Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:29 PM JST

PDB ID : 9K2C
Title : Structure of ClpP from Staphylococcus aureus in complex with ZY1
Authors : Li, J.H.; Wu, W.; Zhang, T.; Yang, C.-G.
Deposited on : 2024-10-17
Resolution : 1.98 Å(reported)

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

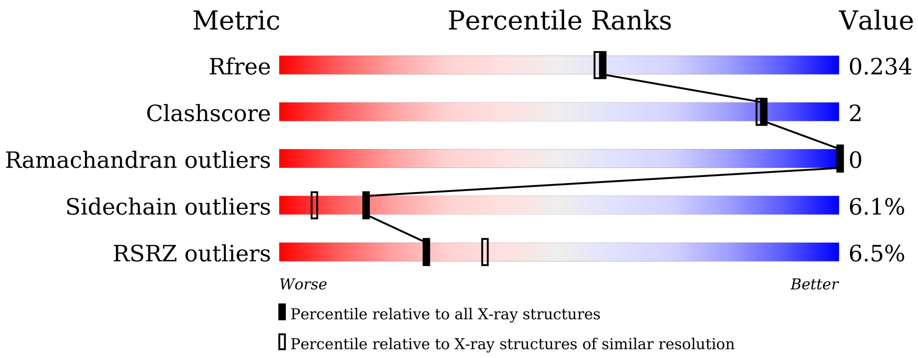
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance ⓘ

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

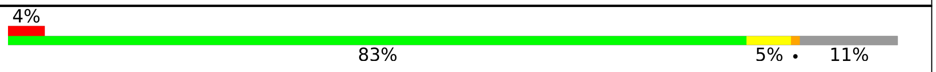
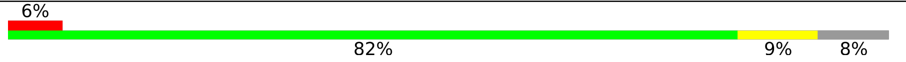
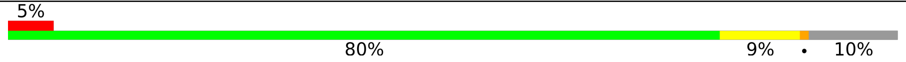
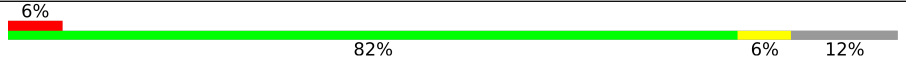
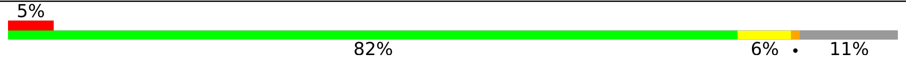
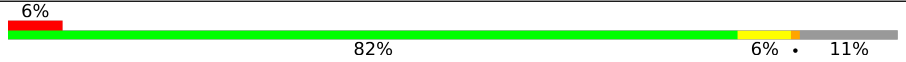
The reported resolution of this entry is 1.98 Å.

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	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	203	
1	B	203	
1	C	203	
1	D	203	
1	E	203	
1	F	203	

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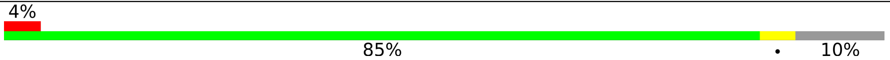
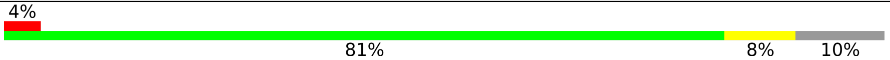
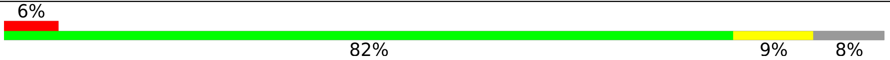
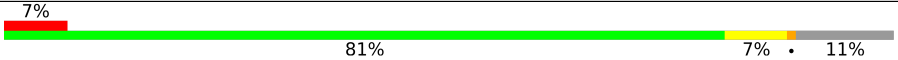
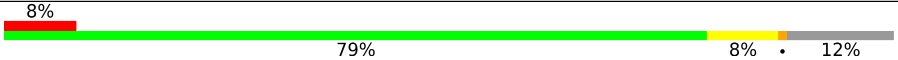
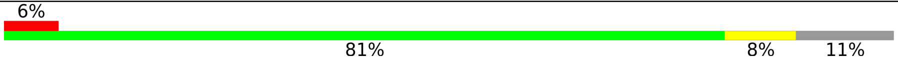
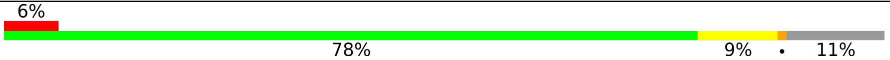
Mol	Chain	Length	Quality of chain
1	G	203	
1	H	203	
1	I	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21198 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	181	1389	877	235	271	6	0	0	0
1	B	186	1404	886	239	273	6	0	0	0
1	C	183	1405	887	238	273	7	0	1	0
1	D	179	1380	871	234	269	6	0	0	0
1	E	180	1381	871	234	270	6	0	0	0
1	F	180	1385	874	235	270	6	0	0	0
1	G	179	1373	867	232	267	7	0	1	0
1	H	182	1398	883	236	273	6	0	0	0
1	I	182	1398	883	237	272	6	0	0	0
1	J	187	1455	916	252	280	7	0	1	0
1	K	181	1393	879	235	273	6	0	0	0
1	L	179	1378	869	234	269	6	0	0	0
1	M	180	1378	868	235	269	6	0	0	0
1	N	180	1381	871	234	270	6	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	LEU	-	expression tag	UNP A7WZR9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	-	expression tag	UNP A7WZR9
A	198	HIS	-	expression tag	UNP A7WZR9
A	199	HIS	-	expression tag	UNP A7WZR9
A	200	HIS	-	expression tag	UNP A7WZR9
A	201	HIS	-	expression tag	UNP A7WZR9
A	202	HIS	-	expression tag	UNP A7WZR9
A	203	HIS	-	expression tag	UNP A7WZR9
B	196	LEU	-	expression tag	UNP A7WZR9
B	197	GLU	-	expression tag	UNP A7WZR9
B	198	HIS	-	expression tag	UNP A7WZR9
B	199	HIS	-	expression tag	UNP A7WZR9
B	200	HIS	-	expression tag	UNP A7WZR9
B	201	HIS	-	expression tag	UNP A7WZR9
B	202	HIS	-	expression tag	UNP A7WZR9
B	203	HIS	-	expression tag	UNP A7WZR9
C	196	LEU	-	expression tag	UNP A7WZR9
C	197	GLU	-	expression tag	UNP A7WZR9
C	198	HIS	-	expression tag	UNP A7WZR9
C	199	HIS	-	expression tag	UNP A7WZR9
C	200	HIS	-	expression tag	UNP A7WZR9
C	201	HIS	-	expression tag	UNP A7WZR9
C	202	HIS	-	expression tag	UNP A7WZR9
C	203	HIS	-	expression tag	UNP A7WZR9
D	196	LEU	-	expression tag	UNP A7WZR9
D	197	GLU	-	expression tag	UNP A7WZR9
D	198	HIS	-	expression tag	UNP A7WZR9
D	199	HIS	-	expression tag	UNP A7WZR9
D	200	HIS	-	expression tag	UNP A7WZR9
D	201	HIS	-	expression tag	UNP A7WZR9
D	202	HIS	-	expression tag	UNP A7WZR9
D	203	HIS	-	expression tag	UNP A7WZR9
E	196	LEU	-	expression tag	UNP A7WZR9
E	197	GLU	-	expression tag	UNP A7WZR9
E	198	HIS	-	expression tag	UNP A7WZR9
E	199	HIS	-	expression tag	UNP A7WZR9
E	200	HIS	-	expression tag	UNP A7WZR9
E	201	HIS	-	expression tag	UNP A7WZR9
E	202	HIS	-	expression tag	UNP A7WZR9
E	203	HIS	-	expression tag	UNP A7WZR9
F	196	LEU	-	expression tag	UNP A7WZR9
F	197	GLU	-	expression tag	UNP A7WZR9
F	198	HIS	-	expression tag	UNP A7WZR9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	HIS	-	expression tag	UNP A7WZR9
F	200	HIS	-	expression tag	UNP A7WZR9
F	201	HIS	-	expression tag	UNP A7WZR9
F	202	HIS	-	expression tag	UNP A7WZR9
F	203	HIS	-	expression tag	UNP A7WZR9
G	196	LEU	-	expression tag	UNP A7WZR9
G	197	GLU	-	expression tag	UNP A7WZR9
G	198	HIS	-	expression tag	UNP A7WZR9
G	199	HIS	-	expression tag	UNP A7WZR9
G	200	HIS	-	expression tag	UNP A7WZR9
G	201	HIS	-	expression tag	UNP A7WZR9
G	202	HIS	-	expression tag	UNP A7WZR9
G	203	HIS	-	expression tag	UNP A7WZR9
H	196	LEU	-	expression tag	UNP A7WZR9
H	197	GLU	-	expression tag	UNP A7WZR9
H	198	HIS	-	expression tag	UNP A7WZR9
H	199	HIS	-	expression tag	UNP A7WZR9
H	200	HIS	-	expression tag	UNP A7WZR9
H	201	HIS	-	expression tag	UNP A7WZR9
H	202	HIS	-	expression tag	UNP A7WZR9
H	203	HIS	-	expression tag	UNP A7WZR9
I	196	LEU	-	expression tag	UNP A7WZR9
I	197	GLU	-	expression tag	UNP A7WZR9
I	198	HIS	-	expression tag	UNP A7WZR9
I	199	HIS	-	expression tag	UNP A7WZR9
I	200	HIS	-	expression tag	UNP A7WZR9
I	201	HIS	-	expression tag	UNP A7WZR9
I	202	HIS	-	expression tag	UNP A7WZR9
I	203	HIS	-	expression tag	UNP A7WZR9
J	196	LEU	-	expression tag	UNP A7WZR9
J	197	GLU	-	expression tag	UNP A7WZR9
J	198	HIS	-	expression tag	UNP A7WZR9
J	199	HIS	-	expression tag	UNP A7WZR9
J	200	HIS	-	expression tag	UNP A7WZR9
J	201	HIS	-	expression tag	UNP A7WZR9
J	202	HIS	-	expression tag	UNP A7WZR9
J	203	HIS	-	expression tag	UNP A7WZR9
K	196	LEU	-	expression tag	UNP A7WZR9
K	197	GLU	-	expression tag	UNP A7WZR9
K	198	HIS	-	expression tag	UNP A7WZR9
K	199	HIS	-	expression tag	UNP A7WZR9
K	200	HIS	-	expression tag	UNP A7WZR9

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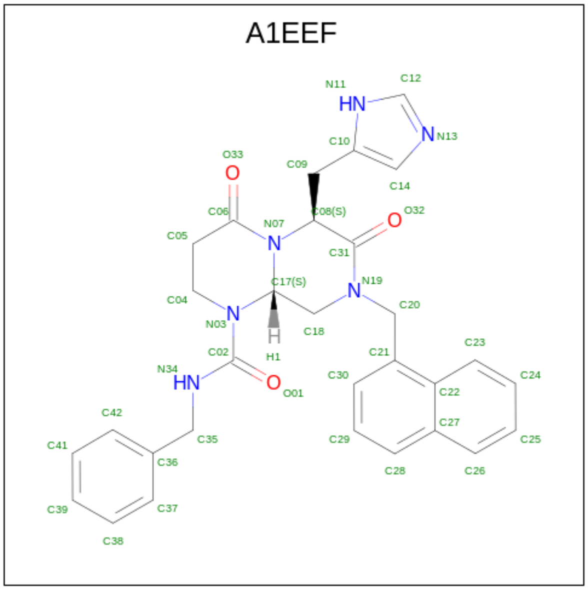
Chain	Residue	Modelled	Actual	Comment	Reference
K	201	HIS	-	expression tag	UNP A7WZR9
K	202	HIS	-	expression tag	UNP A7WZR9
K	203	HIS	-	expression tag	UNP A7WZR9
L	196	LEU	-	expression tag	UNP A7WZR9
L	197	GLU	-	expression tag	UNP A7WZR9
L	198	HIS	-	expression tag	UNP A7WZR9
L	199	HIS	-	expression tag	UNP A7WZR9
L	200	HIS	-	expression tag	UNP A7WZR9
L	201	HIS	-	expression tag	UNP A7WZR9
L	202	HIS	-	expression tag	UNP A7WZR9
L	203	HIS	-	expression tag	UNP A7WZR9
M	196	LEU	-	expression tag	UNP A7WZR9
M	197	GLU	-	expression tag	UNP A7WZR9
M	198	HIS	-	expression tag	UNP A7WZR9
M	199	HIS	-	expression tag	UNP A7WZR9
M	200	HIS	-	expression tag	UNP A7WZR9
M	201	HIS	-	expression tag	UNP A7WZR9
M	202	HIS	-	expression tag	UNP A7WZR9
M	203	HIS	-	expression tag	UNP A7WZR9
N	196	LEU	-	expression tag	UNP A7WZR9
N	197	GLU	-	expression tag	UNP A7WZR9
N	198	HIS	-	expression tag	UNP A7WZR9
N	199	HIS	-	expression tag	UNP A7WZR9
N	200	HIS	-	expression tag	UNP A7WZR9
N	201	HIS	-	expression tag	UNP A7WZR9
N	202	HIS	-	expression tag	UNP A7WZR9
N	203	HIS	-	expression tag	UNP A7WZR9

- Molecule 2 is (6 {S},9 {a} {S})-6-(1 {H}-imidazol-5-ylmethyl)-8-(naphthalen-1-ylmethyl) -4,7-bis(oxidanylidene)- {N}-(phenylmethyl)-3,6,9,9 {a}-tetrahydro-2 {H}-pyrazino[1,2-a]pyrimidine-1-carboxamide (three-letter code: A1EEF) (formula: $C_{30}H_{30}N_6O_3$) (labeled as "Ligand of Interest" by depositor).

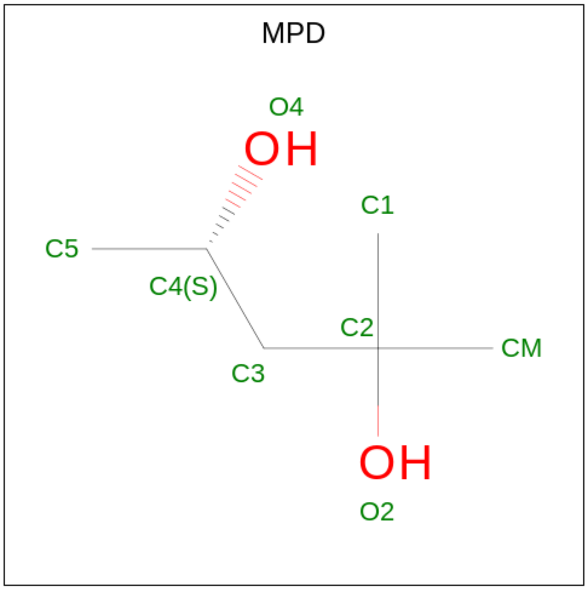


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	39	30	6	3	0	0
2	B	1	39	30	6	3	0	0
2	C	1	39	30	6	3	0	0
2	D	1	39	30	6	3	0	0
2	E	1	39	30	6	3	0	0
2	F	1	39	30	6	3	0	0
2	G	1	39	30	6	3	0	0
2	H	1	39	30	6	3	0	0
2	I	1	39	30	6	3	0	0
2	J	1	39	30	6	3	0	0
2	K	1	39	30	6	3	0	0
2	L	1	39	30	6	3	0	0
2	M	1	39	30	6	3	0	0
2	N	1	39	30	6	3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0
4	G	1	Total C O 8 6 2	0	0
4	H	1	Total C O 8 6 2	0	0
4	I	1	Total C O 8 6 2	0	0
4	J	1	Total C O 8 6 2	0	0
4	K	1	Total C O 8 6 2	0	0
4	L	1	Total C O 8 6 2	0	0
4	M	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

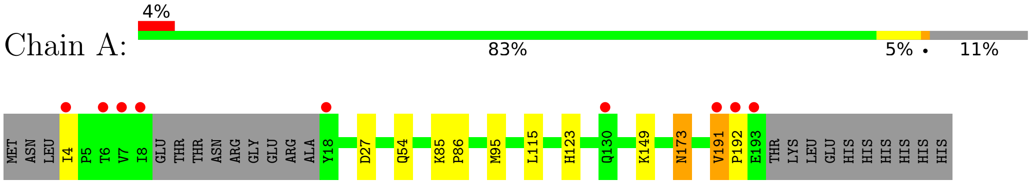
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	107	Total O 107 107	0	0
5	B	99	Total O 99 99	0	0
5	C	85	Total O 85 85	0	0
5	D	58	Total O 58 58	0	0
5	E	58	Total O 58 58	0	0
5	F	62	Total O 62 62	0	0
5	G	83	Total O 83 83	0	0
5	H	78	Total O 78 78	0	0
5	I	83	Total O 83 83	0	0
5	J	79	Total O 79 79	0	0
5	K	54	Total O 54 54	0	0
5	L	49	Total O 49 49	0	0
5	M	57	Total O 57 57	0	0
5	N	68	Total O 68 68	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.

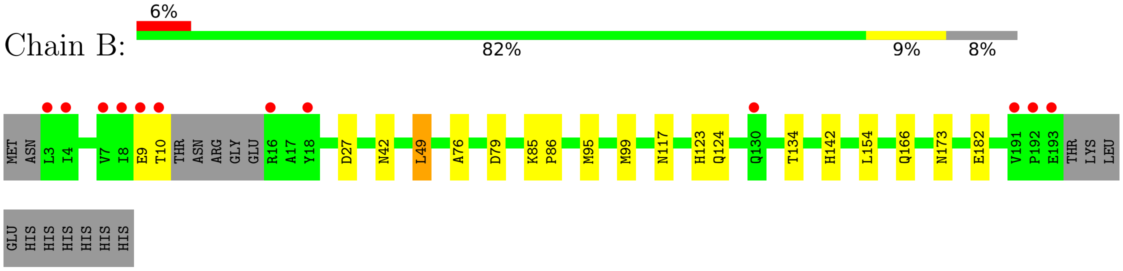
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



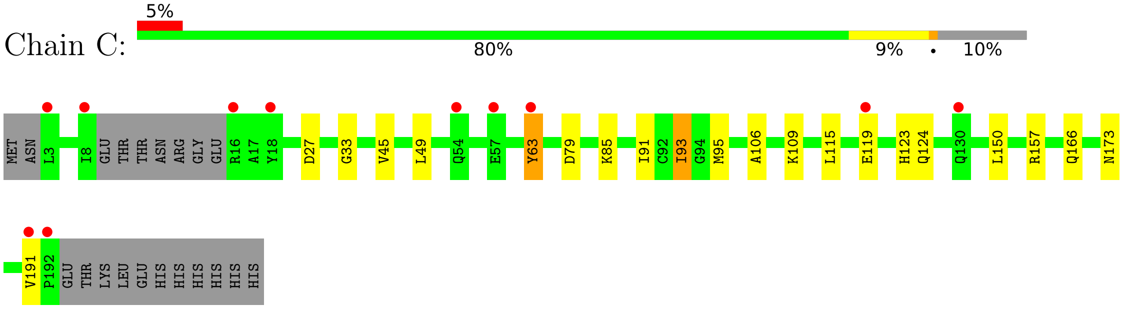
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



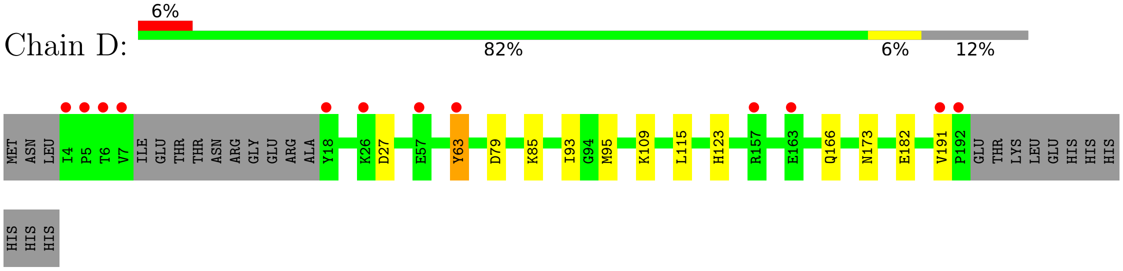
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:

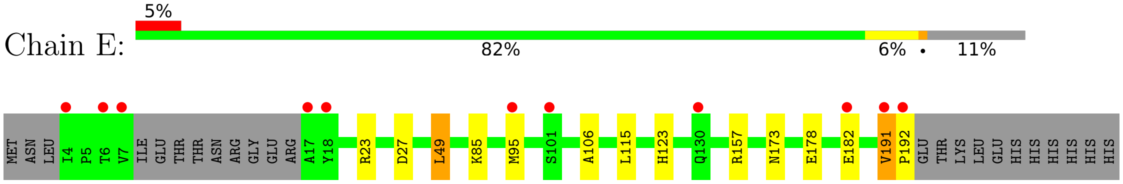


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

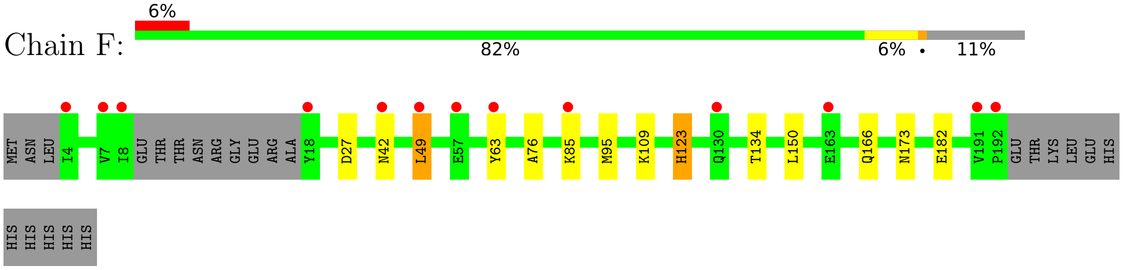
Chain D:



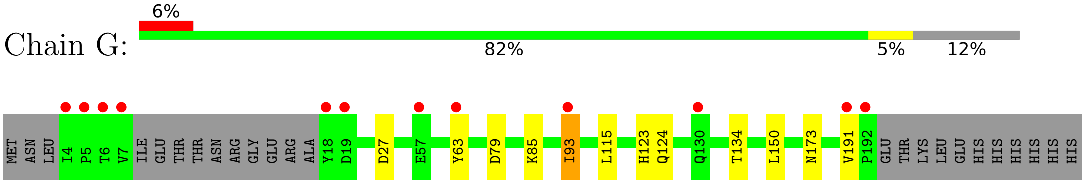
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



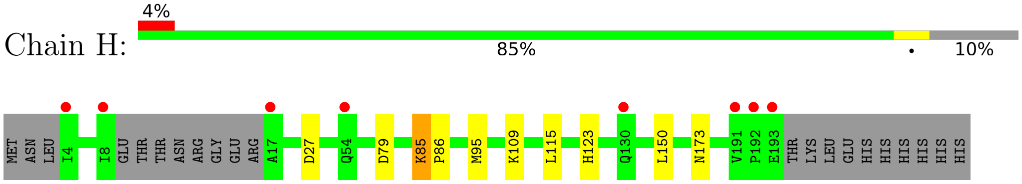
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



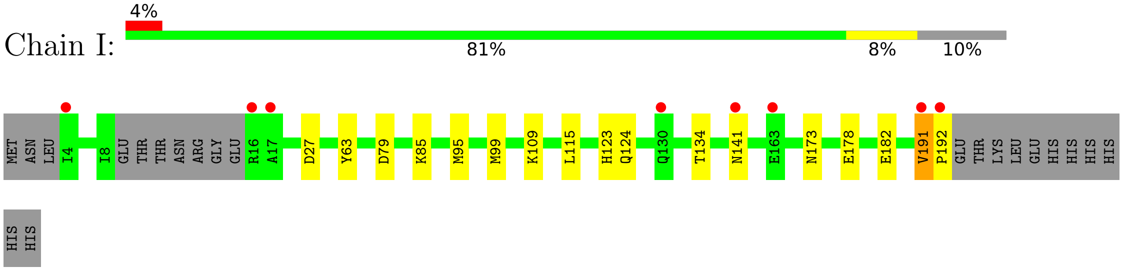
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



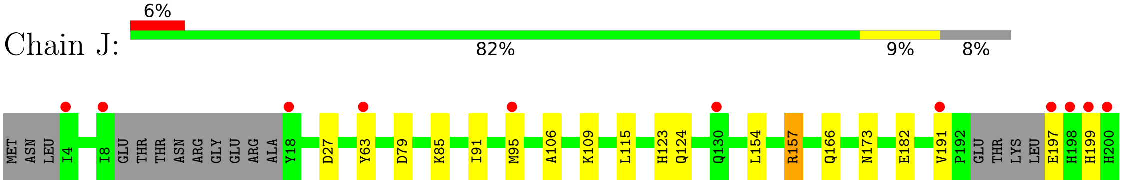
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

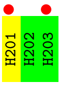


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

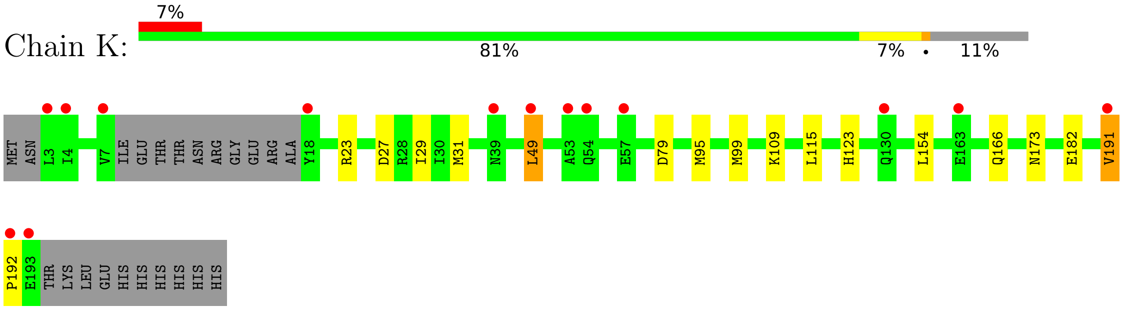


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

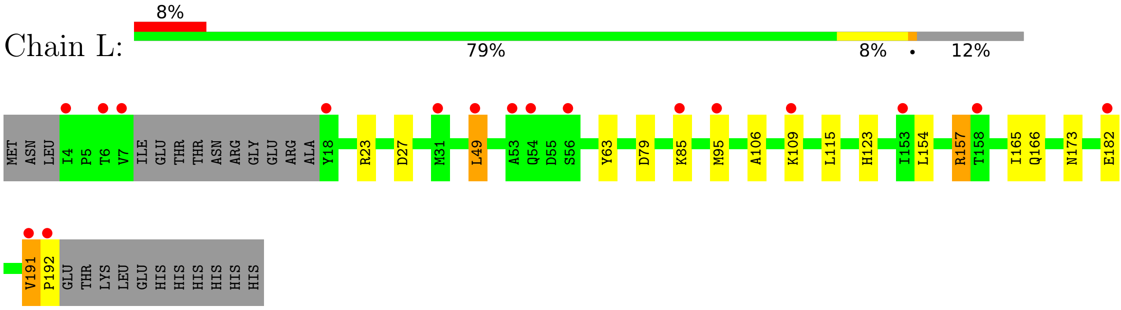




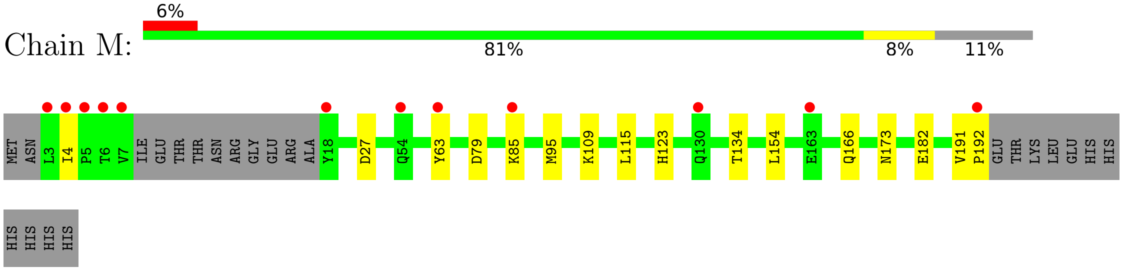
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



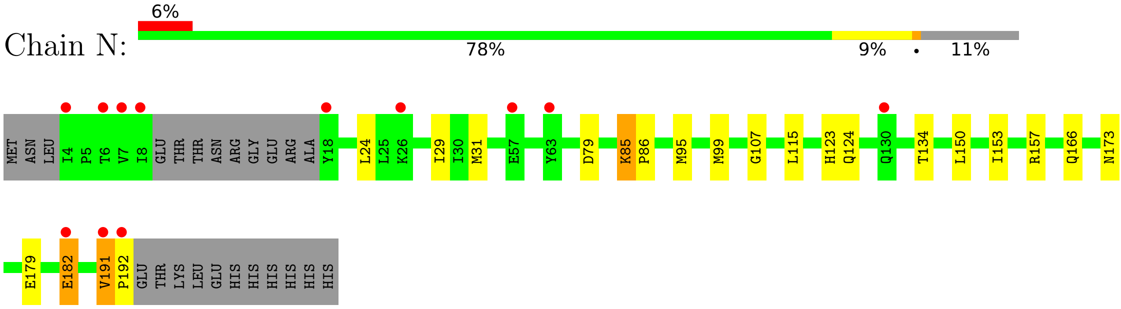
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.70Å 126.01Å 145.80Å 90.00° 93.91° 90.00°	Depositor
Resolution (Å)	29.90 – 1.98 29.90 – 1.98	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.90-1.98) 92.2 (29.90-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.205 , 0.227 0.212 , 0.234	Depositor DCC
R_{free} test set	11623 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21198	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: MG, A1EEF, MPD

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	0.28	0/1407	0.54	0/1901
1	B	0.28	0/1422	0.53	0/1925
1	C	0.28	0/1426	0.51	0/1925
1	D	0.27	0/1398	0.50	0/1887
1	E	0.27	0/1399	0.50	0/1890
1	F	0.27	0/1403	0.50	0/1894
1	G	0.28	0/1394	0.52	0/1884
1	H	0.27	0/1416	0.52	0/1912
1	I	0.28	0/1416	0.53	0/1912
1	J	0.29	0/1480	0.51	0/1995
1	K	0.27	0/1411	0.50	0/1906
1	L	0.27	0/1396	0.50	0/1884
1	M	0.27	0/1395	0.49	0/1883
1	N	0.28	0/1399	0.51	0/1890
All	All	0.28	0/19762	0.51	0/26688

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1389	0	1398	5	0
1	B	1404	0	1397	12	0
1	C	1405	0	1416	12	0
1	D	1380	0	1396	5	0
1	E	1381	0	1390	5	0
1	F	1385	0	1398	6	0
1	G	1373	0	1379	6	0
1	H	1398	0	1412	4	0
1	I	1398	0	1414	7	0
1	J	1455	0	1449	7	0
1	K	1393	0	1402	8	0
1	L	1378	0	1389	7	0
1	M	1378	0	1391	6	0
1	N	1381	0	1387	14	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
2	C	39	0	0	2	0
2	D	39	0	0	1	0
2	E	39	0	0	0	0
2	F	39	0	0	1	0
2	G	39	0	0	1	0
2	H	39	0	0	0	0
2	I	39	0	0	0	0
2	J	39	0	0	0	0
2	K	39	0	0	0	0
2	L	39	0	0	2	0
2	M	39	0	0	2	0
2	N	39	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	28	0	0
4	C	8	0	14	1	0
4	D	8	0	14	0	0
4	E	8	0	14	0	0
4	F	8	0	14	2	0
4	G	8	0	14	1	0
4	H	8	0	14	1	0
4	I	8	0	14	0	0
4	J	8	0	14	0	0
4	K	8	0	14	0	0
4	L	8	0	14	0	0
4	M	8	0	14	0	0
4	N	8	0	14	1	0
5	A	107	0	0	1	0
5	B	99	0	0	1	0
5	C	85	0	0	0	0
5	D	58	0	0	0	0
5	E	58	0	0	0	0
5	F	62	0	0	1	0
5	G	83	0	0	0	0
5	H	78	0	0	0	0
5	I	83	0	0	1	0
5	J	79	0	0	0	0
5	K	54	0	0	0	0
5	L	49	0	0	0	0
5	M	57	0	0	0	0
5	N	68	0	0	0	0
All	All	21198	0	19828	81	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 2.

All (81) 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:N:29:ILE:HG22	1:N:31:MET:CE	2.18	0.73
1:N:29:ILE:HG22	1:N:31:MET:HE3	1.74	0.68
1:K:29:ILE:HG22	1:K:31:MET:CE	2.26	0.65
1:I:141:ASN:HB3	5:I:480:HOH:O	1.99	0.62
1:A:173:ASN:ND2	5:A:401:HOH:O	2.34	0.60
1:I:191:VAL:HG12	1:I:192:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:HG22	1:C:93:ILE:HD12	1.86	0.57
1:N:107:GLY:O	1:N:157:ARG:NH2	2.37	0.57
1:G:150:LEU:HD13	4:G:303:MPD:H52	1.87	0.57
1:J:199:HIS:HD2	1:J:201:HIS:H	1.52	0.56
1:I:79:ASP:HB3	1:J:115:LEU:HD23	1.87	0.56
1:B:49:LEU:HD21	2:C:301:A1EEF:C26	2.35	0.56
1:B:42:ASN:HB3	5:B:467:HOH:O	2.05	0.55
1:A:191:VAL:HG12	1:A:192:PRO:HD2	1.87	0.55
1:A:115:LEU:HD23	1:G:79:ASP:HB3	1.90	0.54
1:I:178:GLU:O	1:I:182:GLU:HG3	2.08	0.54
1:C:45:VAL:HG21	1:D:93:ILE:HD11	1.90	0.54
1:B:9:GLU:O	1:B:10:THR:C	2.46	0.54
1:F:42:ASN:HB3	5:F:459:HOH:O	2.09	0.53
1:G:124:GLN:HE22	1:I:134:THR:H	1.56	0.53
1:G:134:THR:H	1:I:124:GLN:HE22	1.56	0.53
1:K:29:ILE:HG22	1:K:31:MET:HE3	1.90	0.52
1:E:178:GLU:O	1:E:182:GLU:HG3	2.10	0.52
1:K:191:VAL:HG12	1:K:192:PRO:HD2	1.92	0.52
1:C:79:ASP:HB3	1:D:115:LEU:HD23	1.92	0.51
1:L:191:VAL:HG12	1:L:192:PRO:HD2	1.91	0.51
1:A:149:LYS:HD2	1:B:117:ASN:HD22	1.76	0.51
1:J:106:ALA:HA	1:J:157:ARG:HD2	1.92	0.51
1:F:150:LEU:HD13	4:F:303:MPD:H53	1.94	0.50
1:N:153:ILE:O	1:N:157:ARG:HG2	2.13	0.49
1:M:79:ASP:HB3	1:N:115:LEU:HD23	1.95	0.49
1:N:29:ILE:CG2	1:N:31:MET:CE	2.90	0.48
1:C:124:GLN:HE22	1:M:134:THR:H	1.62	0.48
1:K:79:ASP:HB3	1:L:115:LEU:HD23	1.96	0.47
1:F:49:LEU:HD11	2:G:301:A1EEF:C28	2.44	0.47
1:C:63:TYR:HB2	2:C:301:A1EEF:C29	2.45	0.47
1:F:123:HIS:O	4:F:303:MPD:H52	2.15	0.47
1:B:124:GLN:HE22	1:N:134:THR:H	1.63	0.47
1:H:79:ASP:HB3	1:I:115:LEU:HD23	1.96	0.47
1:L:79:ASP:HB3	1:M:115:LEU:HD23	1.97	0.46
1:M:191:VAL:HG12	1:M:192:PRO:HD2	1.97	0.46
1:D:79:ASP:HB3	1:E:115:LEU:HD23	1.98	0.45
1:K:49:LEU:HD11	2:L:301:A1EEF:C28	2.46	0.45
1:B:42:ASN:ND2	1:C:33:GLY:O	2.44	0.45
1:H:150:LEU:HD13	4:H:303:MPD:H52	1.99	0.45
1:K:49:LEU:HD11	2:L:301:A1EEF:C26	2.47	0.44
1:L:49:LEU:HD11	2:M:301:A1EEF:C28	2.48	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:D:63:TYR:CE2	1:D:93:ILE:HG12	2.52	0.44
1:G:93:ILE:HD11	1:G:115:LEU:HD22	2.00	0.44
1:B:134:THR:H	1:N:124:GLN:HE22	1.66	0.44
1:E:191:VAL:HG12	1:E:192:PRO:HD2	1.99	0.44
1:L:154:LEU:HB3	1:L:165:ILE:HD13	2.00	0.43
1:F:134:THR:H	1:J:124:GLN:HE22	1.65	0.43
1:B:142:HIS:HE1	1:C:119:GLU:OE1	2.02	0.43
1:J:91:ILE:HD11	1:J:115:LEU:CD1	2.48	0.43
1:C:106:ALA:HA	1:C:157:ARG:HD2	2.01	0.42
1:E:49:LEU:HD11	2:F:301:A1EEF:C28	2.48	0.42
1:J:79:ASP:HB3	1:K:115:LEU:HD23	2.01	0.42
1:L:106:ALA:HA	1:L:157:ARG:HD2	1.99	0.42
1:N:24:LEU:HG	2:N:301:A1EEF:C38	2.49	0.42
1:N:179:GLU:HA	1:N:182:GLU:HG3	2.01	0.42
1:B:79:ASP:HB3	1:C:115:LEU:HD23	2.01	0.42
1:J:154:LEU:HD23	1:J:154:LEU:HA	1.94	0.42
1:E:106:ALA:HA	1:E:157:ARG:HD2	2.01	0.42
1:M:154:LEU:HD23	1:M:154:LEU:HA	1.90	0.41
1:M:4:ILE:H	1:M:4:ILE:HG13	1.73	0.41
1:C:49:LEU:HD21	2:D:301:A1EEF:C26	2.50	0.41
1:A:85:LYS:N	1:A:86:PRO:CD	2.84	0.41
1:K:154:LEU:HD23	1:K:154:LEU:HA	1.93	0.41
1:N:191:VAL:HG12	1:N:192:PRO:HD2	2.01	0.41
1:N:150:LEU:HD13	4:N:303:MPD:H52	2.03	0.41
1:B:76:ALA:HB1	1:C:93:ILE:CG2	2.50	0.41
1:C:150:LEU:HD13	4:C:303:MPD:H52	2.02	0.41
1:H:115:LEU:HD23	1:N:79:ASP:HB3	2.03	0.41
1:B:85:LYS:N	1:B:86:PRO:CD	2.84	0.40
1:F:76:ALA:HB1	1:G:93:ILE:CG2	2.51	0.40
1:H:85:LYS:N	1:H:86:PRO:CD	2.84	0.40
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.93	0.40
1:D:63:TYR:HE2	1:D:93:ILE:HD11	1.85	0.40
1:L:49:LEU:HD11	2:M:301:A1EEF:C26	2.51	0.40
1:N:85:LYS:N	1:N:86:PRO:CD	2.85	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	177/203 (87%)	175 (99%)	2 (1%)	0	100	100
1	B	182/203 (90%)	180 (99%)	2 (1%)	0	100	100
1	C	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
1	D	175/203 (86%)	173 (99%)	2 (1%)	0	100	100
1	E	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
1	F	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
1	G	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
1	H	178/203 (88%)	176 (99%)	2 (1%)	0	100	100
1	I	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	J	182/203 (90%)	179 (98%)	3 (2%)	0	100	100
1	K	177/203 (87%)	174 (98%)	3 (2%)	0	100	100
1	L	175/203 (86%)	174 (99%)	1 (1%)	0	100	100
1	M	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
1	N	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
All	All	2484/2842 (87%)	2454 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	149/171 (87%)	142 (95%)	7 (5%)	22	11
1	B	147/171 (86%)	139 (95%)	8 (5%)	18	8
1	C	150/171 (88%)	139 (93%)	11 (7%)	11	4
1	D	149/171 (87%)	139 (93%)	10 (7%)	13	5
1	E	148/171 (86%)	140 (95%)	8 (5%)	18	8
1	F	149/171 (87%)	139 (93%)	10 (7%)	13	5
1	G	147/171 (86%)	140 (95%)	7 (5%)	21	10
1	H	150/171 (88%)	144 (96%)	6 (4%)	27	16
1	I	150/171 (88%)	141 (94%)	9 (6%)	16	6
1	J	156/171 (91%)	143 (92%)	13 (8%)	9	2
1	K	150/171 (88%)	139 (93%)	11 (7%)	11	4
1	L	148/171 (86%)	135 (91%)	13 (9%)	8	2
1	M	148/171 (86%)	139 (94%)	9 (6%)	15	6
1	N	148/171 (86%)	140 (95%)	8 (5%)	18	8
All	All	2089/2394 (87%)	1959 (94%)	130 (6%)	15	6

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	27	ASP
1	A	54	GLN
1	A	95	MET
1	A	123	HIS
1	A	173	ASN
1	A	191	VAL
1	B	27	ASP
1	B	49	LEU
1	B	95	MET
1	B	99	MET
1	B	123	HIS
1	B	166	GLN
1	B	173	ASN
1	B	182	GLU
1	C	27	ASP
1	C	63	TYR
1	C	85	LYS
1	C	93	ILE

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Mol	Chain	Res	Type
1	C	95[A]	MET
1	C	95[B]	MET
1	C	109	LYS
1	C	123	HIS
1	C	166	GLN
1	C	173	ASN
1	C	191	VAL
1	D	27	ASP
1	D	63	TYR
1	D	85	LYS
1	D	95	MET
1	D	109	LYS
1	D	123	HIS
1	D	166	GLN
1	D	173	ASN
1	D	182	GLU
1	D	191	VAL
1	E	23	ARG
1	E	27	ASP
1	E	49	LEU
1	E	85	LYS
1	E	95	MET
1	E	123	HIS
1	E	173	ASN
1	E	191	VAL
1	F	27	ASP
1	F	49	LEU
1	F	63	TYR
1	F	85	LYS
1	F	95	MET
1	F	109	LYS
1	F	123	HIS
1	F	166	GLN
1	F	173	ASN
1	F	182	GLU
1	G	27	ASP
1	G	63	TYR
1	G	85	LYS
1	G	93	ILE
1	G	123	HIS
1	G	173	ASN
1	G	191	VAL

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Mol	Chain	Res	Type
1	H	27	ASP
1	H	85	LYS
1	H	95	MET
1	H	109	LYS
1	H	123	HIS
1	H	173	ASN
1	I	27	ASP
1	I	63	TYR
1	I	85	LYS
1	I	95	MET
1	I	99	MET
1	I	109	LYS
1	I	123	HIS
1	I	173	ASN
1	I	191	VAL
1	J	27	ASP
1	J	63	TYR
1	J	85	LYS
1	J	95[A]	MET
1	J	95[B]	MET
1	J	109	LYS
1	J	123	HIS
1	J	157	ARG
1	J	166	GLN
1	J	173	ASN
1	J	182	GLU
1	J	191	VAL
1	J	197	GLU
1	K	23	ARG
1	K	27	ASP
1	K	49	LEU
1	K	95	MET
1	K	99	MET
1	K	109	LYS
1	K	123	HIS
1	K	166	GLN
1	K	173	ASN
1	K	182	GLU
1	K	191	VAL
1	L	23	ARG
1	L	27	ASP
1	L	49	LEU

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Mol	Chain	Res	Type
1	L	63	TYR
1	L	85	LYS
1	L	95	MET
1	L	109	LYS
1	L	123	HIS
1	L	157	ARG
1	L	166	GLN
1	L	173	ASN
1	L	182	GLU
1	L	191	VAL
1	M	27	ASP
1	M	63	TYR
1	M	85	LYS
1	M	95	MET
1	M	109	LYS
1	M	123	HIS
1	M	166	GLN
1	M	173	ASN
1	M	182	GLU
1	N	85	LYS
1	N	95	MET
1	N	99	MET
1	N	123	HIS
1	N	166	GLN
1	N	173	ASN
1	N	182	GLU
1	N	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	54	GLN
1	A	82	GLN
1	A	117	ASN
1	A	124	GLN
1	A	173	ASN
1	B	82	GLN
1	B	117	ASN
1	B	124	GLN
1	B	142	HIS
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	173	ASN
1	C	82	GLN
1	C	117	ASN
1	C	124	GLN
1	C	166	GLN
1	C	173	ASN
1	D	52	GLN
1	D	82	GLN
1	D	117	ASN
1	D	124	GLN
1	D	166	GLN
1	D	173	ASN
1	E	82	GLN
1	E	117	ASN
1	E	124	GLN
1	E	142	HIS
1	E	173	ASN
1	F	82	GLN
1	F	117	ASN
1	F	124	GLN
1	F	166	GLN
1	F	173	ASN
1	G	82	GLN
1	G	117	ASN
1	G	124	GLN
1	G	173	ASN
1	H	52	GLN
1	H	82	GLN
1	H	117	ASN
1	H	124	GLN
1	H	142	HIS
1	H	173	ASN
1	I	82	GLN
1	I	117	ASN
1	I	124	GLN
1	I	173	ASN
1	J	82	GLN
1	J	117	ASN
1	J	124	GLN
1	J	142	HIS
1	J	166	GLN
1	J	173	ASN

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Mol	Chain	Res	Type
1	J	199	HIS
1	K	82	GLN
1	K	117	ASN
1	K	124	GLN
1	K	166	GLN
1	K	173	ASN
1	L	82	GLN
1	L	117	ASN
1	L	124	GLN
1	L	166	GLN
1	L	173	ASN
1	M	42	ASN
1	M	82	GLN
1	M	117	ASN
1	M	124	GLN
1	M	142	HIS
1	M	166	GLN
1	M	173	ASN
1	N	52	GLN
1	N	82	GLN
1	N	117	ASN
1	N	124	GLN
1	N	166	GLN
1	N	173	ASN

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 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
4	MPD	D	303	-	7,7,7	0.13	0	9,10,10	0.39	0
4	MPD	M	303	-	7,7,7	0.09	0	9,10,10	0.33	0
2	A1EEF	L	301	-	38,44,44	0.24	0	47,62,62	0.48	0
2	A1EEF	G	301	-	38,44,44	0.27	0	47,62,62	0.51	0
2	A1EEF	D	301	-	38,44,44	0.25	0	47,62,62	0.47	0
4	MPD	J	303	-	7,7,7	0.10	0	9,10,10	0.27	0
2	A1EEF	M	301	-	38,44,44	0.25	0	47,62,62	0.51	0
4	MPD	F	303	-	7,7,7	0.13	0	9,10,10	0.45	0
4	MPD	B	303	-	7,7,7	0.13	0	9,10,10	0.47	0
2	A1EEF	C	301	-	38,44,44	0.25	0	47,62,62	0.49	0
4	MPD	E	303	-	7,7,7	0.12	0	9,10,10	0.37	0
2	A1EEF	H	301	-	38,44,44	0.27	0	47,62,62	0.51	0
2	A1EEF	F	301	-	38,44,44	0.24	0	47,62,62	0.49	0
4	MPD	K	303	-	7,7,7	0.11	0	9,10,10	0.39	0
2	A1EEF	N	301	-	38,44,44	0.25	0	47,62,62	0.52	0
4	MPD	I	303	-	7,7,7	0.12	0	9,10,10	0.39	0
4	MPD	C	303	-	7,7,7	0.13	0	9,10,10	0.36	0
4	MPD	G	303	-	7,7,7	0.11	0	9,10,10	0.39	0
2	A1EEF	E	301	-	38,44,44	0.27	0	47,62,62	0.51	0
4	MPD	A	303	-	7,7,7	0.12	0	9,10,10	0.38	0
2	A1EEF	A	301	-	38,44,44	0.26	0	47,62,62	0.48	0
2	A1EEF	J	301	-	38,44,44	0.26	0	47,62,62	0.48	0
2	A1EEF	B	301	-	38,44,44	0.28	0	47,62,62	0.55	0
4	MPD	L	303	-	7,7,7	0.11	0	9,10,10	0.35	0
4	MPD	N	303	-	7,7,7	0.10	0	9,10,10	0.37	0
2	A1EEF	K	301	-	38,44,44	0.27	0	47,62,62	0.49	0
4	MPD	B	304	-	7,7,7	0.12	0	9,10,10	0.43	0
4	MPD	H	303	-	7,7,7	0.12	0	9,10,10	0.40	0
2	A1EEF	I	301	-	38,44,44	0.27	0	47,62,62	0.52	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
4	MPD	D	303	-	-	0/5/5/5	-
4	MPD	M	303	-	-	0/5/5/5	-
2	A1EEF	L	301	-	-	1/17/50/50	0/6/6/6
2	A1EEF	G	301	-	-	3/17/50/50	0/6/6/6
2	A1EEF	D	301	-	-	0/17/50/50	0/6/6/6
4	MPD	J	303	-	-	0/5/5/5	-
2	A1EEF	M	301	-	-	1/17/50/50	0/6/6/6
4	MPD	F	303	-	-	3/5/5/5	-
4	MPD	B	303	-	-	0/5/5/5	-
2	A1EEF	C	301	-	-	2/17/50/50	0/6/6/6
4	MPD	E	303	-	-	0/5/5/5	-
2	A1EEF	H	301	-	-	1/17/50/50	0/6/6/6
2	A1EEF	F	301	-	-	1/17/50/50	0/6/6/6
4	MPD	K	303	-	-	0/5/5/5	-
2	A1EEF	N	301	-	-	3/17/50/50	0/6/6/6
4	MPD	I	303	-	-	0/5/5/5	-
4	MPD	C	303	-	-	0/5/5/5	-
4	MPD	G	303	-	-	0/5/5/5	-
2	A1EEF	E	301	-	-	3/17/50/50	0/6/6/6
4	MPD	A	303	-	-	0/5/5/5	-
2	A1EEF	A	301	-	-	3/17/50/50	0/6/6/6
2	A1EEF	J	301	-	-	1/17/50/50	0/6/6/6
2	A1EEF	B	301	-	-	3/17/50/50	0/6/6/6
4	MPD	L	303	-	-	0/5/5/5	-
4	MPD	N	303	-	-	0/5/5/5	-
2	A1EEF	K	301	-	-	0/17/50/50	0/6/6/6
4	MPD	B	304	-	-	0/5/5/5	-
4	MPD	H	303	-	-	0/5/5/5	-
2	A1EEF	I	301	-	-	0/17/50/50	0/6/6/6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1EEF	C08-C09-C10-N11
2	A	301	A1EEF	N07-C08-C09-C10
2	B	301	A1EEF	C08-C09-C10-N11
2	B	301	A1EEF	N07-C08-C09-C10

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Mol	Chain	Res	Type	Atoms
2	C	301	A1EEF	N07-C08-C09-C10
2	E	301	A1EEF	C08-C09-C10-N11
2	E	301	A1EEF	N07-C08-C09-C10
2	F	301	A1EEF	C08-C09-C10-N11
2	G	301	A1EEF	C08-C09-C10-N11
2	G	301	A1EEF	N07-C08-C09-C10
2	H	301	A1EEF	C08-C09-C10-N11
2	L	301	A1EEF	C08-C09-C10-N11
2	N	301	A1EEF	C08-C09-C10-N11
2	N	301	A1EEF	N07-C08-C09-C10
4	F	303	MPD	C2-C3-C4-O4
2	C	301	A1EEF	C31-C08-C09-C10
2	M	301	A1EEF	N07-C08-C09-C10
2	B	301	A1EEF	C31-C08-C09-C10
2	E	301	A1EEF	C31-C08-C09-C10
2	G	301	A1EEF	C31-C08-C09-C10
2	N	301	A1EEF	C31-C08-C09-C10
4	F	303	MPD	C1-C2-C3-C4
2	J	301	A1EEF	C08-C09-C10-N11
4	F	303	MPD	O2-C2-C3-C4
2	A	301	A1EEF	C08-C09-C10-C14

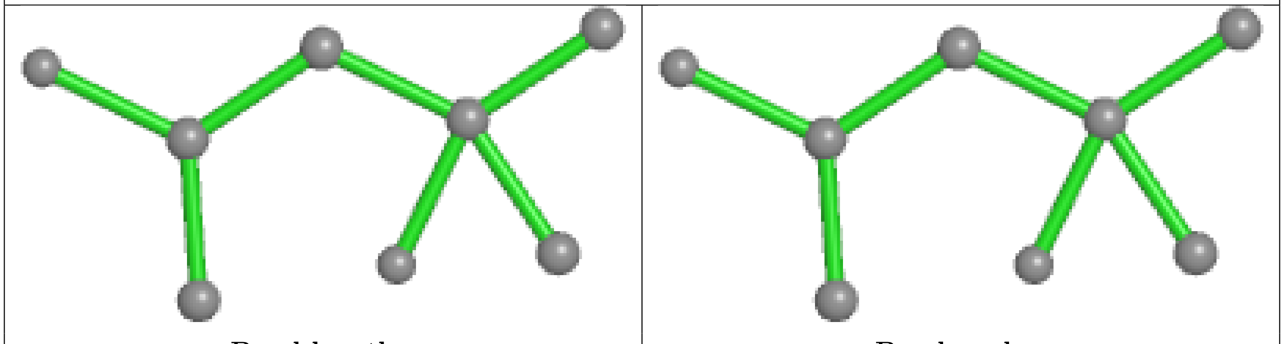
There are no ring outliers.

12 monomers are involved in 16 short contacts:

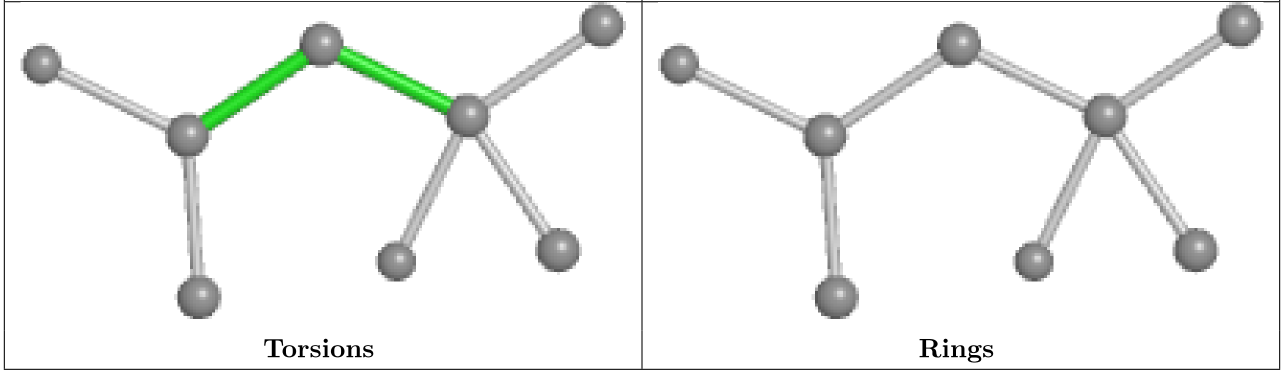
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	A1EEF	2	0
2	G	301	A1EEF	1	0
2	D	301	A1EEF	1	0
2	M	301	A1EEF	2	0
4	F	303	MPD	2	0
2	C	301	A1EEF	2	0
2	F	301	A1EEF	1	0
2	N	301	A1EEF	1	0
4	C	303	MPD	1	0
4	G	303	MPD	1	0
4	N	303	MPD	1	0
4	H	303	MPD	1	0

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.

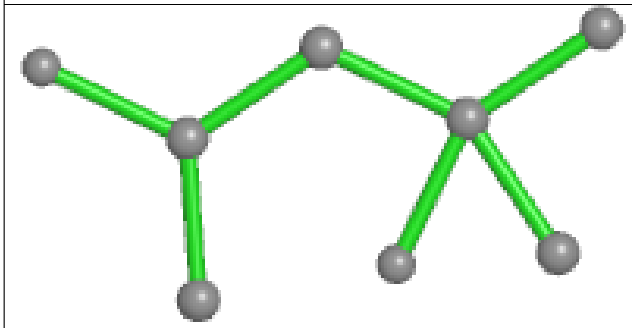
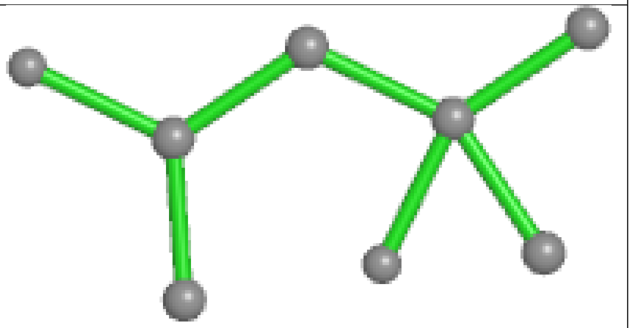
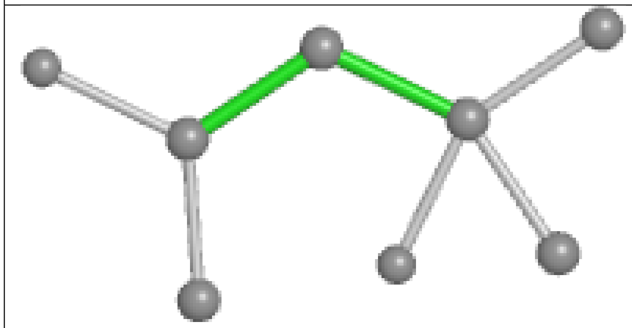
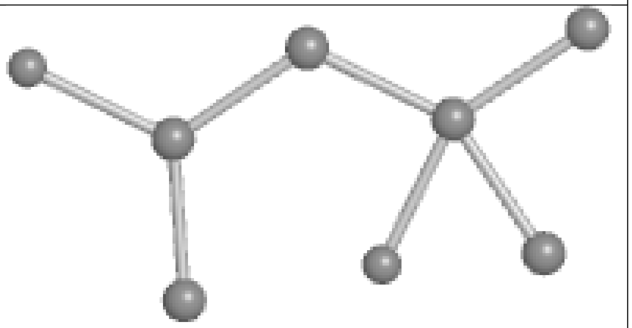
Ligand MPD D 303



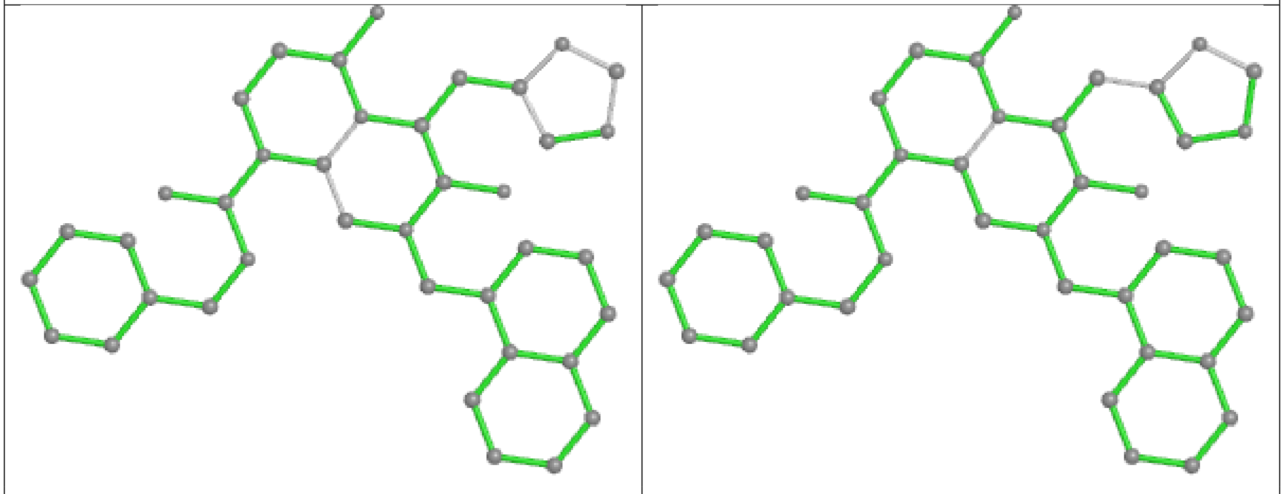
Bond lengths **Bond angles**



Torsions **Rings**

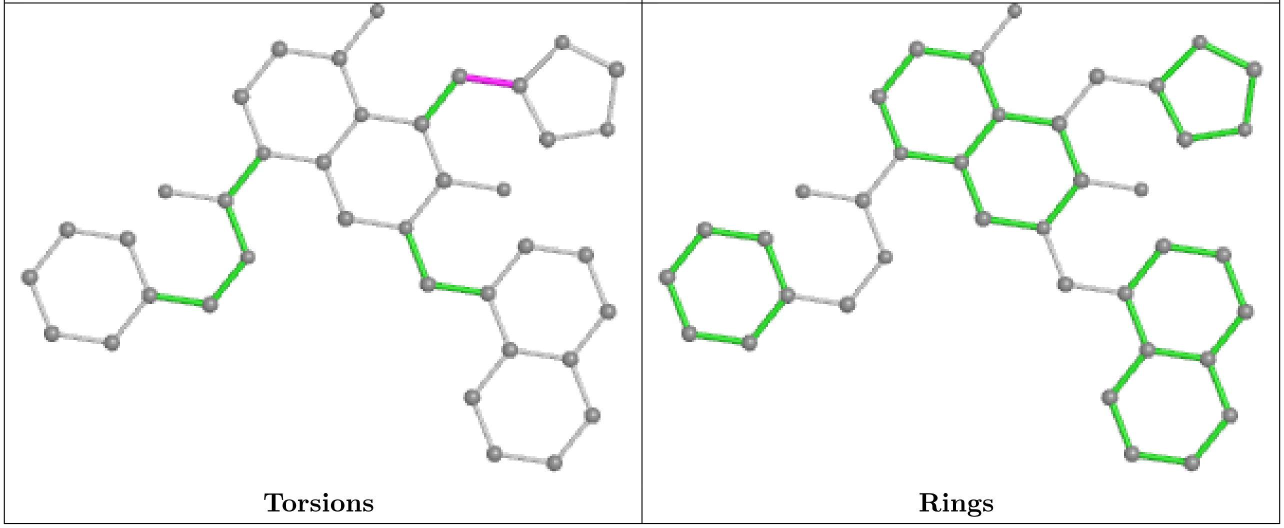
Ligand MPD M 303	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand A1EEF L 301



Bond lengths

Bond angles



Torsions

Rings

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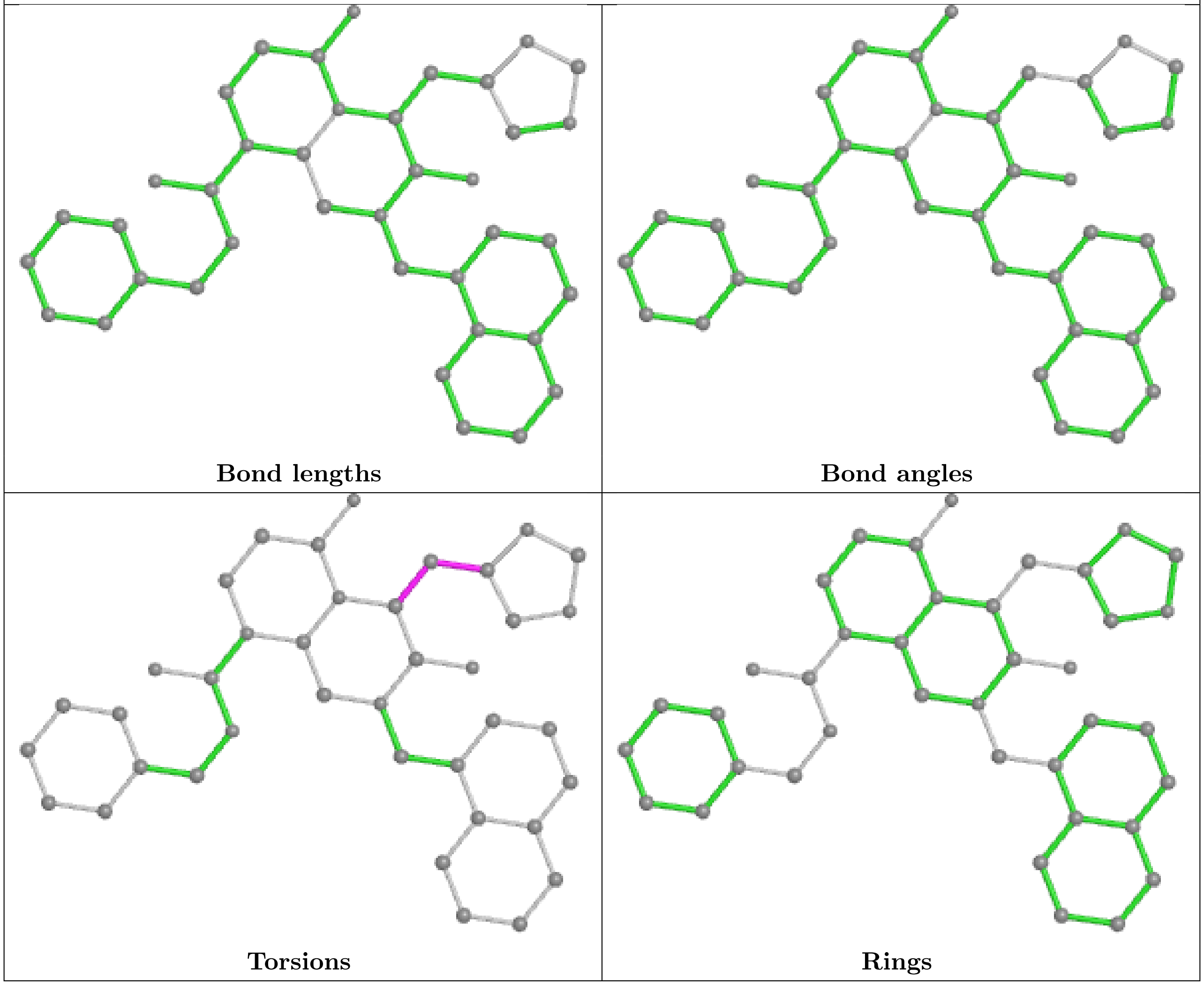
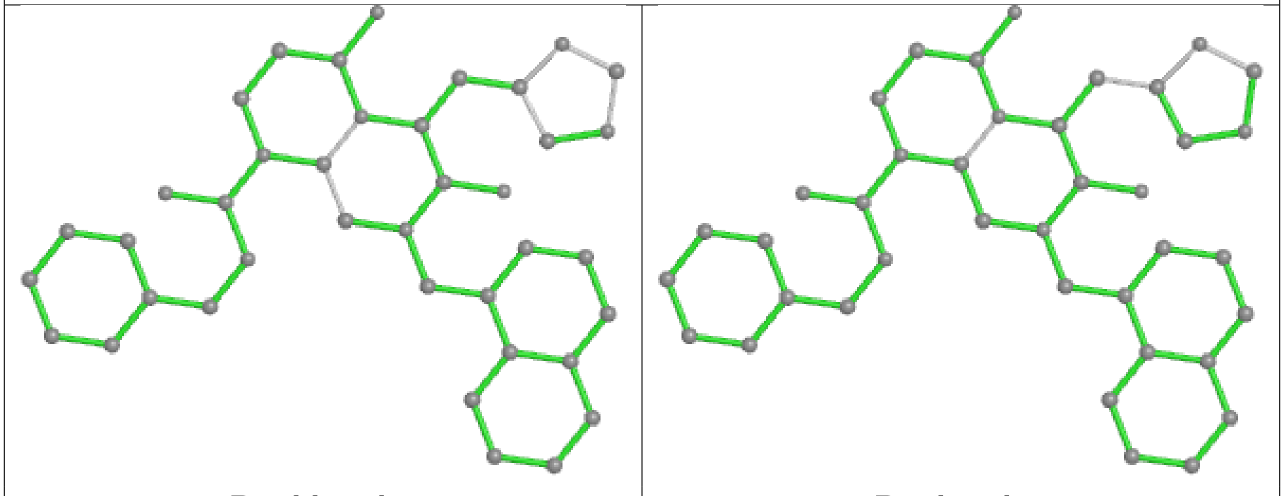
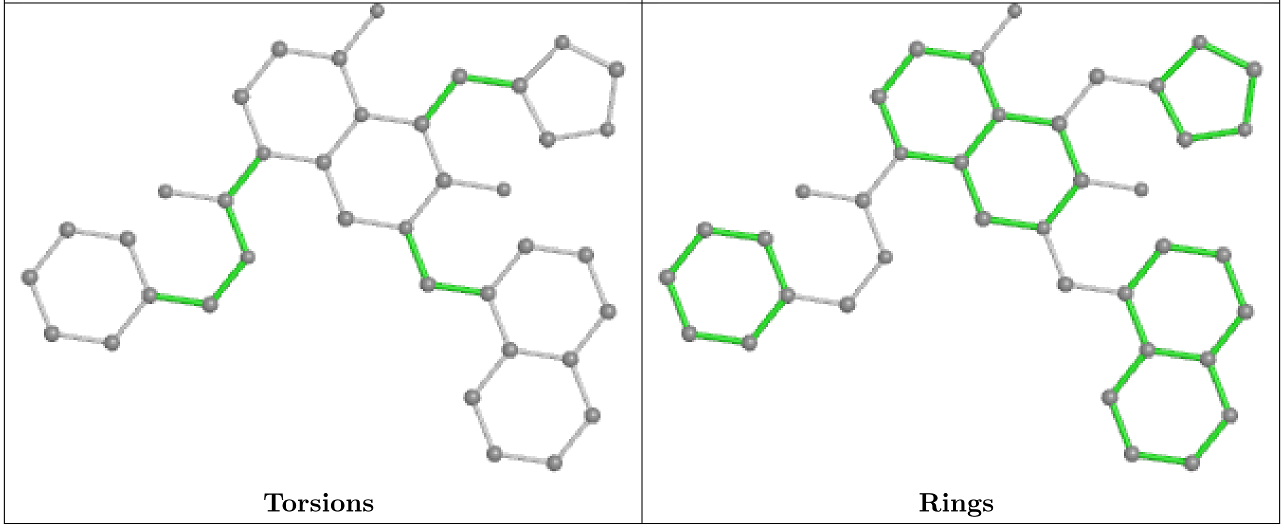


Ligand A1EEF D 301

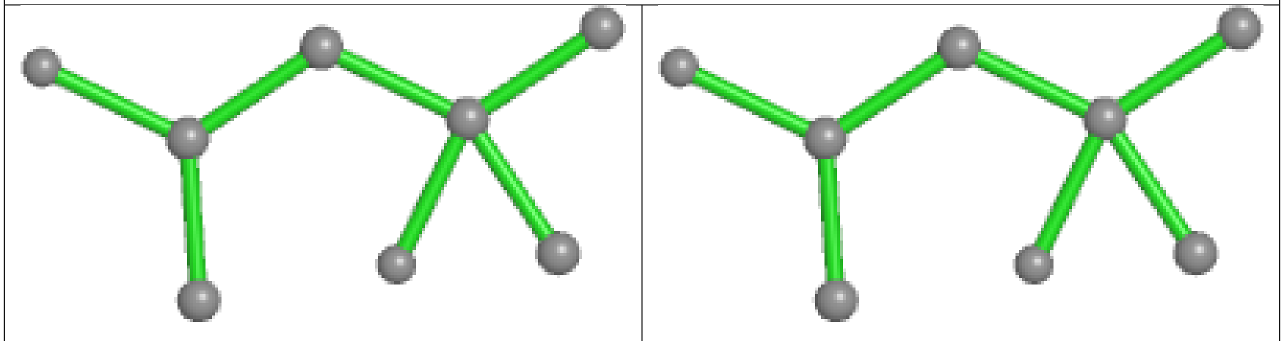


Bond lengths **Bond angles**



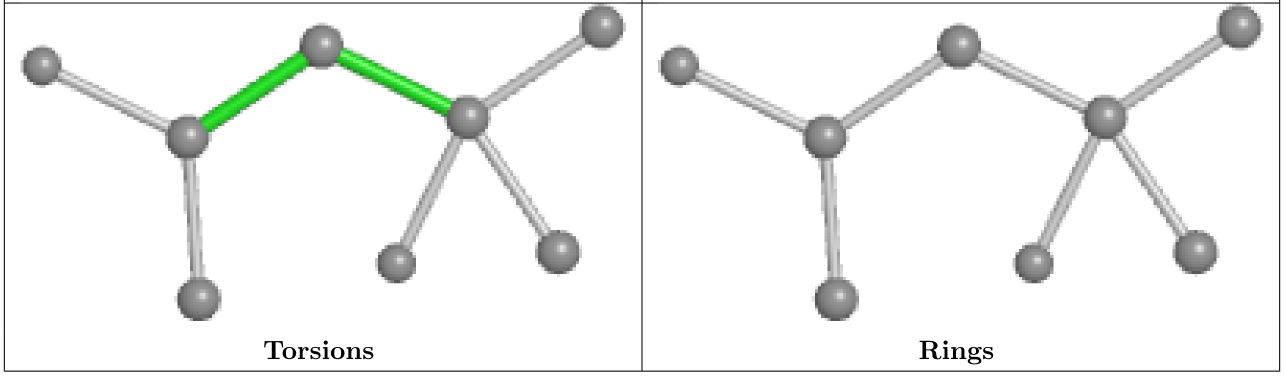
Torsions **Rings**

Ligand MPD J 303



Bond lengths

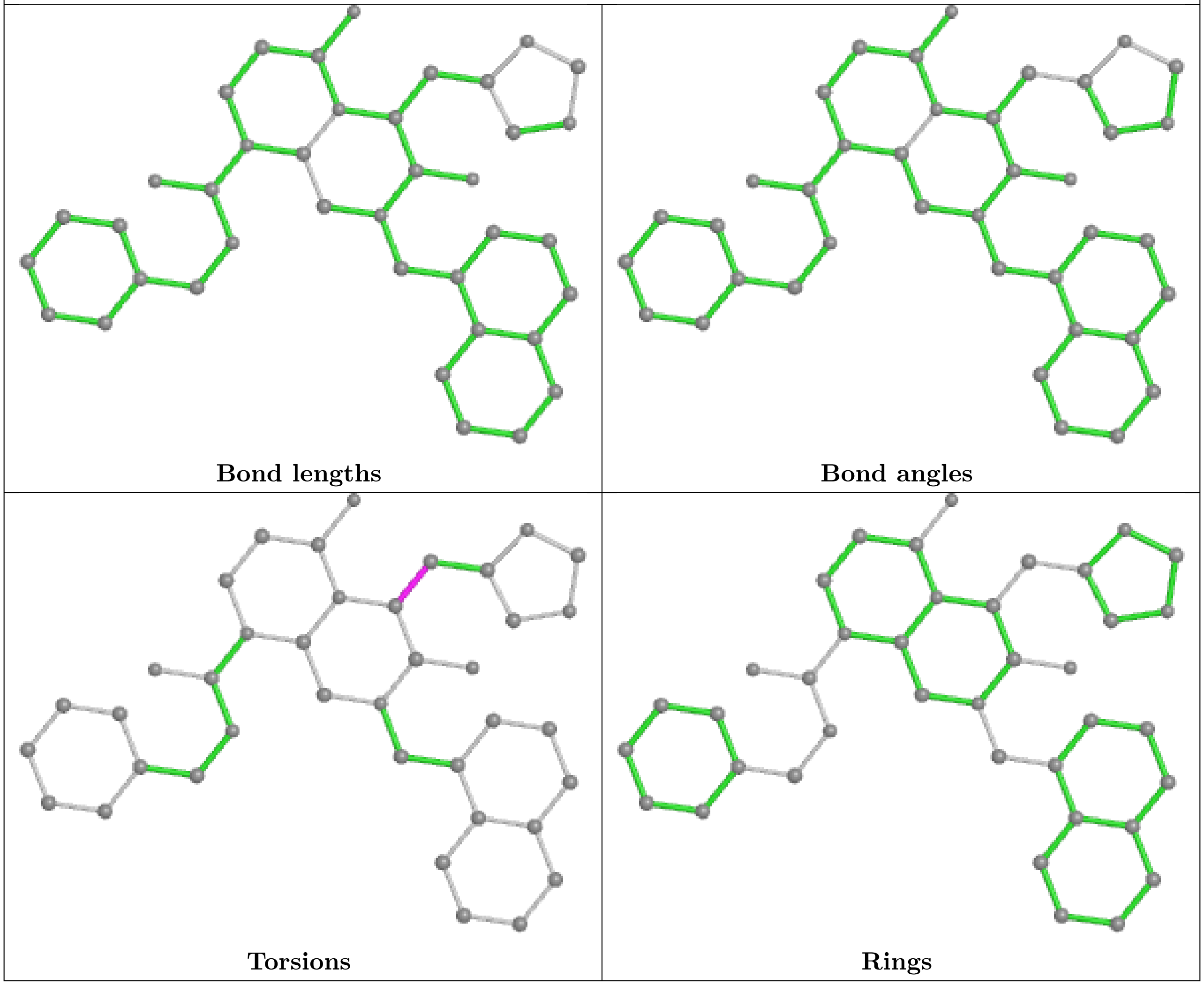
Bond angles



Torsions

Rings

Ligand A1EEF M 301



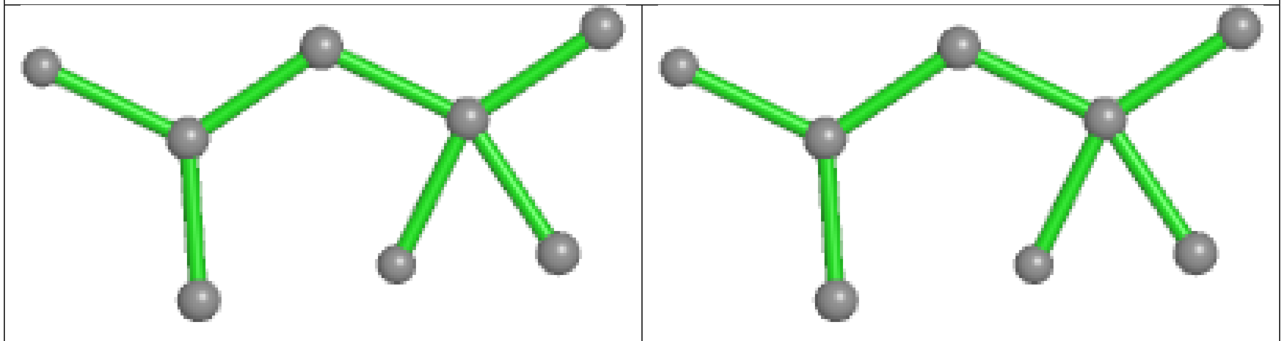
Bond lengths

Bond angles

Torsions

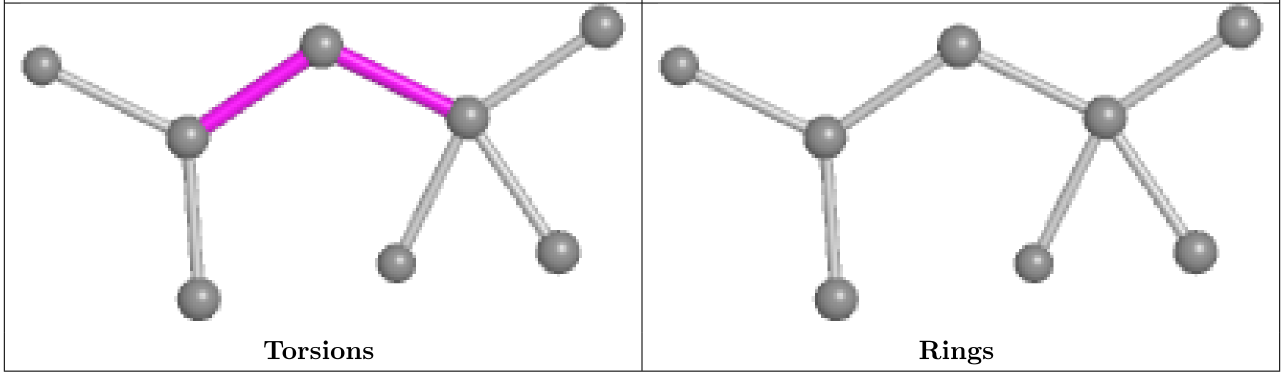
Rings

Ligand MPD F 303



Bond lengths

Bond angles



Torsions

Rings

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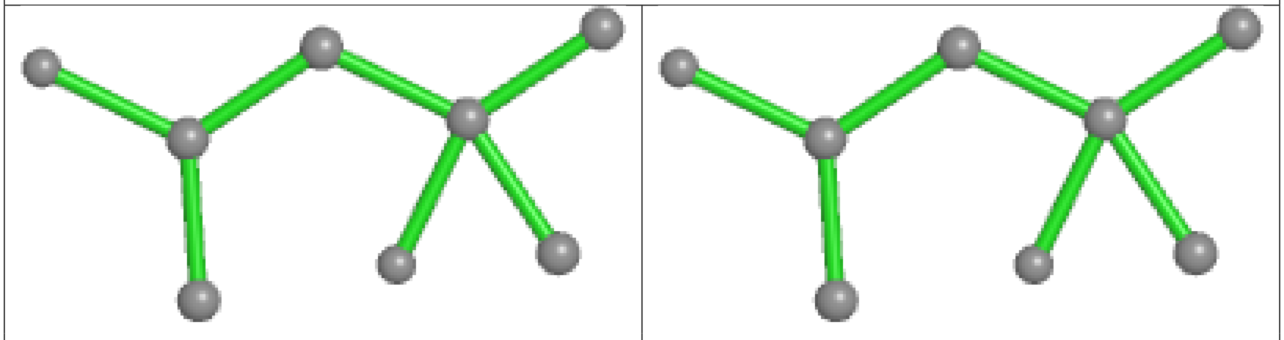
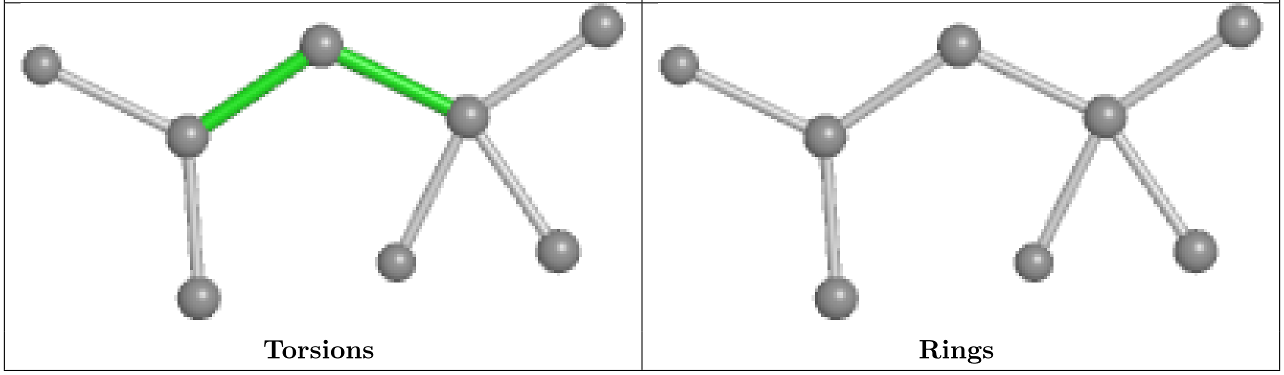


Bond lengths

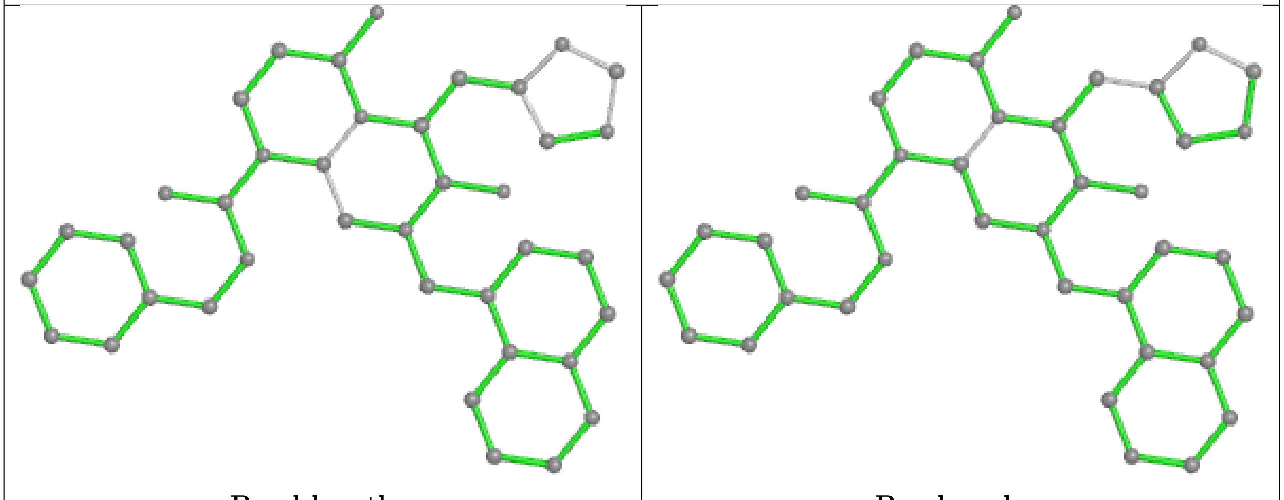
Bond angles



Torsions

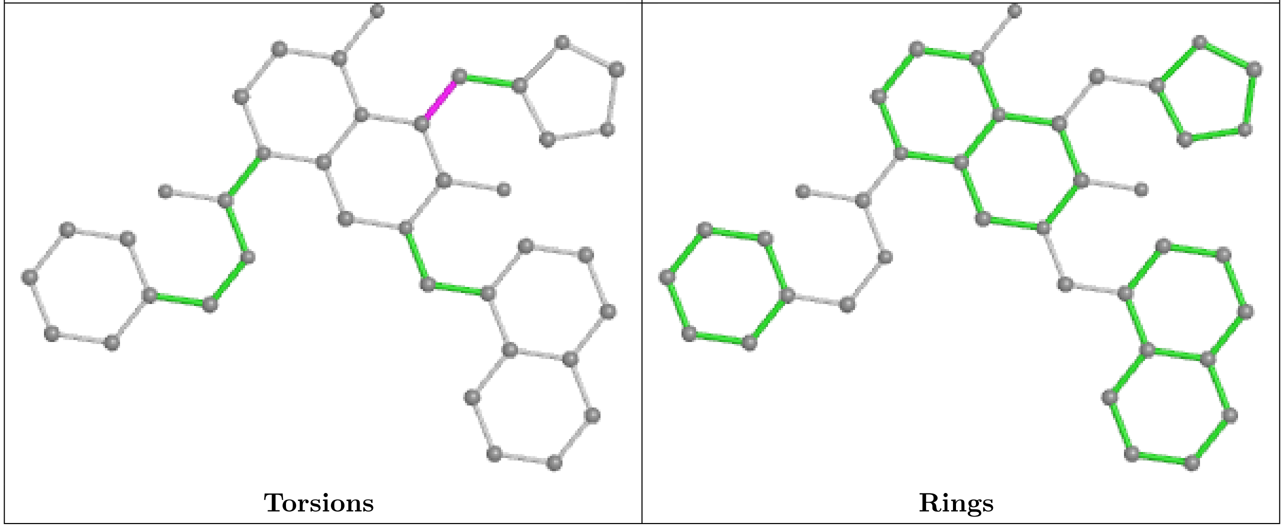
Rings

Ligand A1EEF C 301



Bond lengths

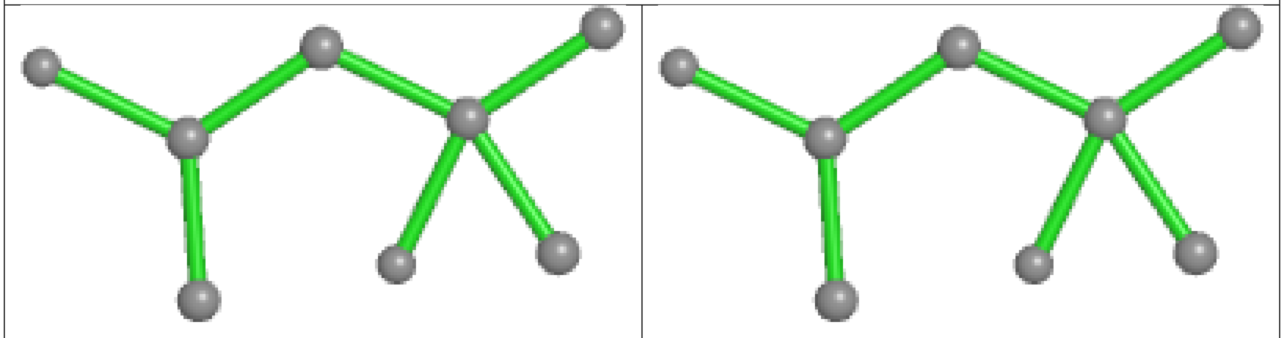
Bond angles



Torsions

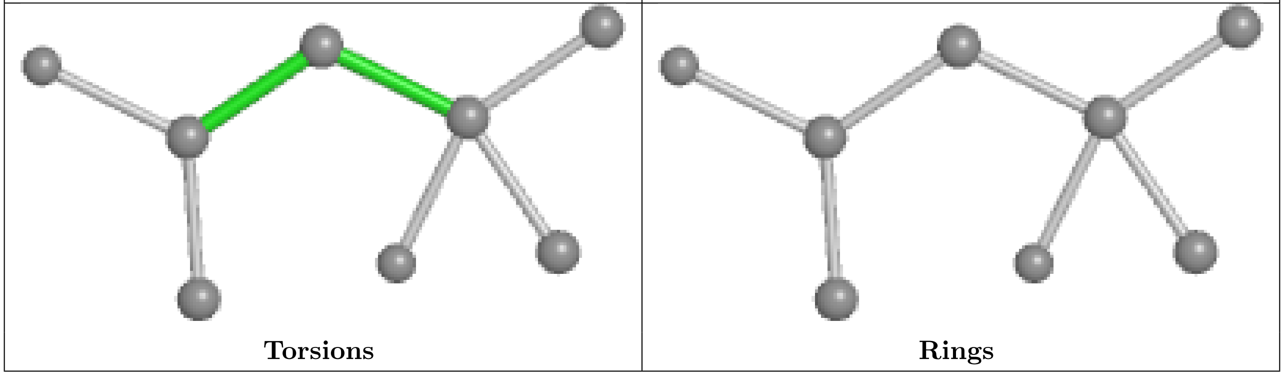
Rings

Ligand MPD E 303



Bond lengths

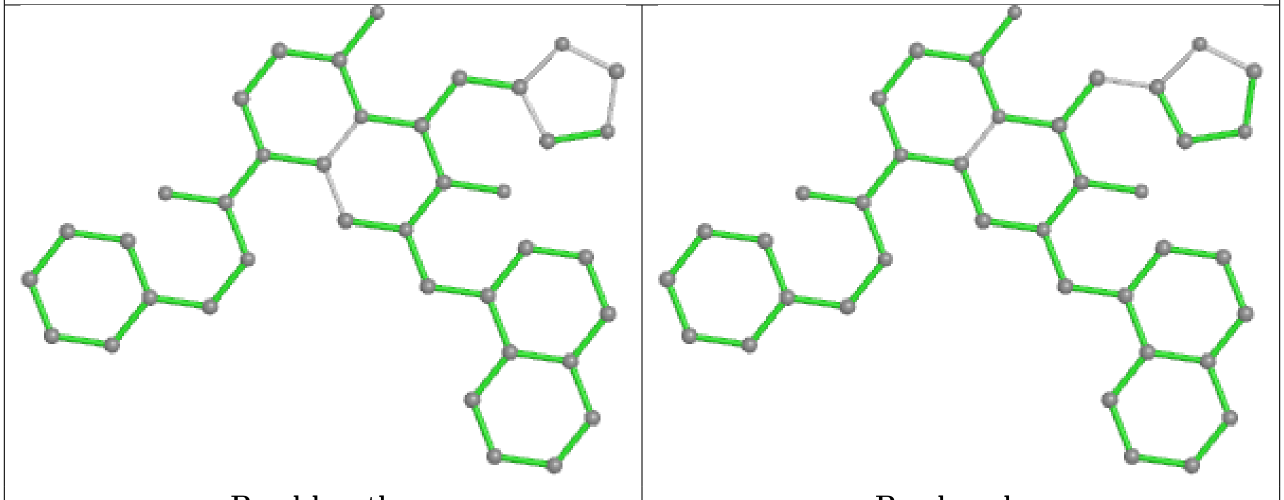
Bond angles



Torsions

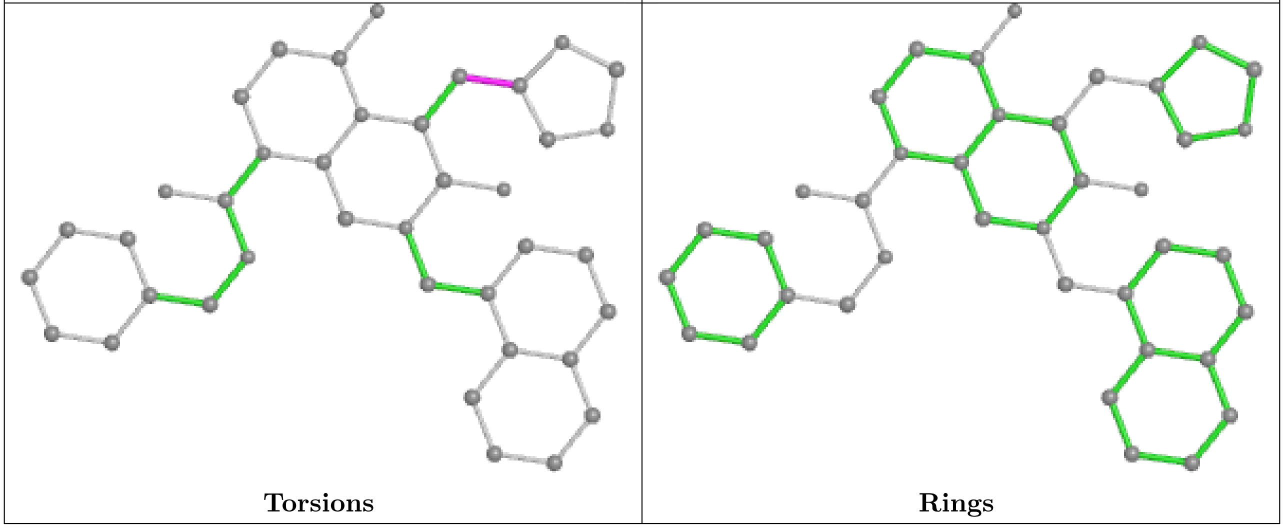
Rings

Ligand A1EEF H 301



Bond lengths

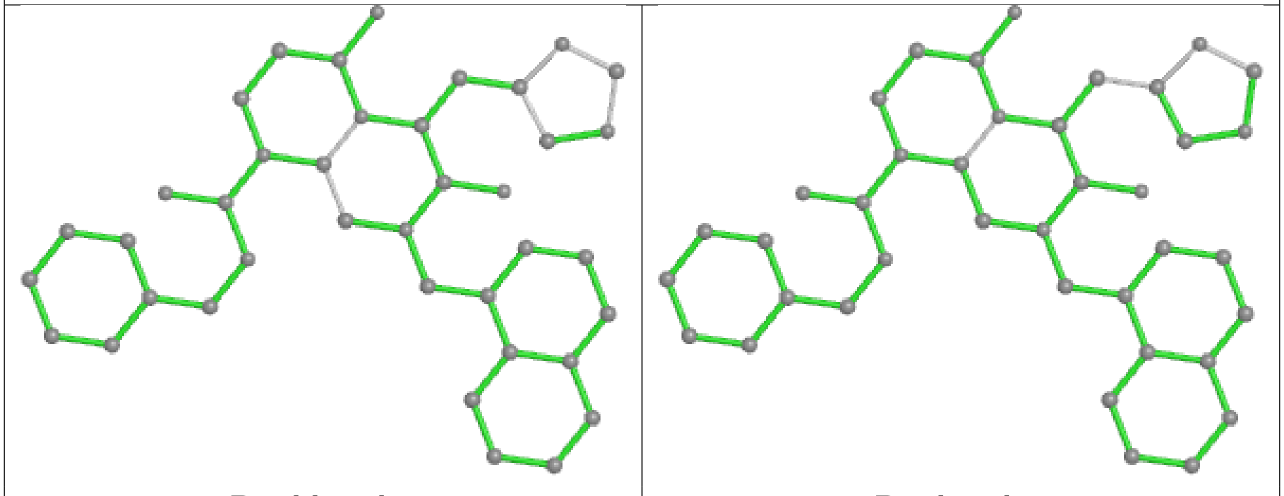
Bond angles



Torsions

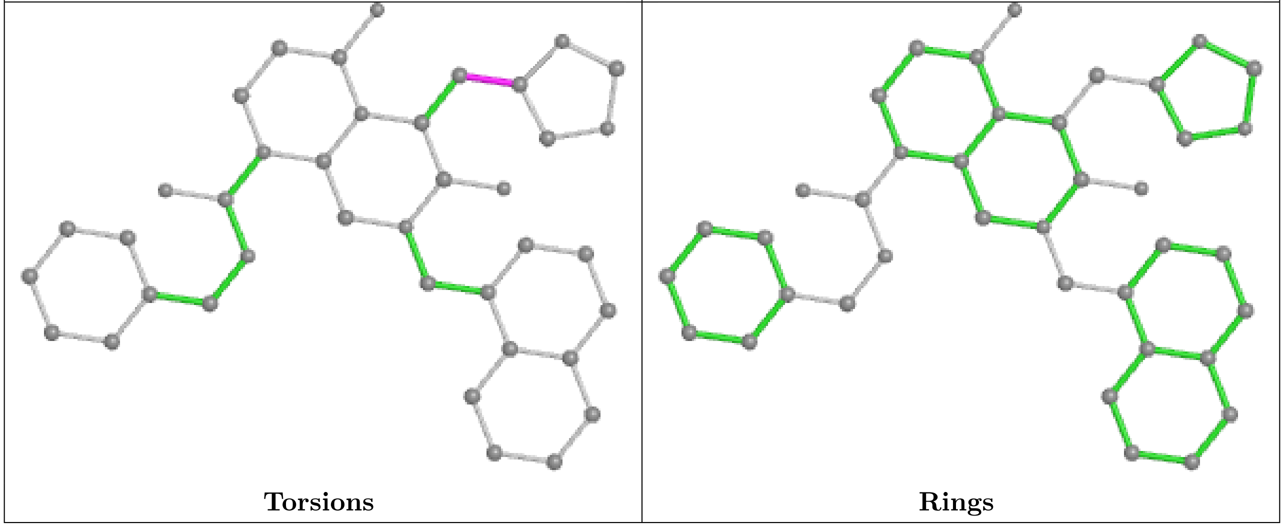
Rings

Ligand A1EEF F 301



Bond lengths

Bond angles



Torsions

Rings

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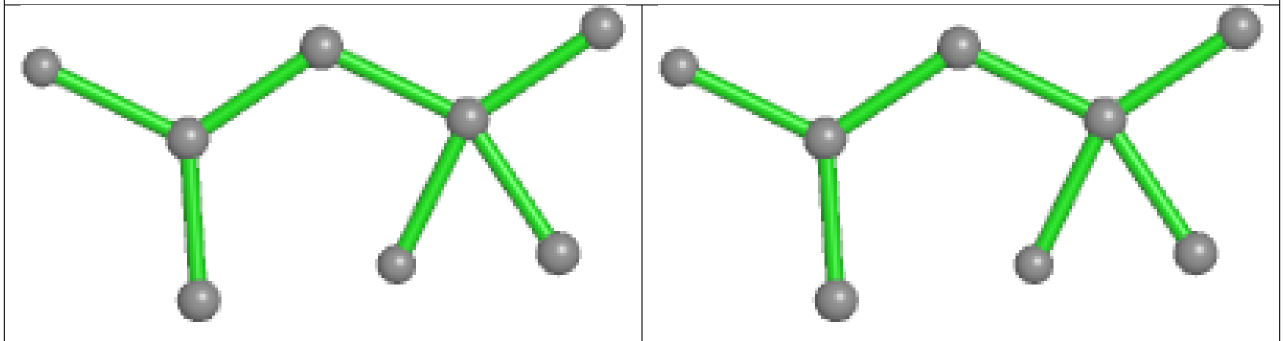
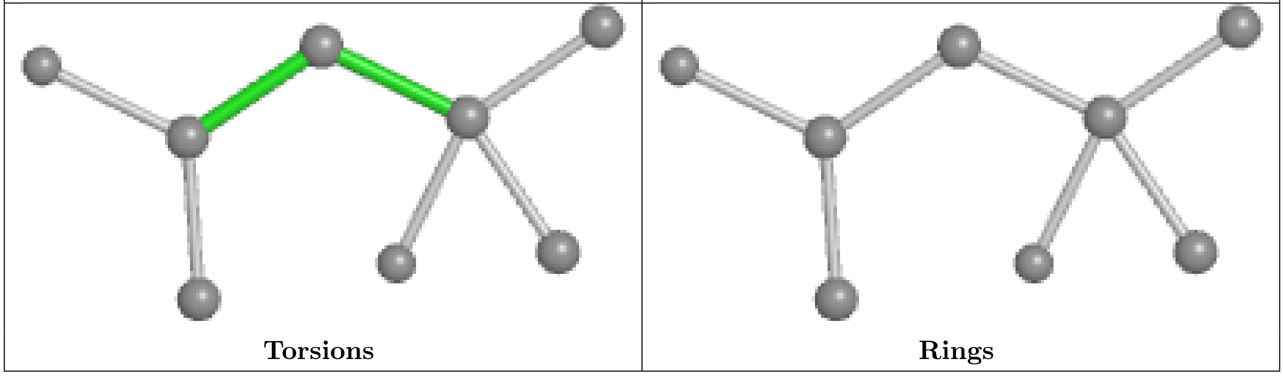
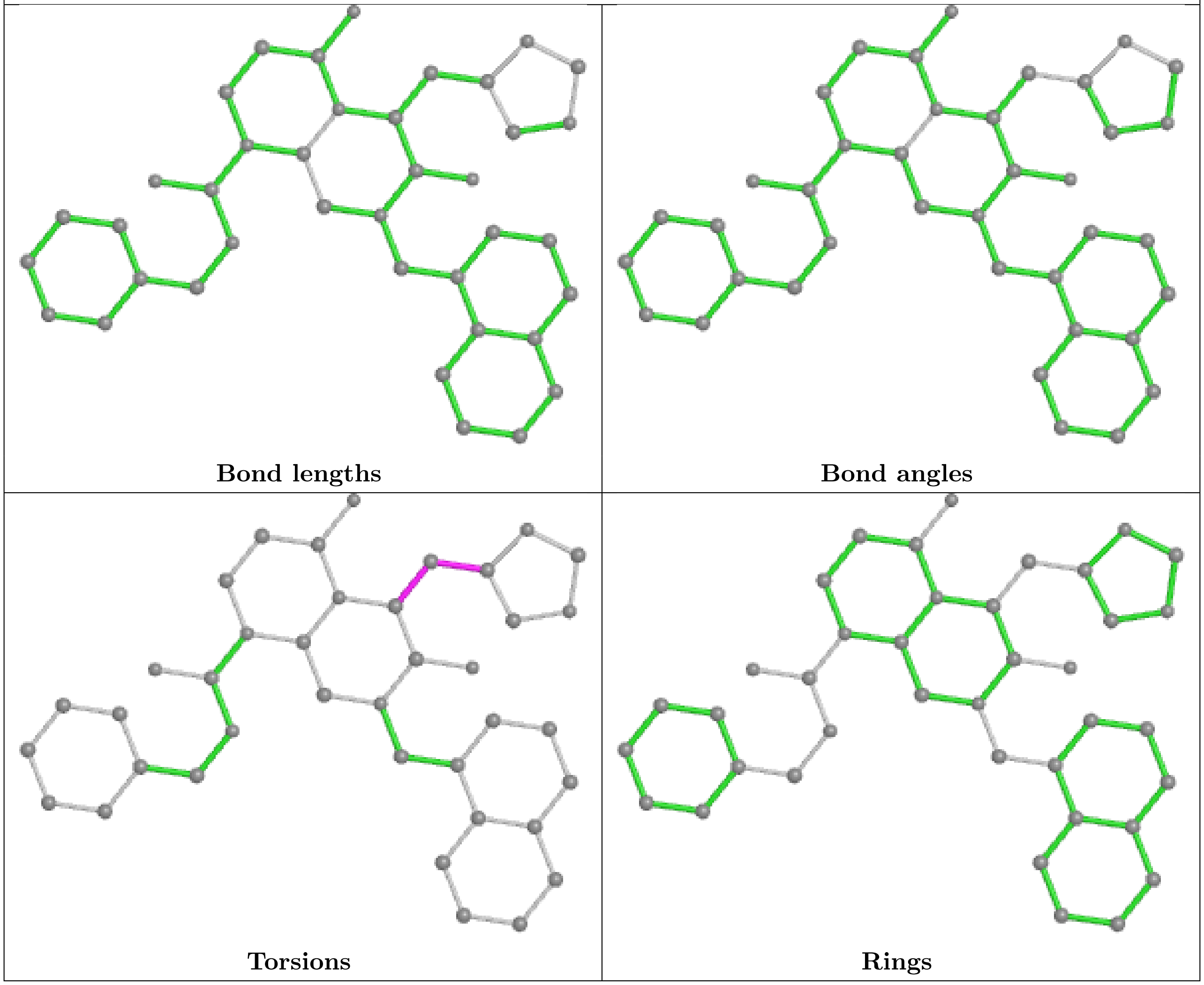


Bond lengths **Bond angles**



Torsions **Rings**

Ligand A1EEF N 301



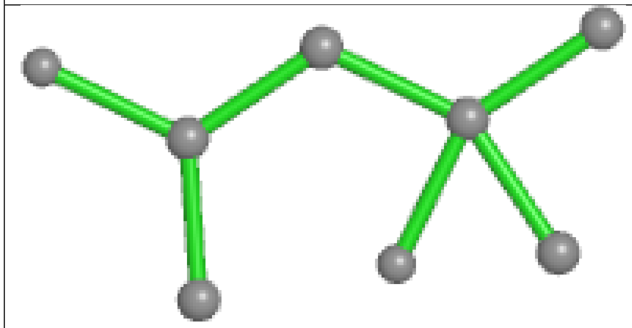
Bond lengths

Bond angles

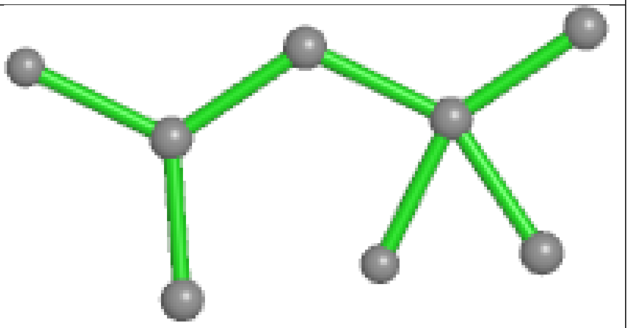
Torsions

Rings

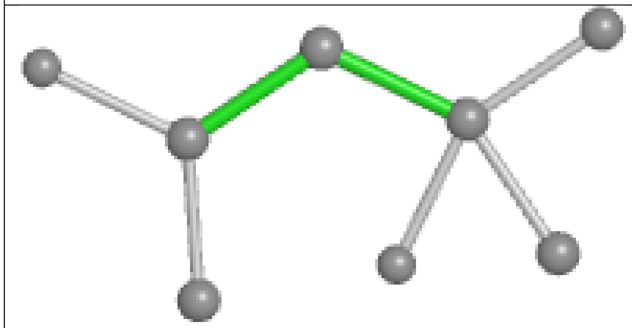
Ligand MPD I 303



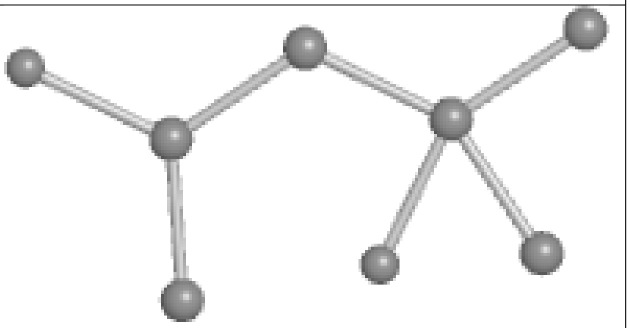
Bond lengths



Bond angles

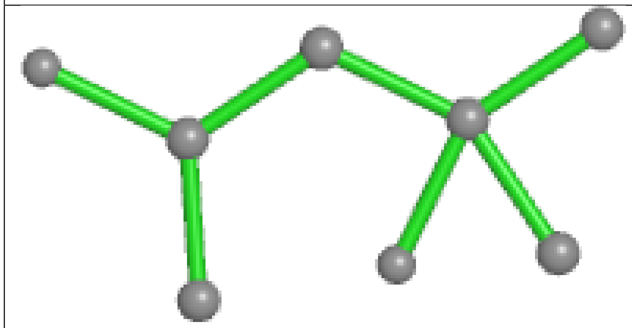


Torsions

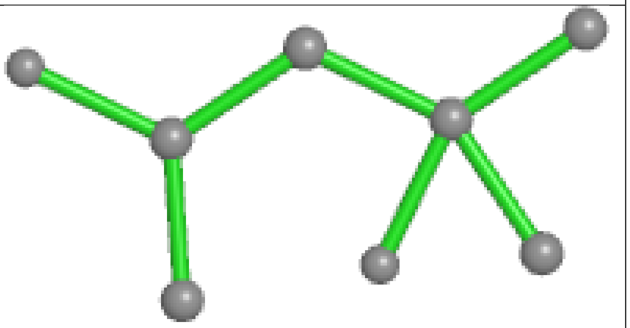


Rings

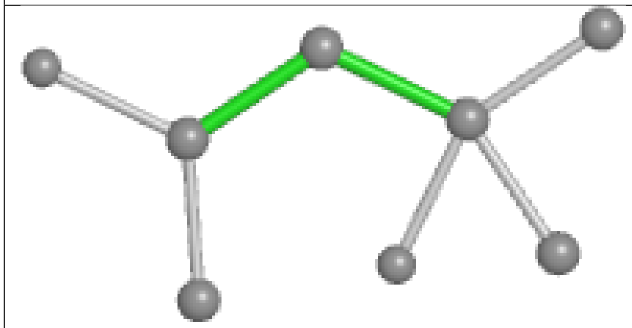
Ligand MPD C 303



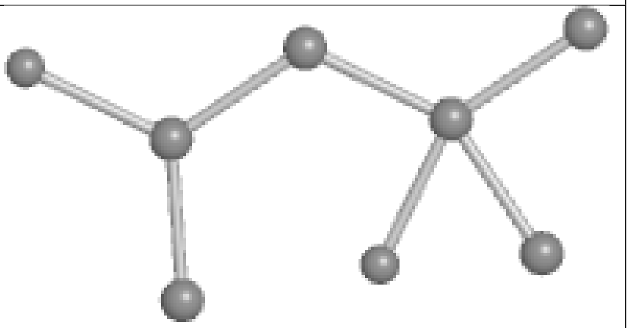
Bond lengths



Bond angles

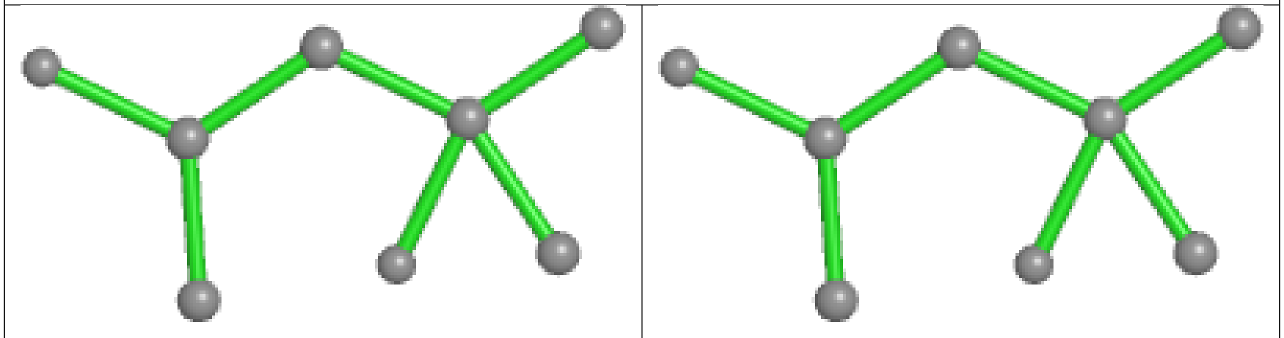


Torsions

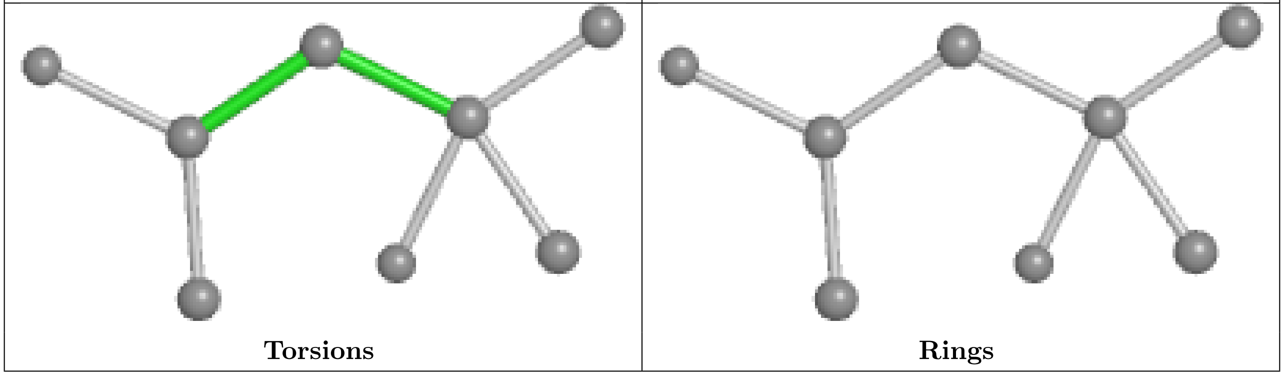


Rings

Ligand MPD G 303

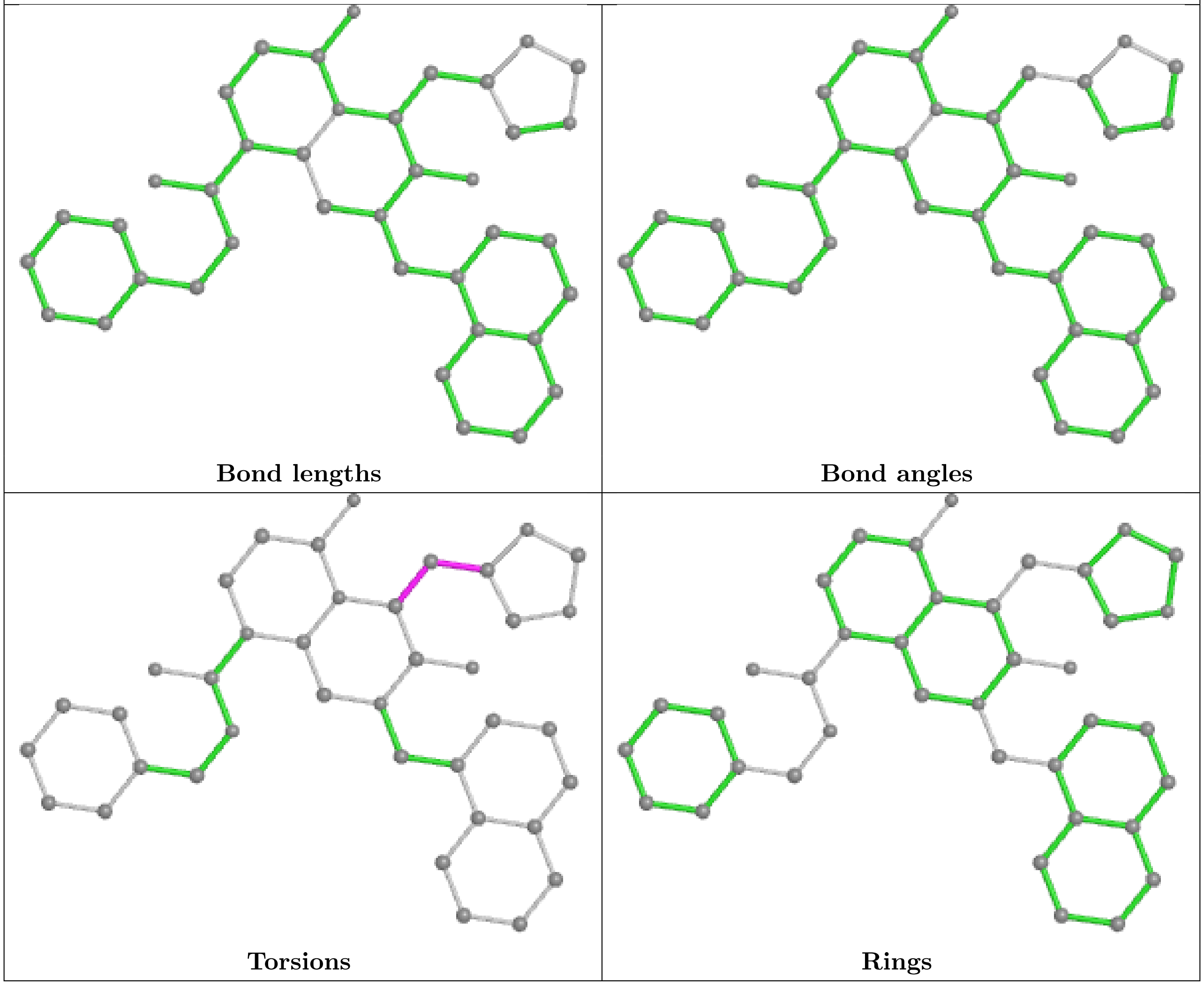


Bond lengths **Bond angles**



Torsions **Rings**

Ligand A1EEF E 301



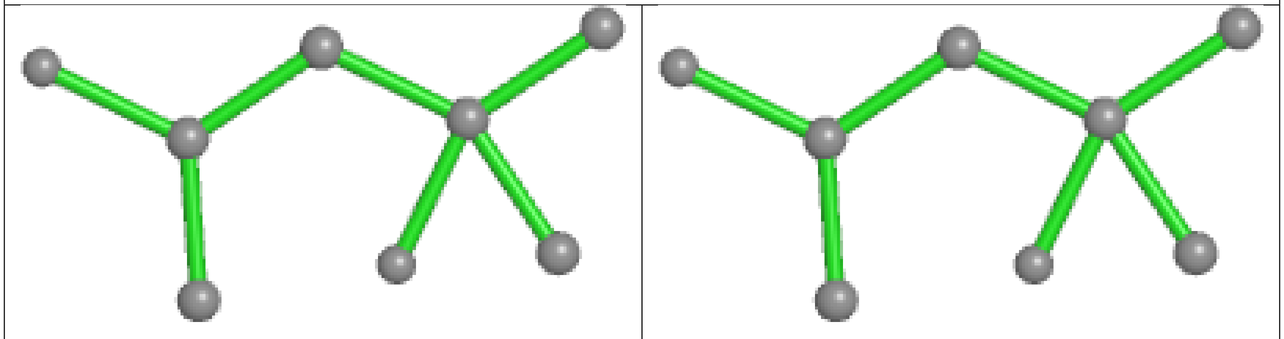
Bond lengths

Bond angles

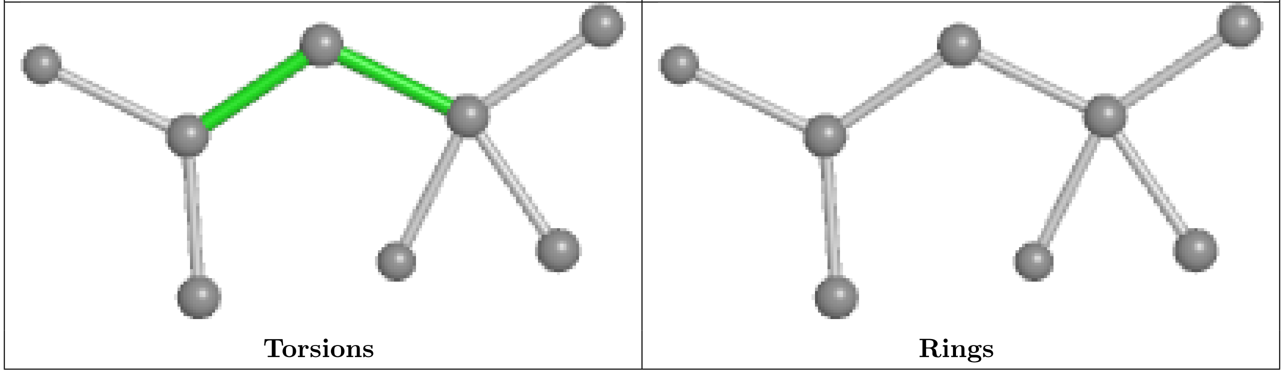
Torsions

Rings

Ligand MPD A 303

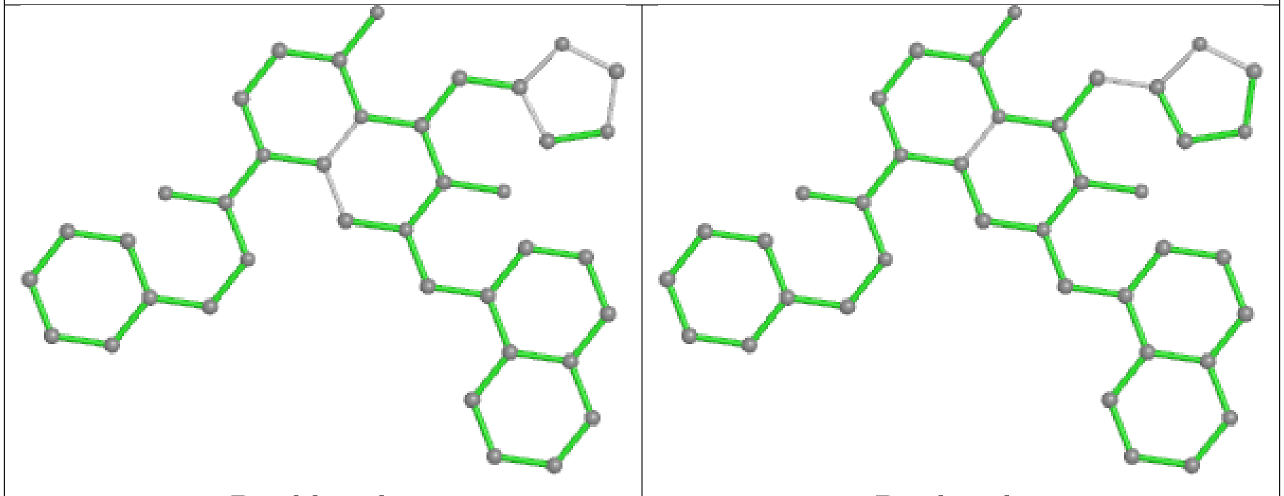


Bond lengths **Bond angles**



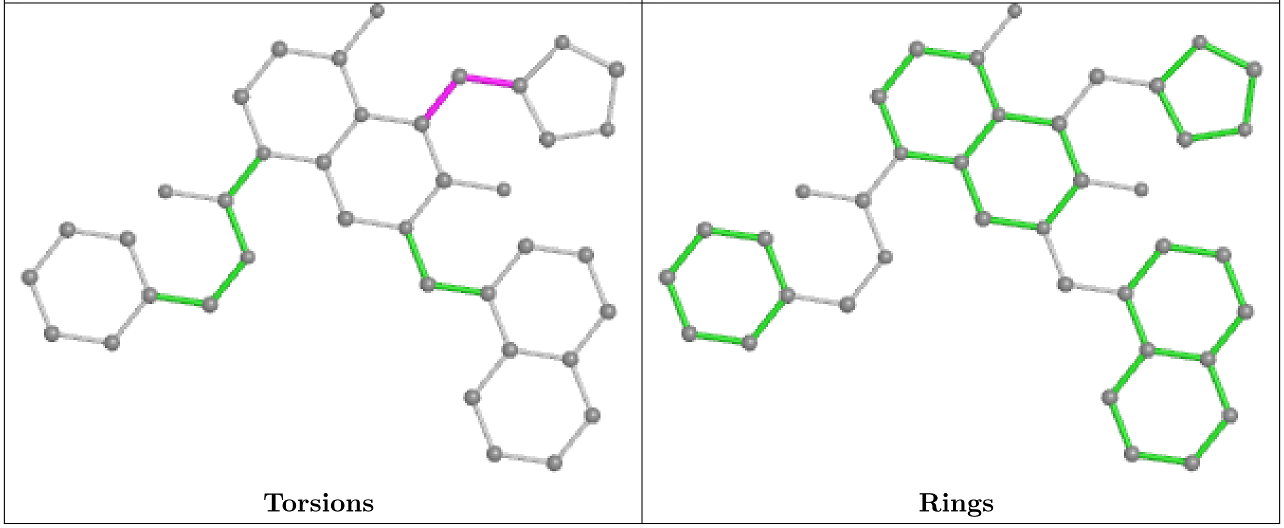
Torsions **Rings**

Ligand A1EEF A 301



Bond lengths

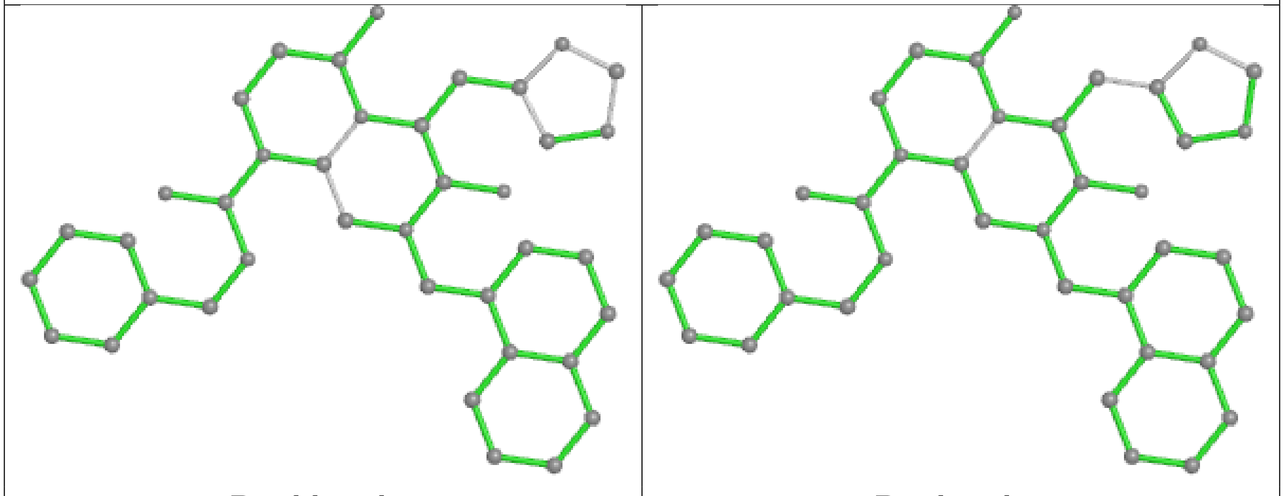
Bond angles



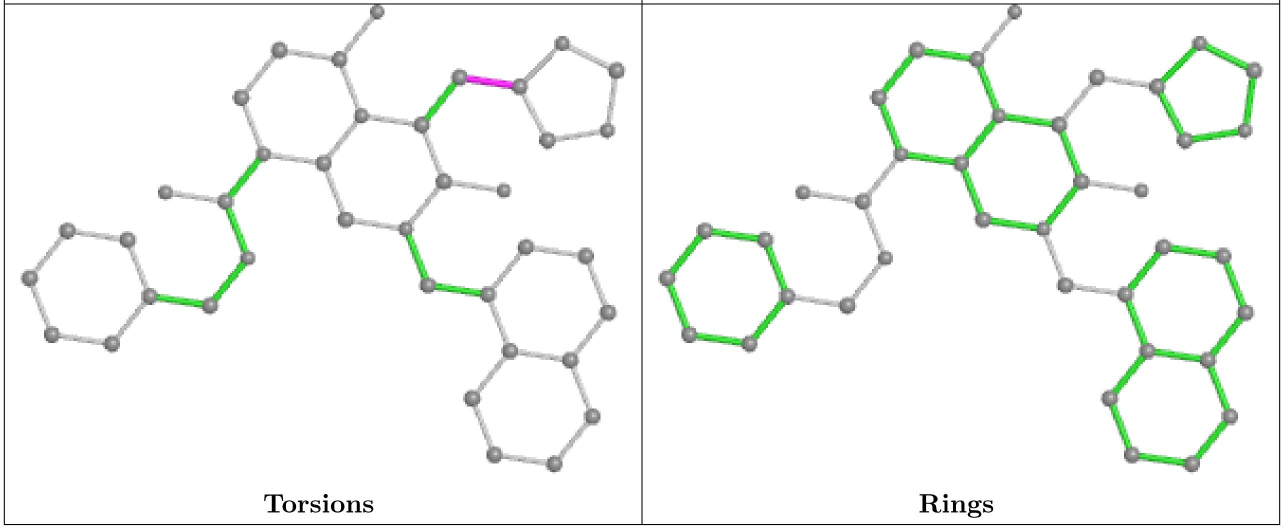
Torsions

Rings

Ligand A1EEF J 301

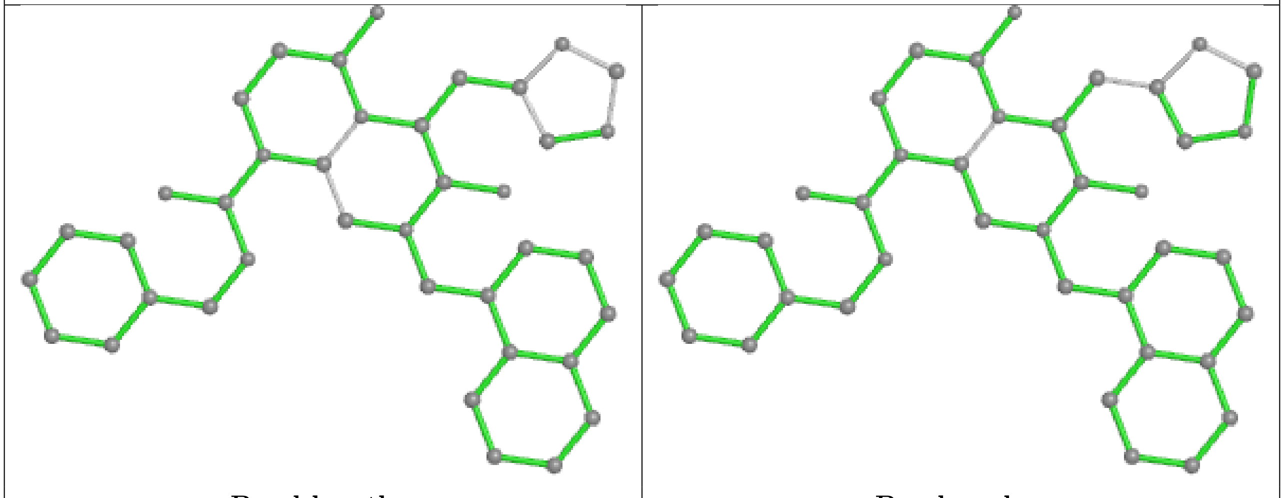


Bond lengths **Bond angles**

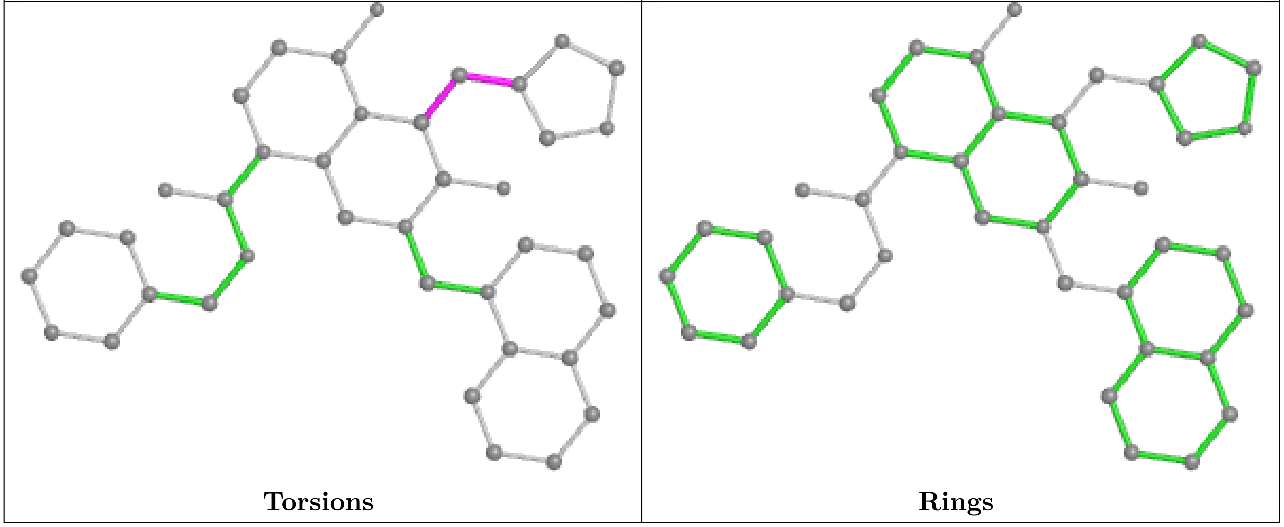


Torsions **Rings**

Ligand A1EEF B 301

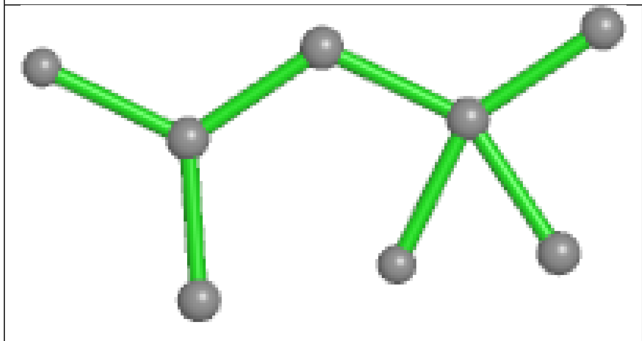


Bond lengths **Bond angles**

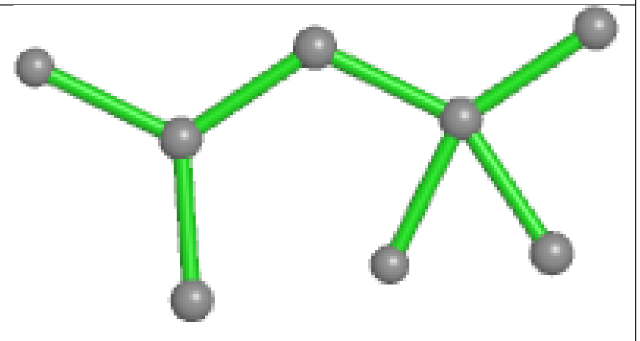


Torsions **Rings**

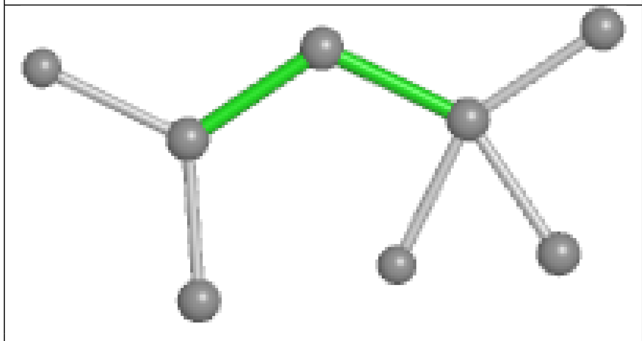
Ligand MPD L 303



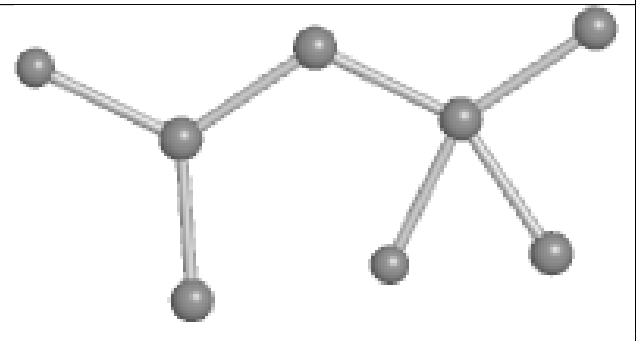
Bond lengths



Bond angles

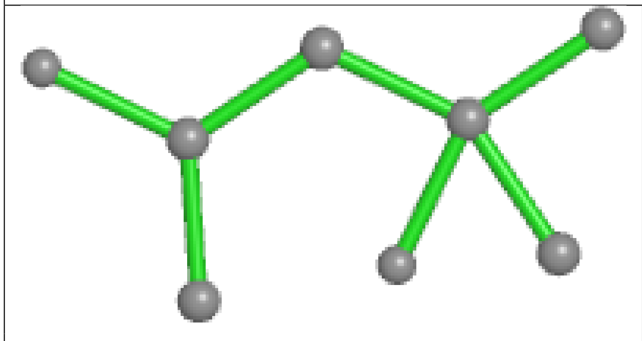


Torsions

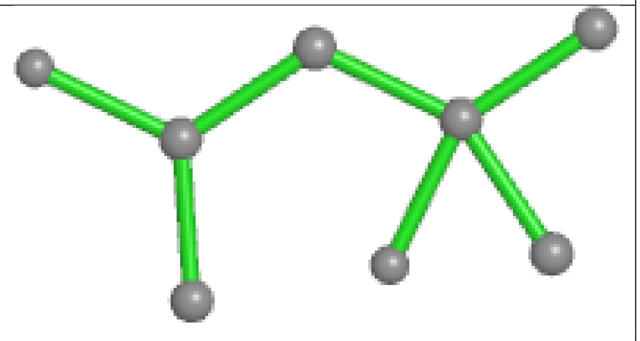


Rings

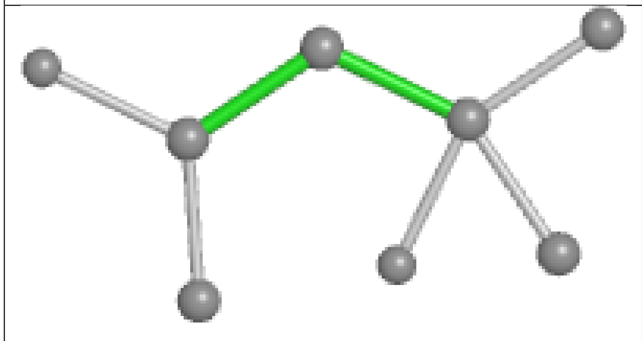
Ligand MPD N 303



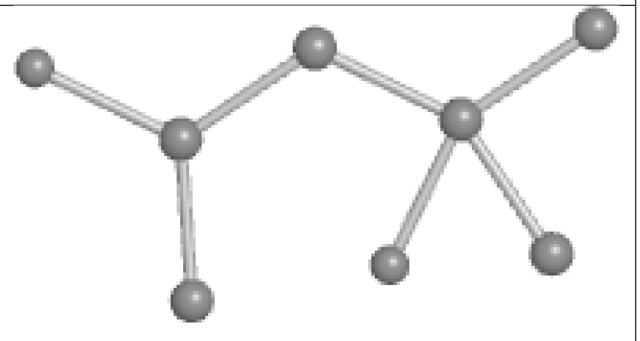
Bond lengths



Bond angles

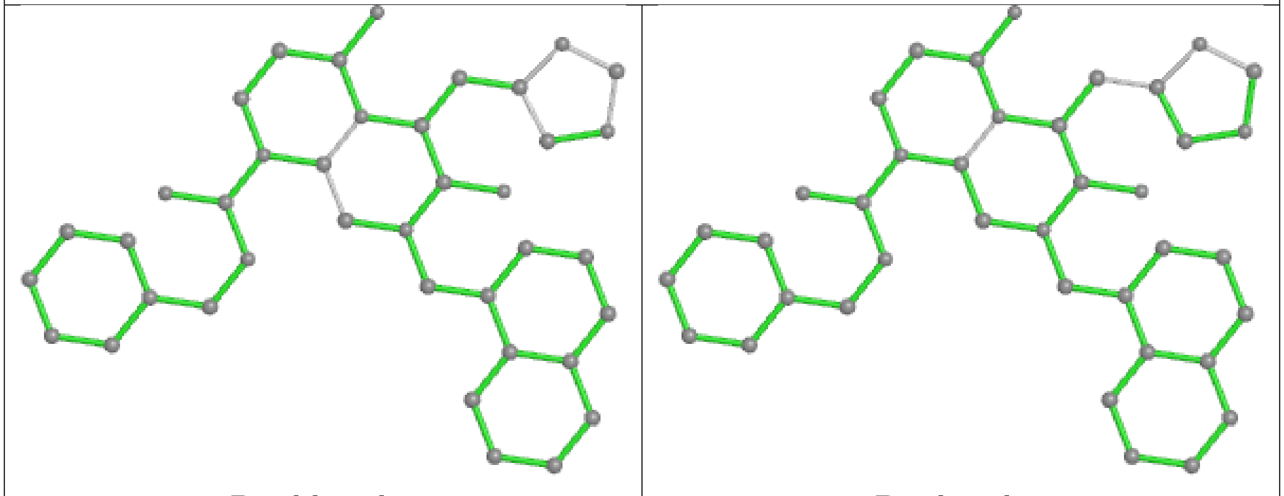


Torsions



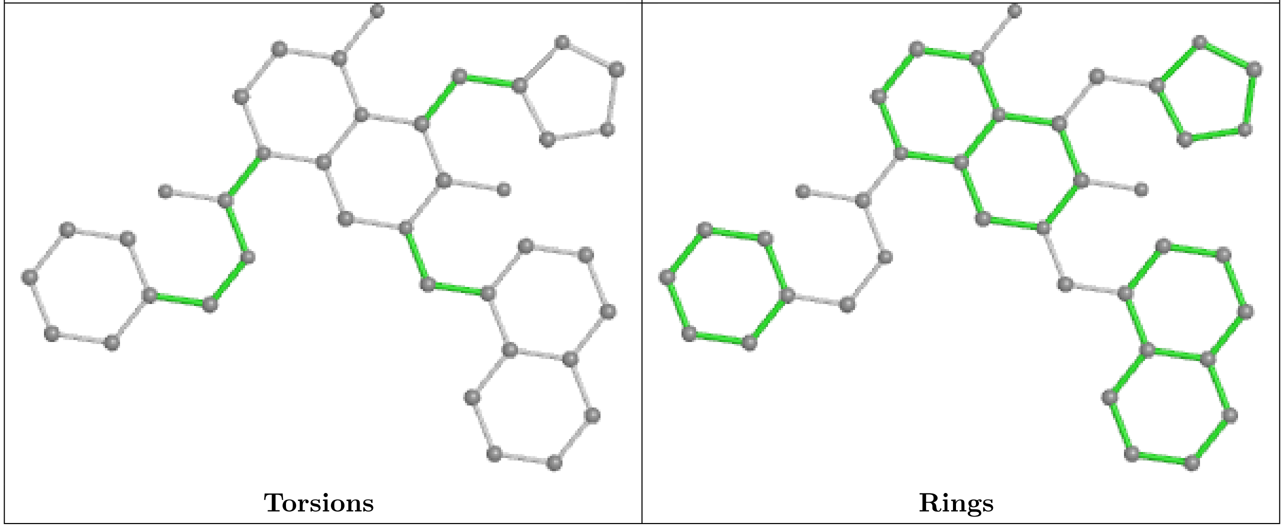
Rings

Ligand A1EEF K 301



Bond lengths

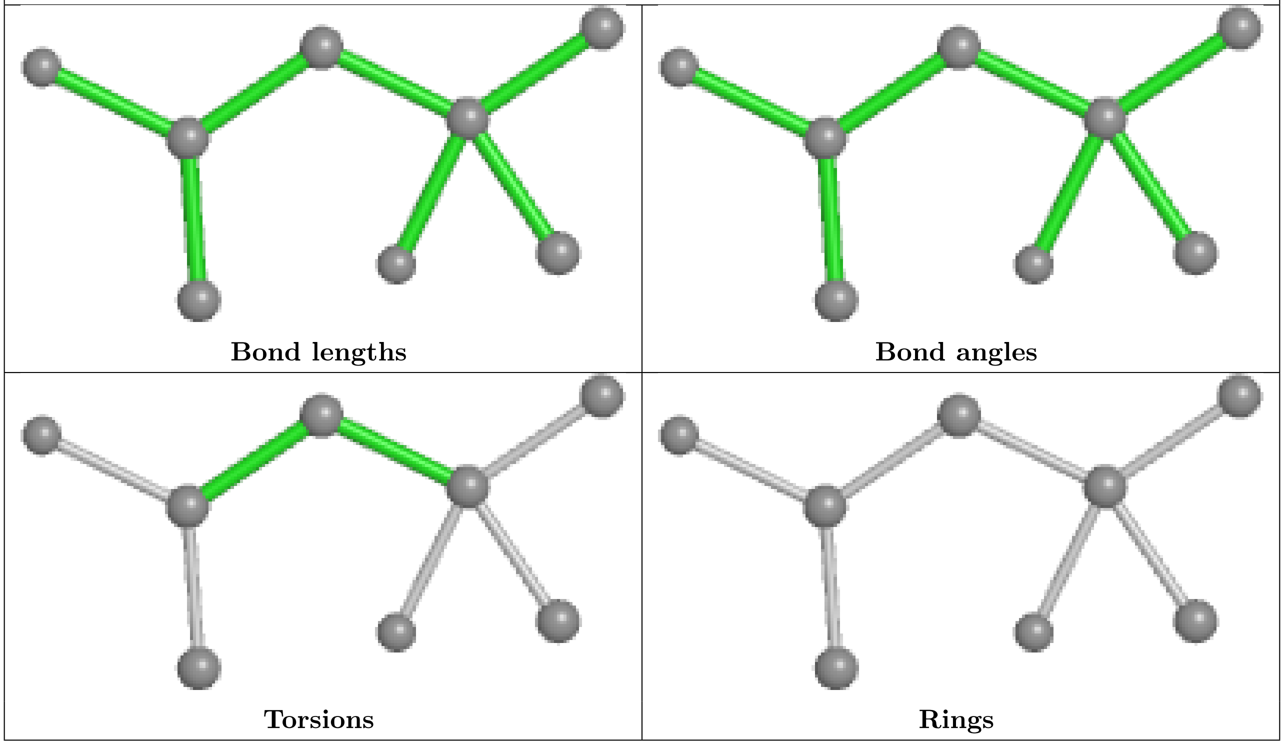
Bond angles



Torsions

Rings

Ligand MPD B 304



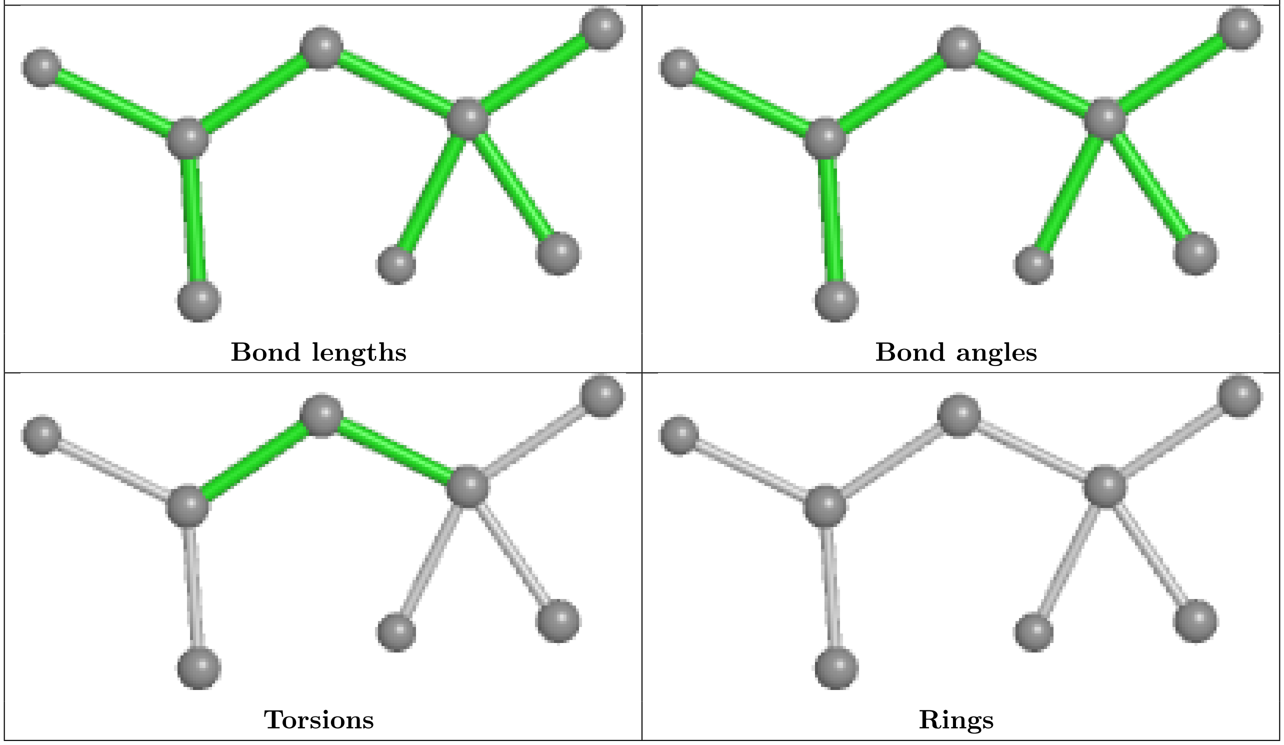
Bond lengths

Bond angles

Torsions

Rings

Ligand MPD H 303



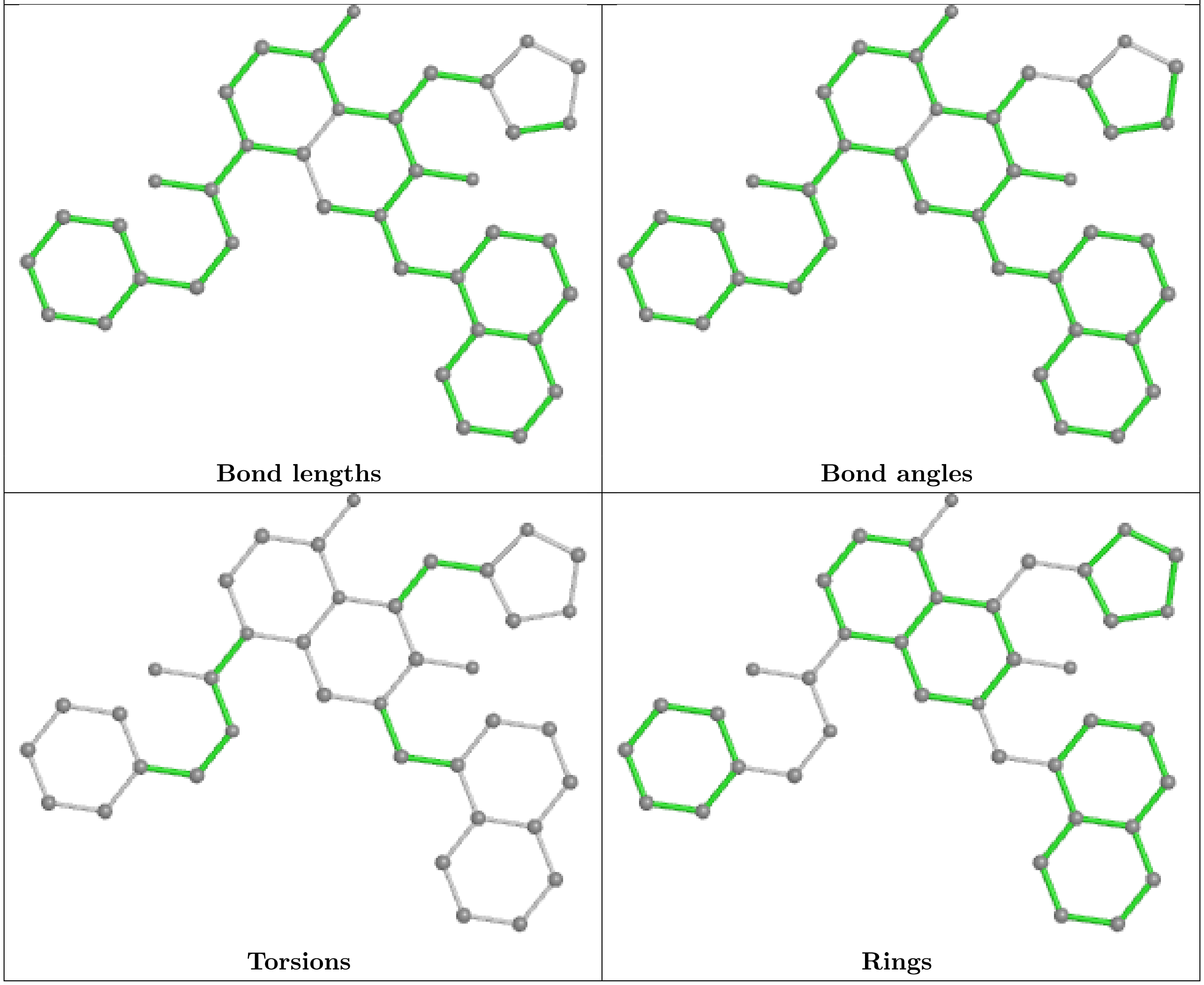
Bond lengths

Bond angles

Torsions

Rings

Ligand A1EEF I 301



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	A	181/203 (89%)	0.13	9 (4%)	35	46	15, 20, 32, 50	0
1	B	186/203 (91%)	0.17	12 (6%)	26	37	16, 20, 34, 54	0
1	C	183/203 (90%)	0.35	11 (6%)	29	39	16, 23, 35, 44	1 (0%)
1	D	179/203 (88%)	0.57	12 (6%)	25	35	23, 28, 41, 51	0
1	E	180/203 (88%)	0.62	11 (6%)	28	39	23, 29, 42, 56	0
1	F	180/203 (88%)	0.48	13 (7%)	23	32	21, 28, 41, 54	0
1	G	179/203 (88%)	0.32	12 (6%)	25	35	15, 22, 36, 56	2 (1%)
1	H	182/203 (89%)	0.20	8 (4%)	39	51	17, 20, 32, 58	0
1	I	182/203 (89%)	0.12	8 (4%)	39	51	16, 20, 32, 47	0
1	J	187/203 (92%)	0.44	13 (6%)	24	33	18, 24, 40, 50	1 (0%)
1	K	181/203 (89%)	0.80	14 (7%)	21	30	25, 31, 44, 56	0
1	L	179/203 (88%)	0.90	17 (9%)	15	22	24, 31, 42, 50	0
1	M	180/203 (88%)	0.68	12 (6%)	25	35	20, 30, 41, 63	0
1	N	180/203 (88%)	0.36	12 (6%)	25	35	18, 24, 37, 53	0
All	All	2539/2842 (89%)	0.44	164 (6%)	26	37	15, 26, 39, 63	4 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	THR	5.5
1	D	18	TYR	5.4
1	J	8	ILE	5.4
1	M	3	LEU	5.3
1	H	8	ILE	5.2
1	D	4	ILE	5.1
1	E	17	ALA	5.1
1	N	8	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	193	GLU	4.9
1	B	10	THR	4.8
1	C	191	VAL	4.7
1	G	4	ILE	4.7
1	F	8	ILE	4.7
1	A	6	THR	4.7
1	G	18	TYR	4.7
1	L	6	THR	4.6
1	A	4	ILE	4.6
1	K	3	LEU	4.5
1	I	192	PRO	4.5
1	B	3	LEU	4.5
1	A	8	ILE	4.4
1	G	7	VAL	4.4
1	L	191	VAL	4.4
1	N	18	TYR	4.3
1	K	7	VAL	4.3
1	H	17	ALA	4.3
1	M	7	VAL	4.3
1	L	49	LEU	4.2
1	G	57	GLU	4.1
1	D	191	VAL	4.0
1	M	4	ILE	4.0
1	H	54	GLN	3.9
1	E	7	VAL	3.9
1	F	191	VAL	3.9
1	L	4	ILE	3.9
1	J	191	VAL	3.8
1	K	191	VAL	3.8
1	D	7	VAL	3.8
1	E	18	TYR	3.7
1	J	4	ILE	3.7
1	C	63	TYR	3.7
1	C	8	ILE	3.7
1	B	130	GLN	3.7
1	C	3	LEU	3.6
1	I	163	GLU	3.5
1	E	130	GLN	3.4
1	J	197	GLU	3.4
1	D	5	PRO	3.4
1	M	6	THR	3.3
1	G	191	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	119	GLU	3.2
1	M	163	GLU	3.2
1	N	7	VAL	3.2
1	C	130	GLN	3.2
1	E	191	VAL	3.2
1	A	18	TYR	3.2
1	L	182	GLU	3.2
1	E	192	PRO	3.2
1	G	130	GLN	3.1
1	L	7	VAL	3.1
1	C	16	ARG	3.1
1	N	4	ILE	3.1
1	D	163	GLU	3.1
1	J	201	HIS	3.1
1	N	191	VAL	3.1
1	M	18	TYR	3.0
1	B	193	GLU	3.0
1	A	193	GLU	3.0
1	G	192	PRO	2.9
1	J	199	HIS	2.9
1	M	130	GLN	2.9
1	N	182	GLU	2.9
1	G	5	PRO	2.9
1	H	4	ILE	2.8
1	L	95	MET	2.8
1	F	18	TYR	2.8
1	A	191	VAL	2.8
1	B	9	GLU	2.8
1	E	4	ILE	2.8
1	G	63	TYR	2.8
1	J	95[A]	MET	2.8
1	F	7	VAL	2.7
1	K	54	GLN	2.7
1	K	193	GLU	2.7
1	K	4	ILE	2.7
1	A	192	PRO	2.7
1	A	130	GLN	2.7
1	J	200	HIS	2.7
1	J	18	TYR	2.7
1	K	18	TYR	2.7
1	B	8	ILE	2.7
1	H	130	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	192	PRO	2.7
1	B	191	VAL	2.6
1	I	191	VAL	2.6
1	L	18	TYR	2.6
1	G	19	ASP	2.6
1	D	192	PRO	2.6
1	K	49	LEU	2.6
1	C	192	PRO	2.6
1	J	203	HIS	2.6
1	I	16	ARG	2.6
1	E	182	GLU	2.6
1	I	17	ALA	2.6
1	J	198	HIS	2.5
1	J	63	TYR	2.5
1	I	141	ASN	2.5
1	D	6	THR	2.5
1	N	26	LYS	2.5
1	H	192	PRO	2.5
1	I	130	GLN	2.5
1	E	101	SER	2.5
1	N	6	THR	2.5
1	K	163	GLU	2.5
1	K	192	PRO	2.5
1	M	192	PRO	2.5
1	L	53	ALA	2.5
1	M	85	LYS	2.4
1	F	49	LEU	2.4
1	N	130	GLN	2.4
1	H	191	VAL	2.4
1	C	18	TYR	2.4
1	N	63	TYR	2.4
1	E	95	MET	2.4
1	F	63	TYR	2.4
1	B	16	ARG	2.3
1	F	192	PRO	2.3
1	K	39	ASN	2.3
1	D	63	TYR	2.3
1	L	109	LYS	2.3
1	C	54	GLN	2.3
1	K	57	GLU	2.3
1	D	57	GLU	2.3
1	L	153	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	192	PRO	2.3
1	B	7	VAL	2.3
1	L	56	SER	2.3
1	F	4	ILE	2.2
1	G	93	ILE	2.2
1	K	130	GLN	2.2
1	L	85	LYS	2.2
1	C	57	GLU	2.2
1	F	85	LYS	2.2
1	B	4	ILE	2.2
1	I	4	ILE	2.2
1	E	6	THR	2.2
1	K	53	ALA	2.2
1	M	5	PRO	2.2
1	B	18	TYR	2.1
1	L	31	MET	2.1
1	M	54	GLN	2.1
1	N	57	GLU	2.1
1	F	57	GLU	2.1
1	F	130	GLN	2.1
1	F	163	GLU	2.1
1	L	54	GLN	2.1
1	N	192	PRO	2.0
1	L	158	THR	2.0
1	D	157	ARG	2.0
1	M	63	TYR	2.0
1	A	7	VAL	2.0
1	D	26	LYS	2.0
1	J	130	GLN	2.0
1	F	42	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($\AA^2$)	Q<0.9
2	A1EEF	G	301	39/39	0.67	0.21	48,53,72,73	0
2	A1EEF	C	301	39/39	0.75	0.18	46,49,70,70	0
2	A1EEF	F	301	39/39	0.78	0.16	47,53,68,69	0
2	A1EEF	N	301	39/39	0.78	0.18	43,49,69,71	0
2	A1EEF	M	301	39/39	0.79	0.16	52,56,71,72	0
2	A1EEF	J	301	39/39	0.80	0.16	39,45,66,67	0
2	A1EEF	D	301	39/39	0.81	0.16	47,50,64,65	0
4	MPD	G	303	8/8	0.81	0.14	35,36,38,40	0
4	MPD	B	303	8/8	0.82	0.17	41,42,43,44	0
2	A1EEF	L	301	39/39	0.82	0.16	51,55,65,66	0
2	A1EEF	I	301	39/39	0.84	0.13	31,34,52,53	0
4	MPD	B	304	8/8	0.85	0.12	32,34,35,36	0
2	A1EEF	K	301	39/39	0.85	0.14	41,48,60,61	0
4	MPD	H	303	8/8	0.85	0.14	31,32,34,35	0
4	MPD	E	303	8/8	0.86	0.16	45,47,48,50	0
2	A1EEF	A	301	39/39	0.86	0.12	33,37,57,60	0
2	A1EEF	H	301	39/39	0.86	0.12	34,36,51,53	0
4	MPD	I	303	8/8	0.86	0.15	30,33,34,35	0
4	MPD	K	303	8/8	0.86	0.15	41,43,44,45	0
4	MPD	D	303	8/8	0.87	0.14	37,39,41,44	0
2	A1EEF	E	301	39/39	0.87	0.12	43,44,57,57	0
4	MPD	L	303	8/8	0.87	0.15	43,45,46,46	0
4	MPD	F	303	8/8	0.88	0.15	42,43,46,48	0
4	MPD	J	303	8/8	0.88	0.12	33,35,37,37	0
4	MPD	C	303	8/8	0.89	0.11	35,38,39,39	0
3	MG	E	302	1/1	0.89	0.24	50,50,50,50	0
3	MG	L	302	1/1	0.90	0.22	51,51,51,51	0
4	MPD	A	303	8/8	0.90	0.11	32,33,33,34	0
4	MPD	N	303	8/8	0.90	0.12	34,35,38,39	0
3	MG	F	302	1/1	0.91	0.10	42,42,42,42	0
2	A1EEF	B	301	39/39	0.91	0.10	26,28,45,46	0
4	MPD	M	303	8/8	0.92	0.11	37,39,41,41	0
3	MG	M	302	1/1	0.95	0.10	47,47,47,47	0
3	MG	D	302	1/1	0.95	0.10	44,44,44,44	0
3	MG	H	302	1/1	0.95	0.07	35,35,35,35	0
3	MG	C	302	1/1	0.95	0.08	36,36,36,36	0
3	MG	N	302	1/1	0.96	0.08	41,41,41,41	0

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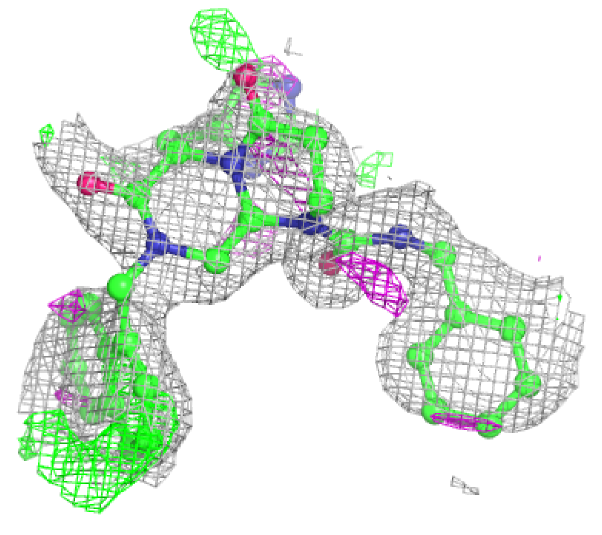
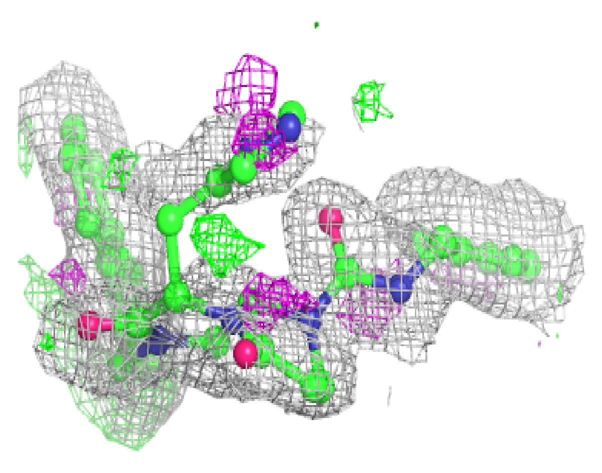
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	302	1/1	0.96	0.14	36,36,36,36	0
3	MG	J	302	1/1	0.97	0.11	43,43,43,43	0
3	MG	I	302	1/1	0.98	0.06	29,29,29,29	0
3	MG	G	302	1/1	0.98	0.09	36,36,36,36	0
3	MG	K	302	1/1	0.98	0.11	48,48,48,48	0
3	MG	A	302	1/1	0.99	0.07	31,31,31,31	0

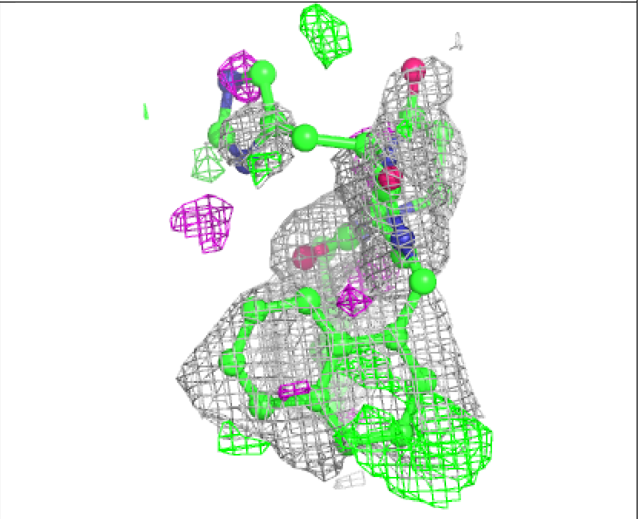
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

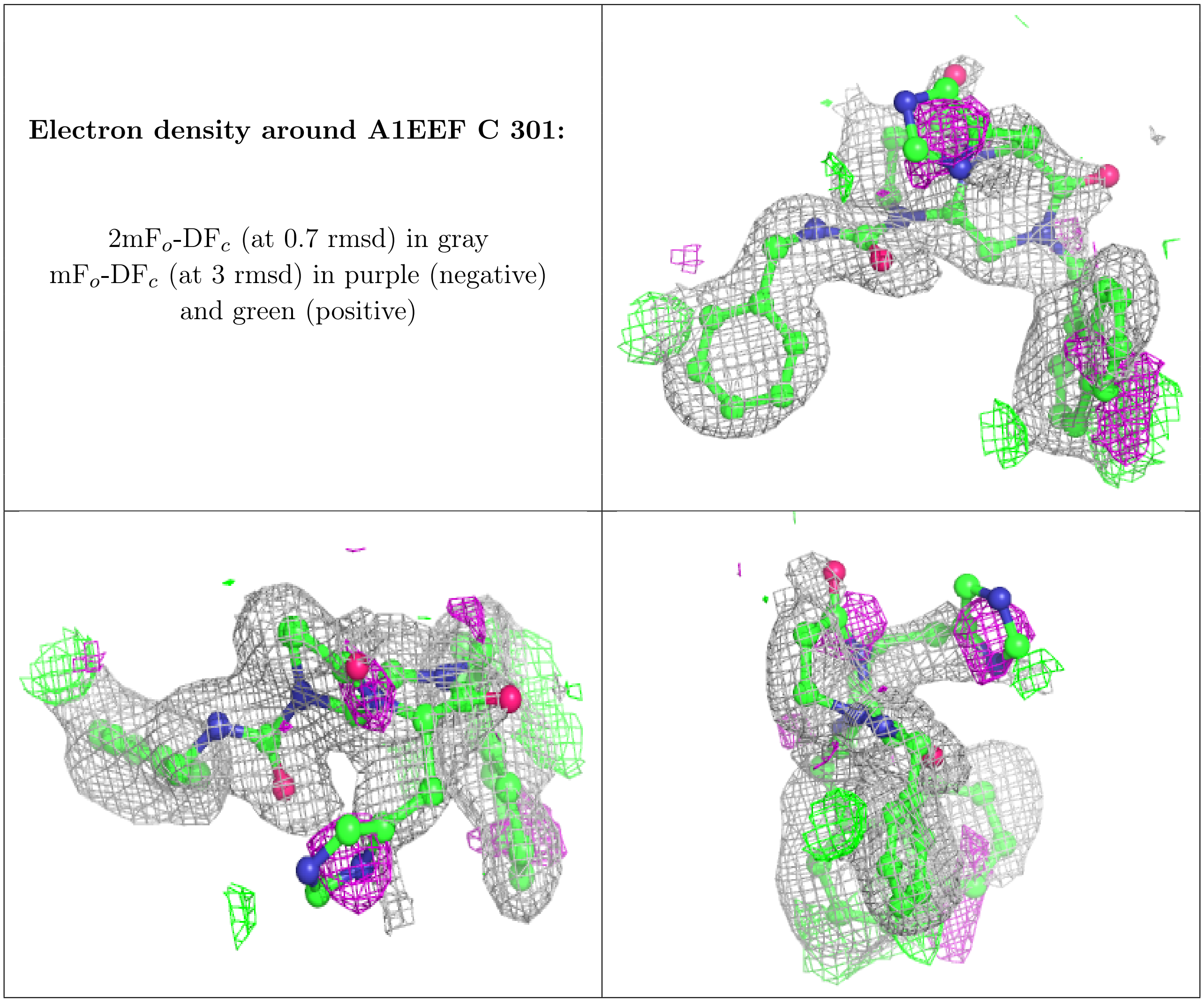
Electron density around A1EEF G 301:

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







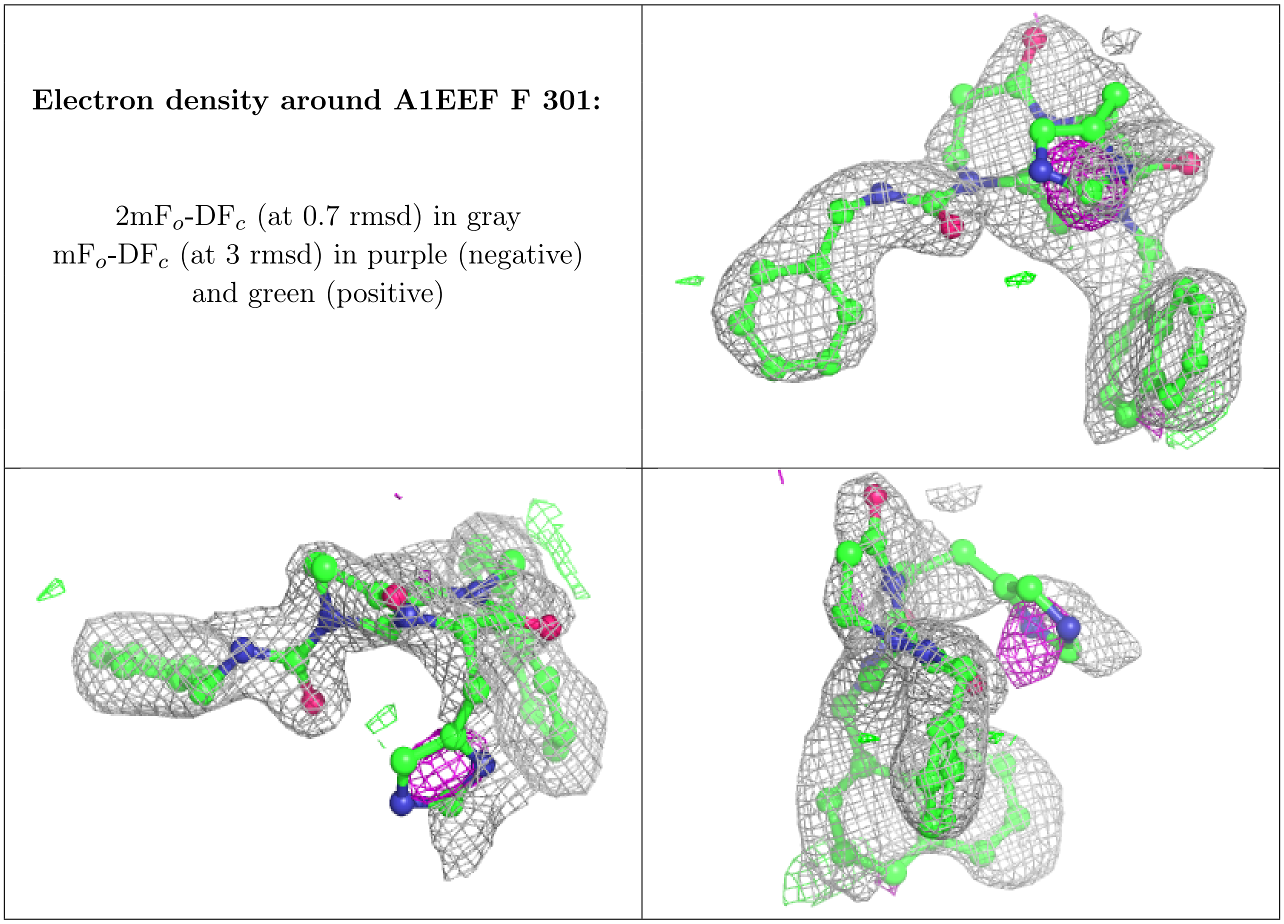


Electron density around A1EEF C 301:

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

Electron density around A1EEF 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 A1EEF N 301:

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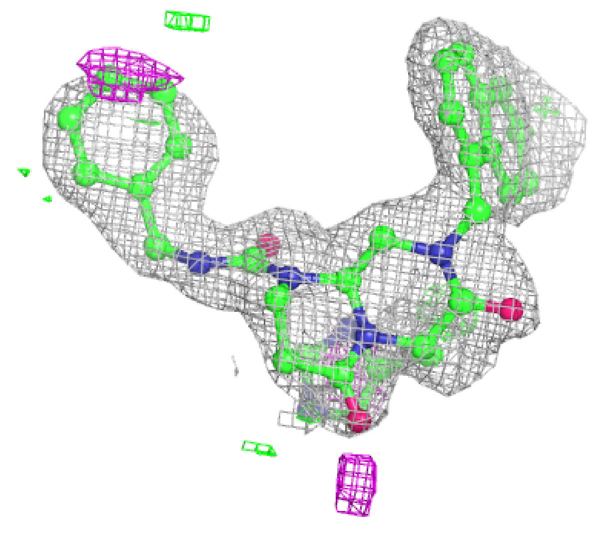
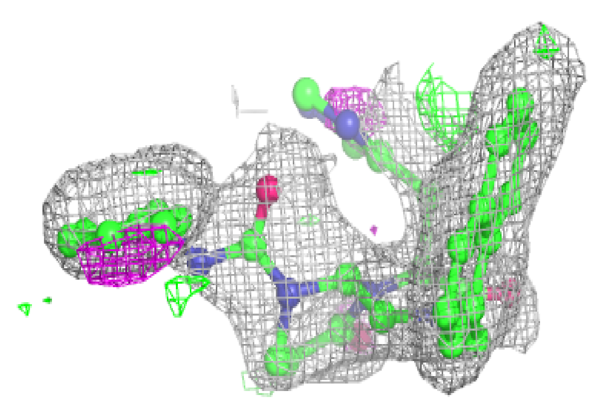
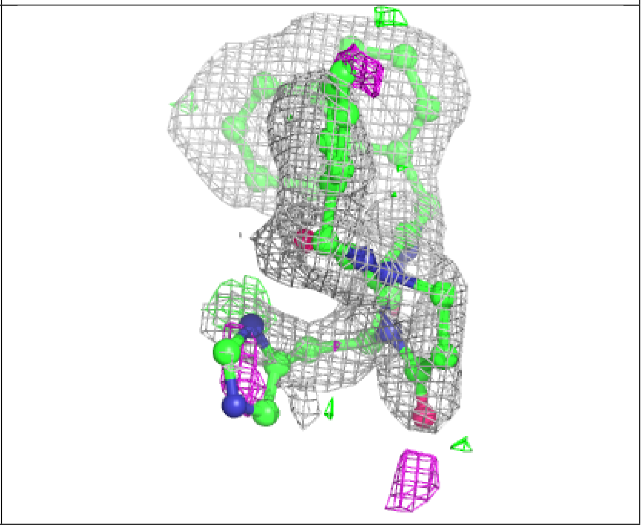
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

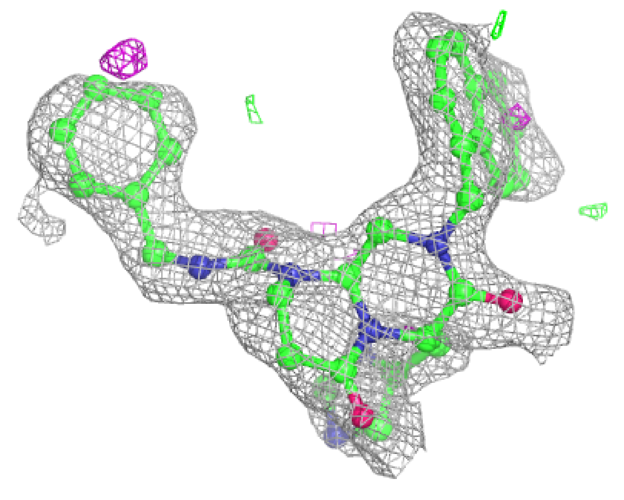


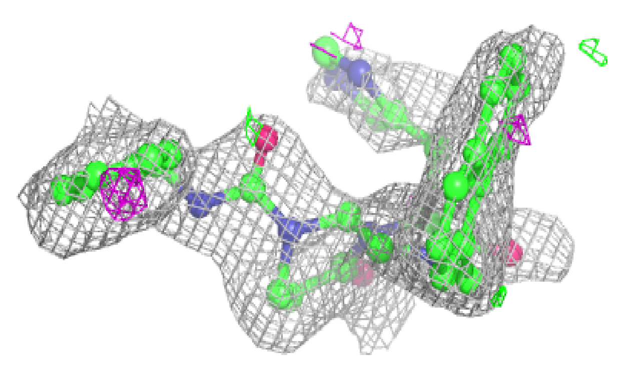


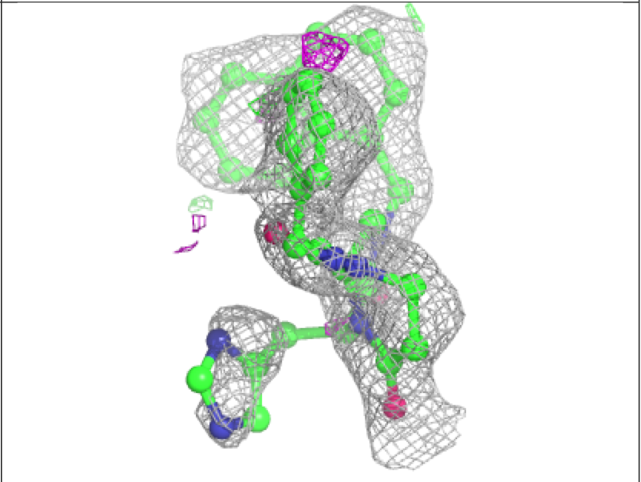


Electron density around A1EEF M 301:

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







Electron density around A1EEF J 301:

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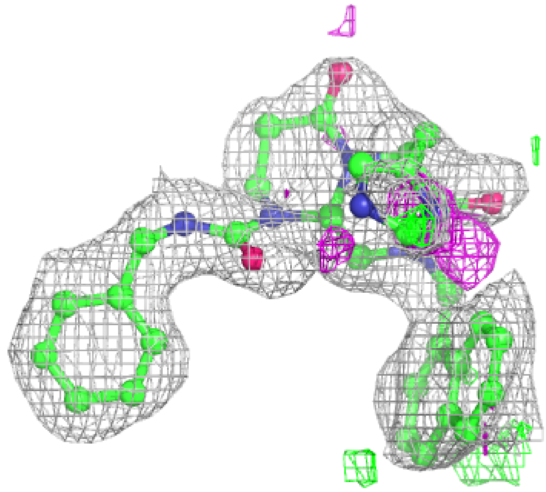
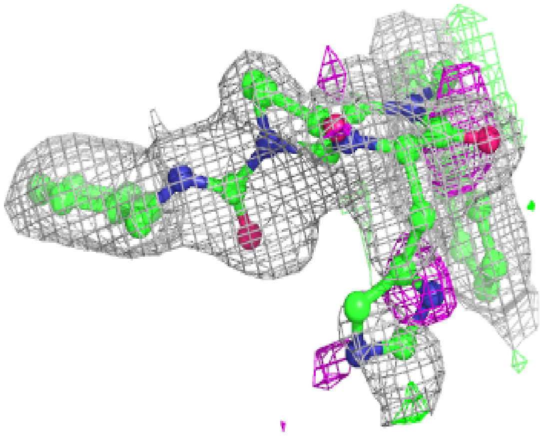
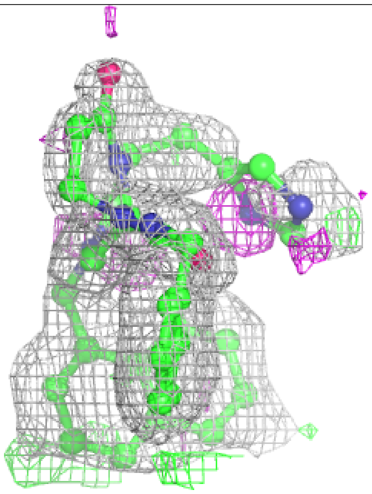
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around A1EEF D 301:

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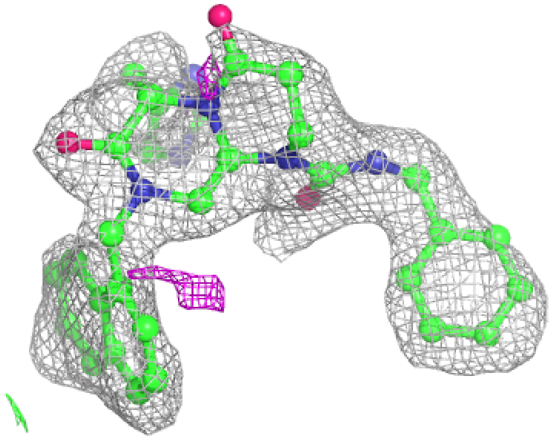
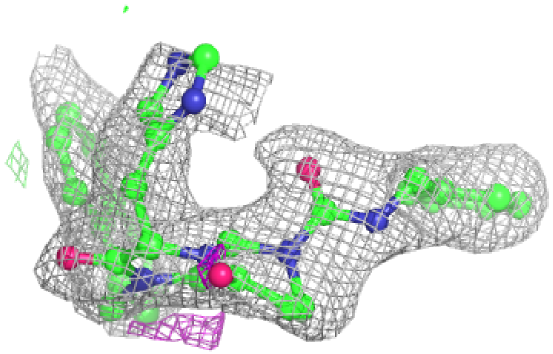
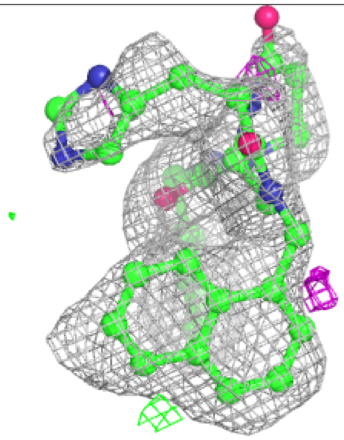
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

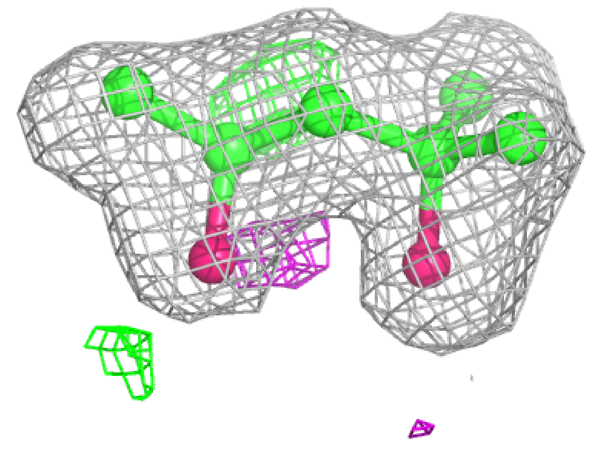


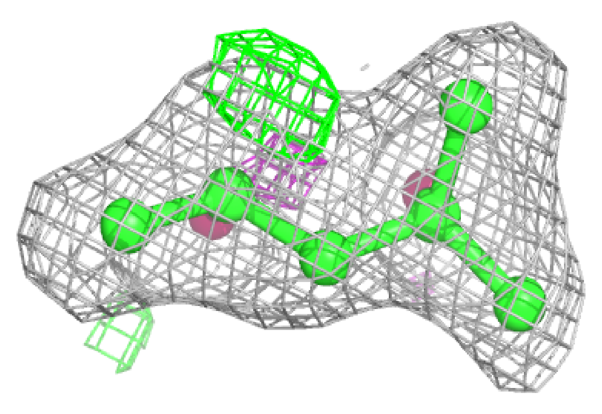


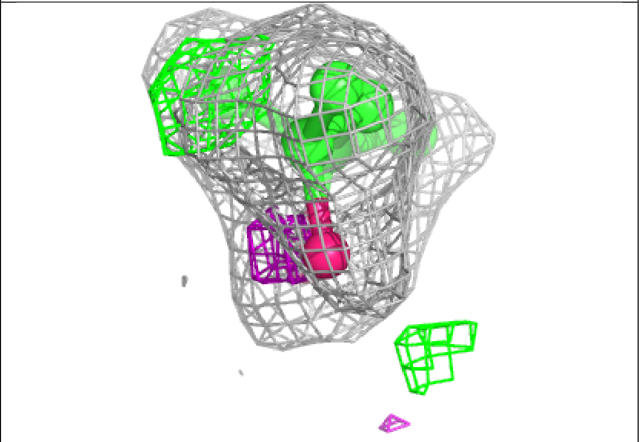


Electron density around MPD G 303:

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

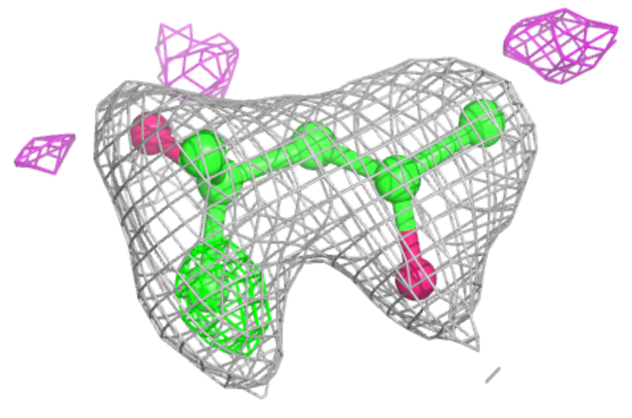


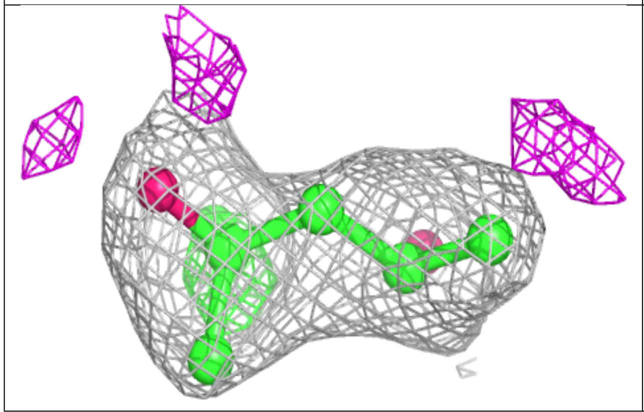


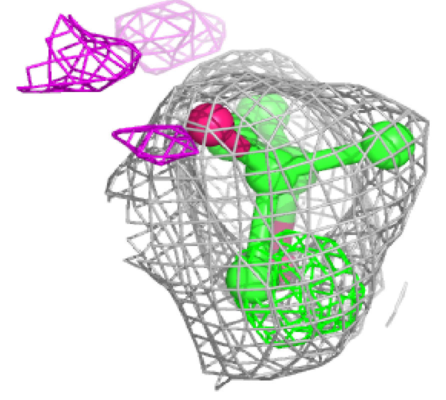


Electron density around MPD B 303:

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

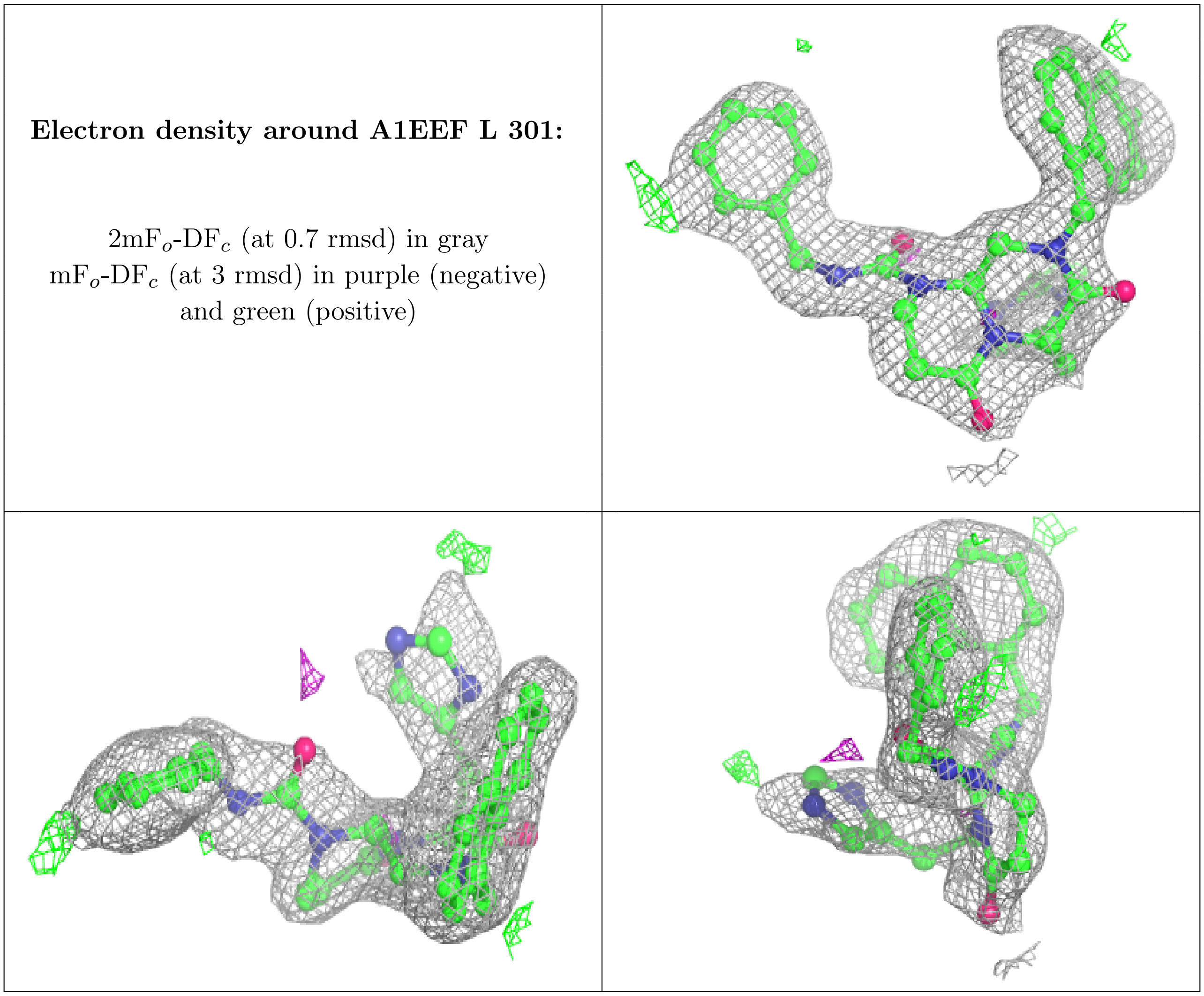


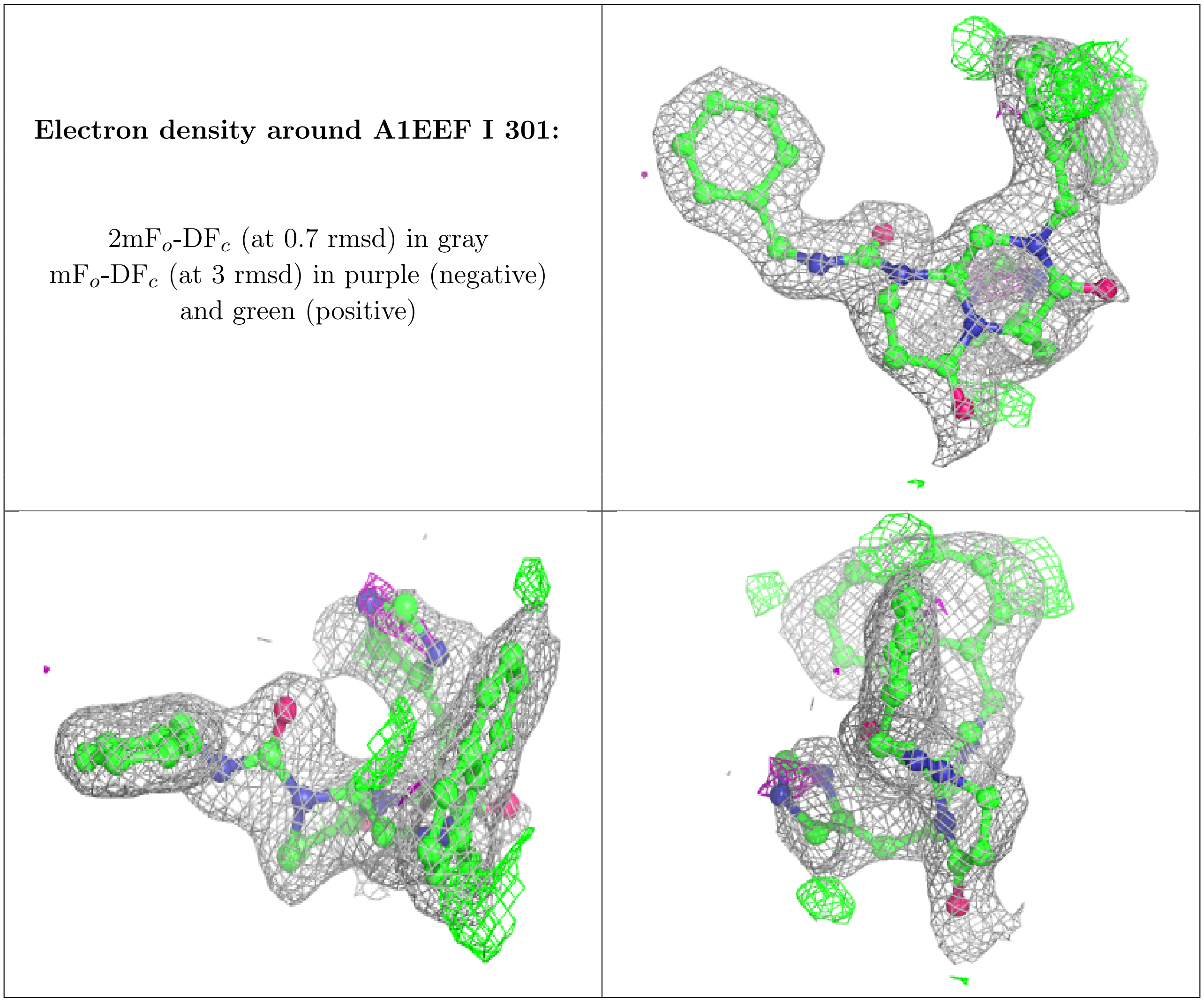




Electron density around A1EEF L 301:

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



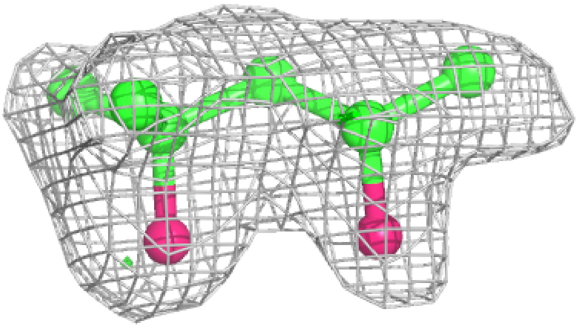


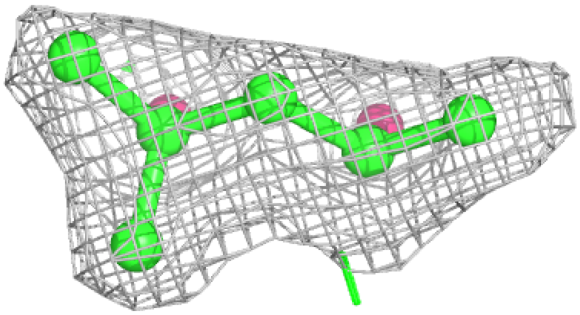
Electron density around A1EEF I 301:

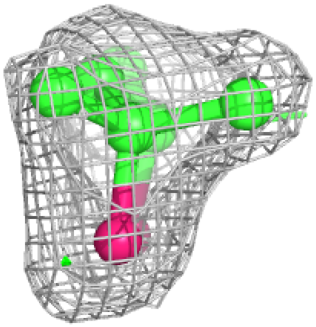
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MPD 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 A1EEF K 301:

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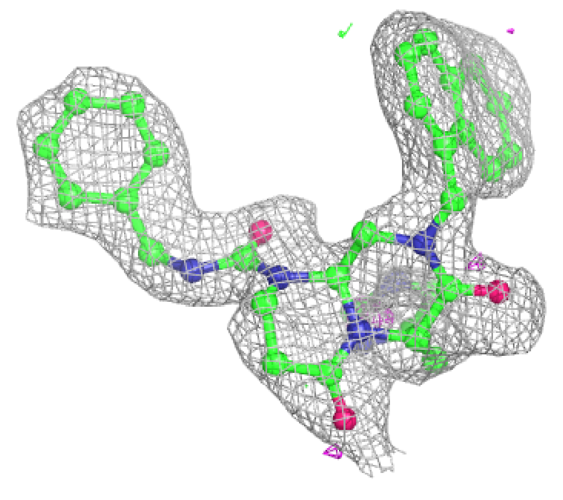
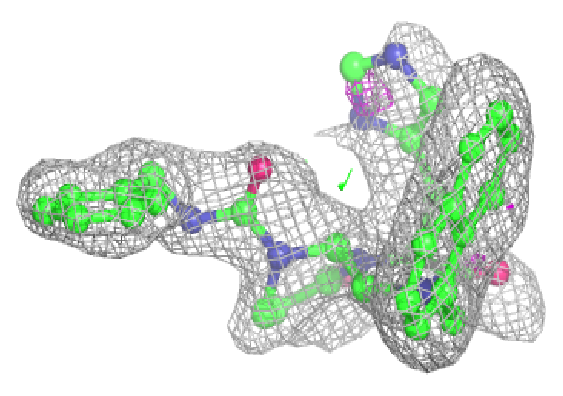
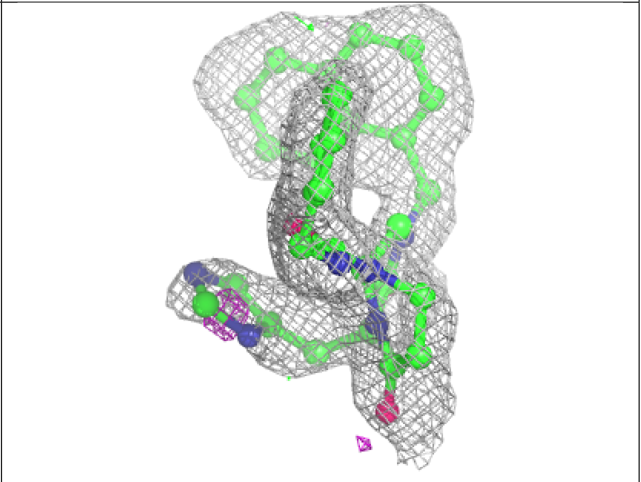
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

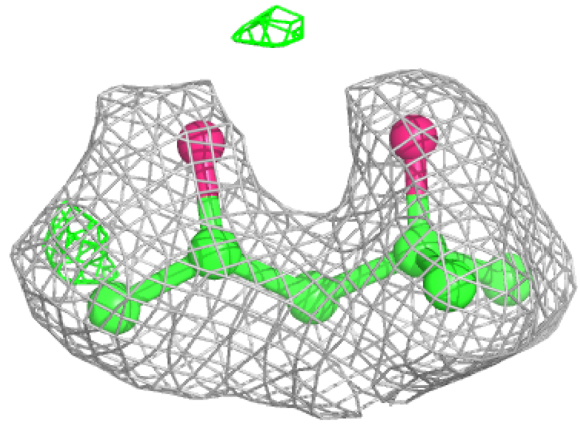


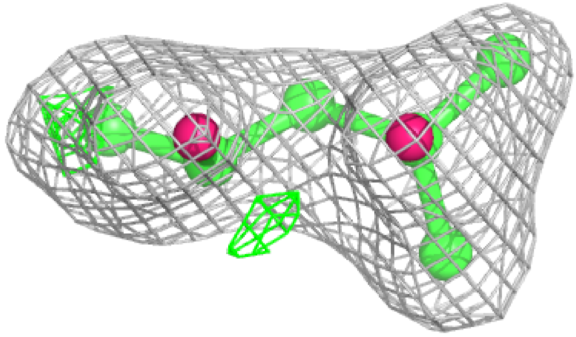


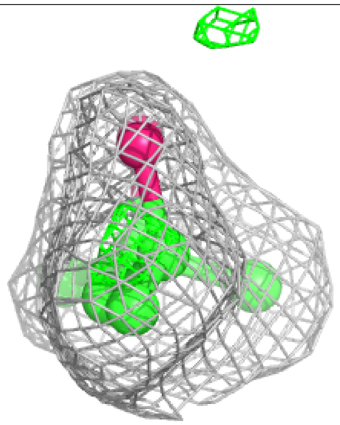


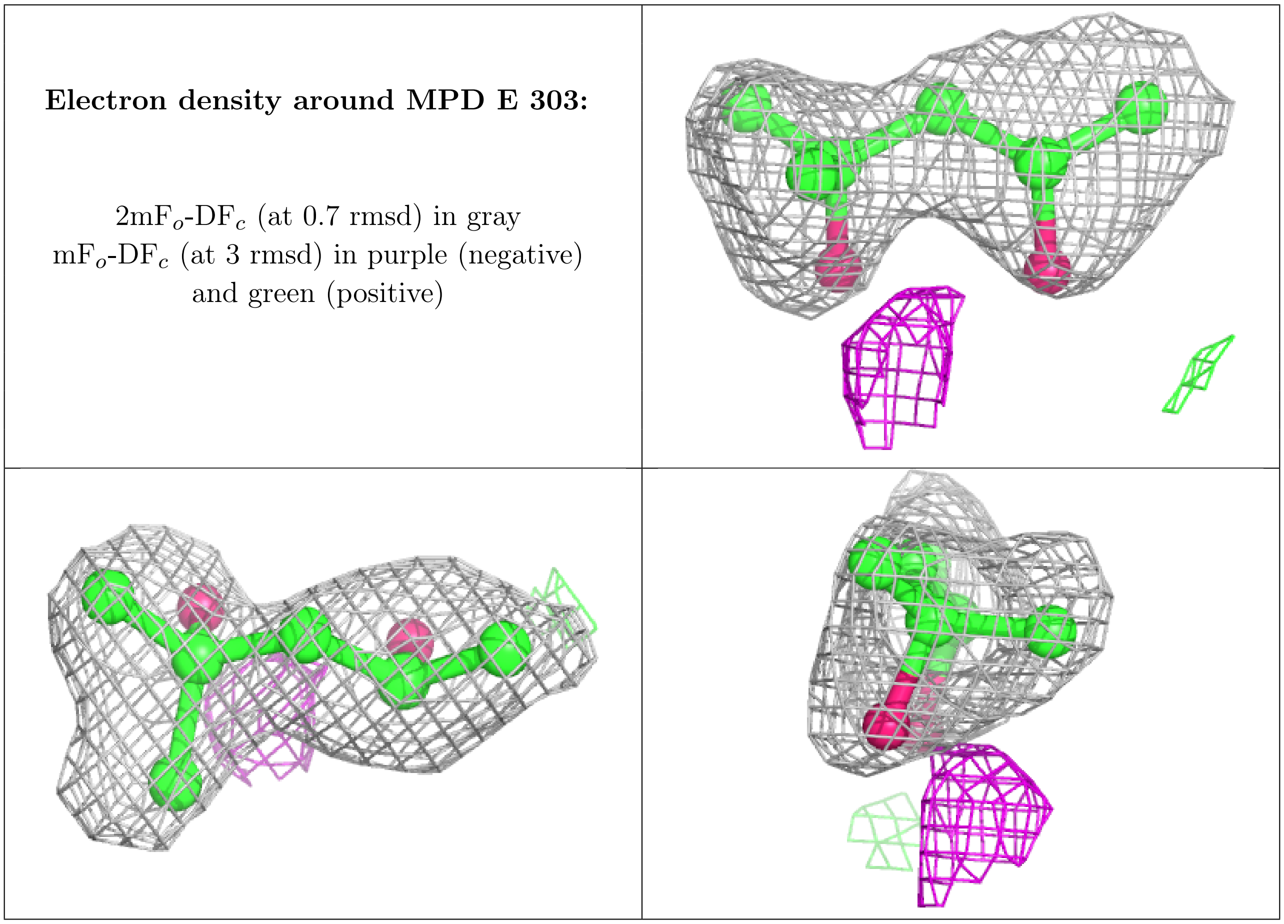
Electron density around MPD H 303:

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







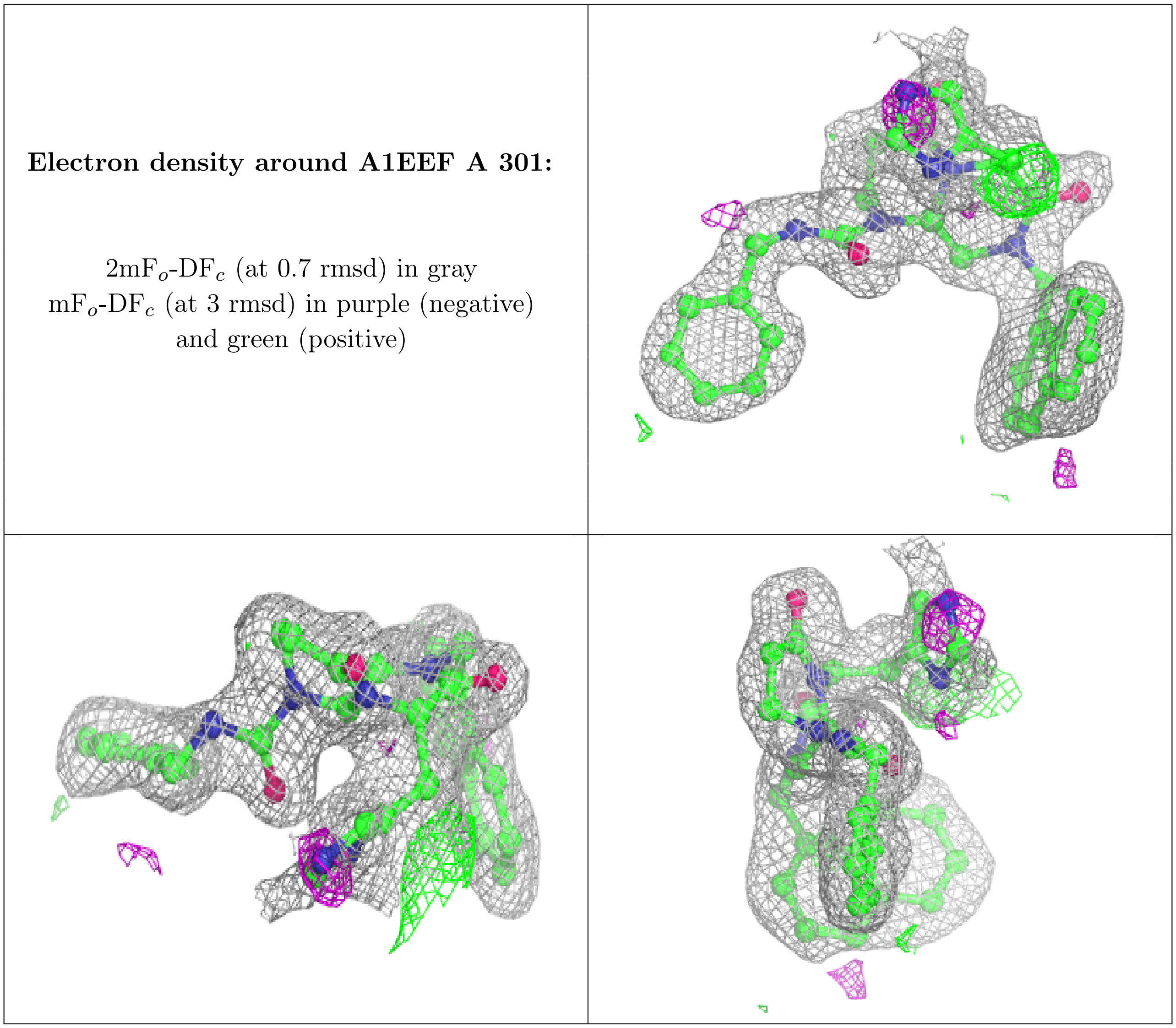


Electron density around MPD E 303:

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 A1EEF 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 A1EEF H 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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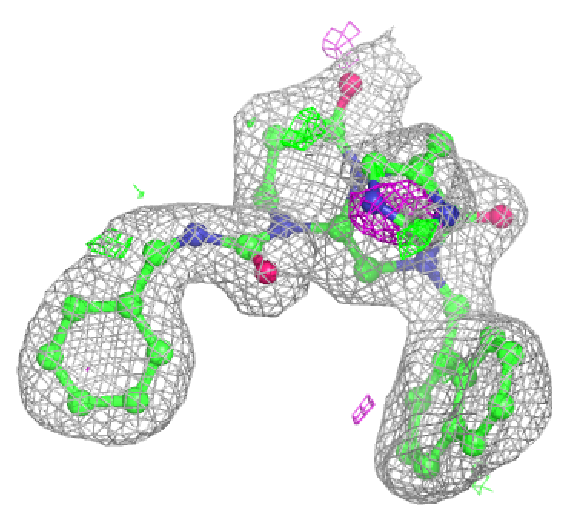
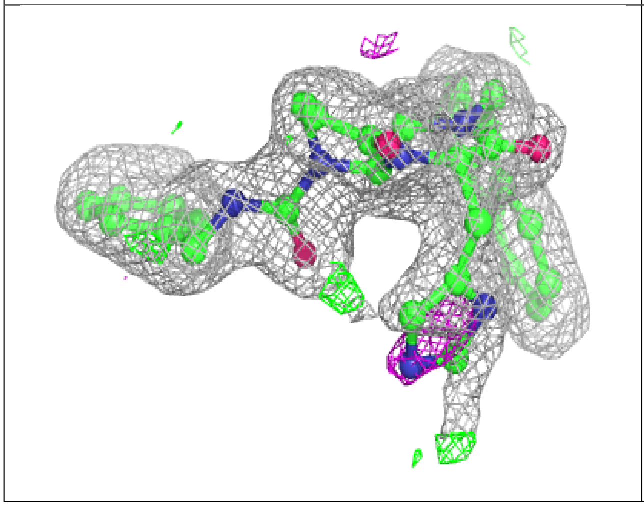
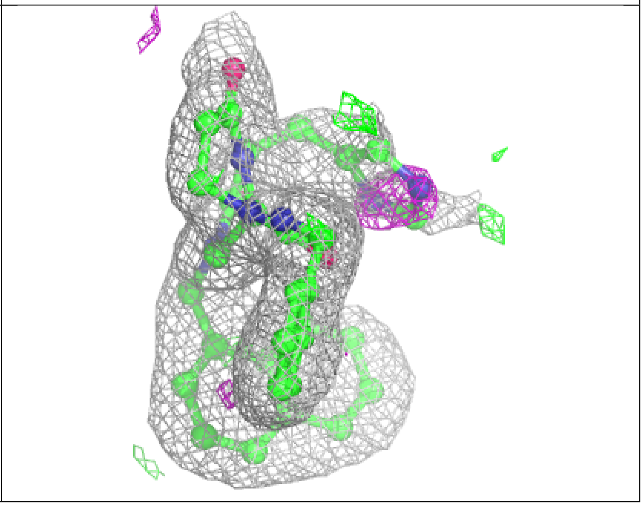
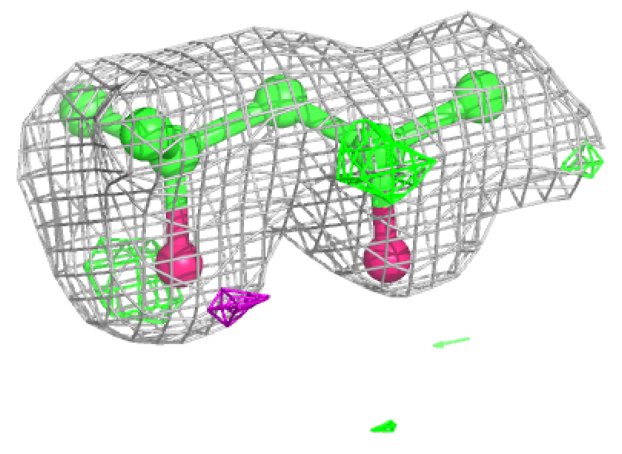


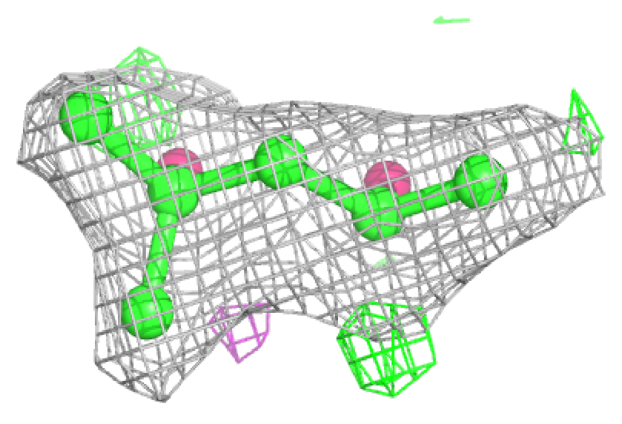


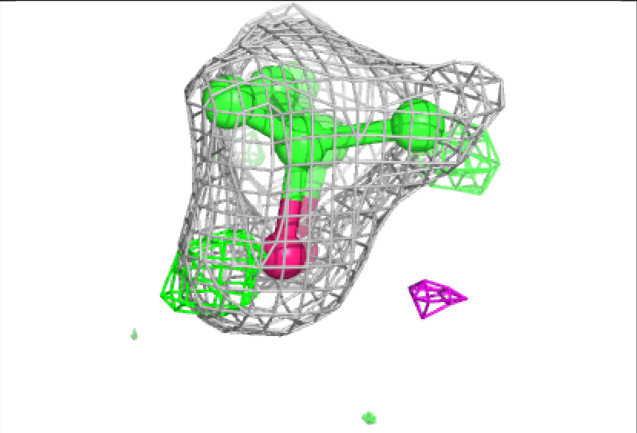


Electron density around MPD I 303:

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

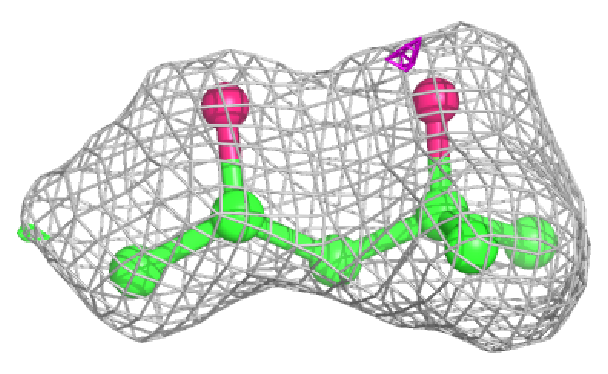


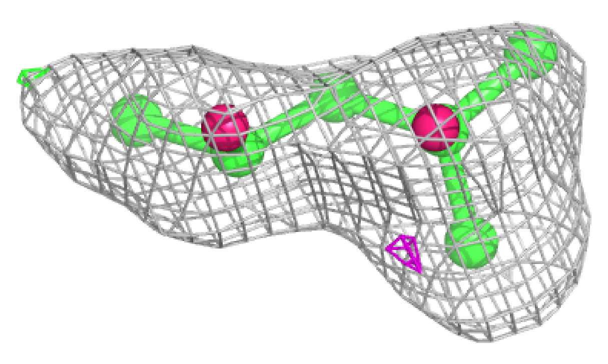


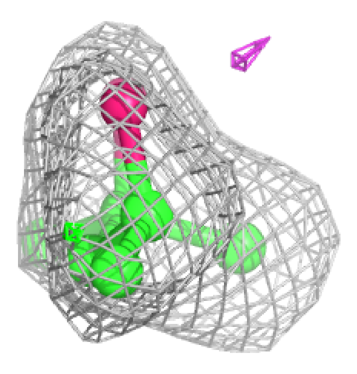


Electron density around MPD K 303:

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

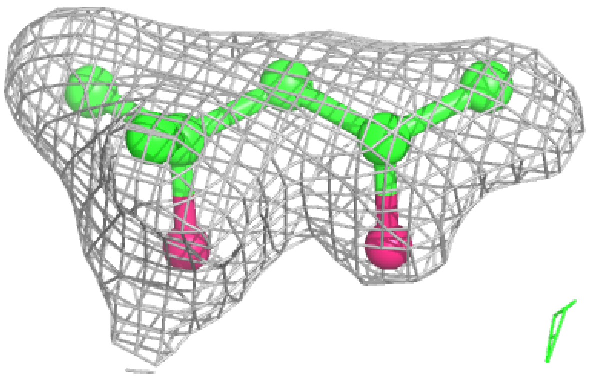


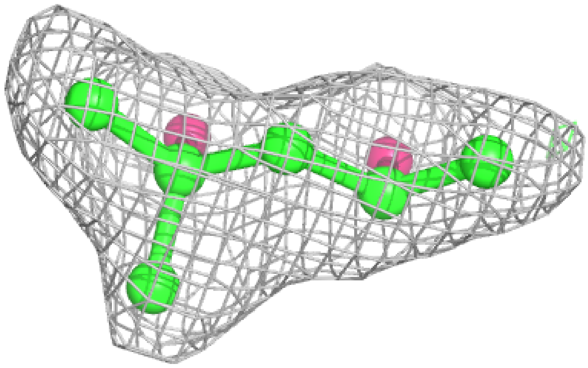


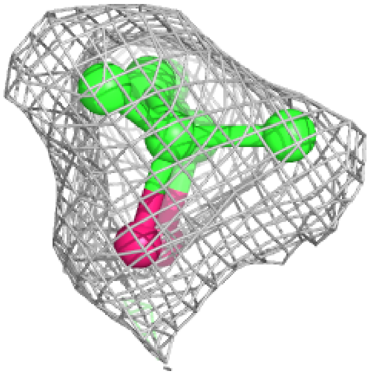


Electron density around MPD D 303:

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

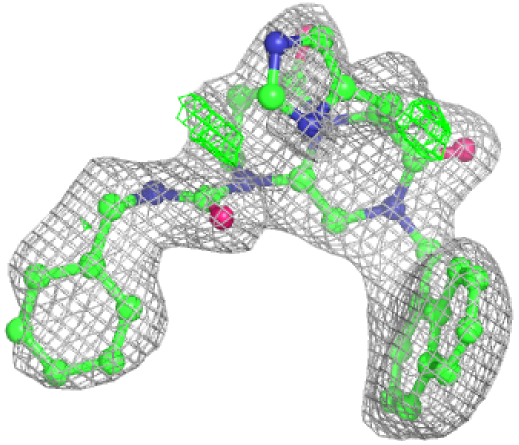


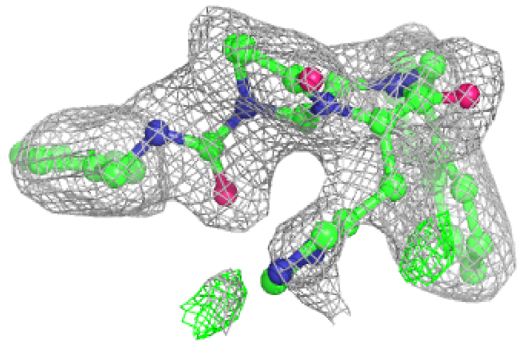


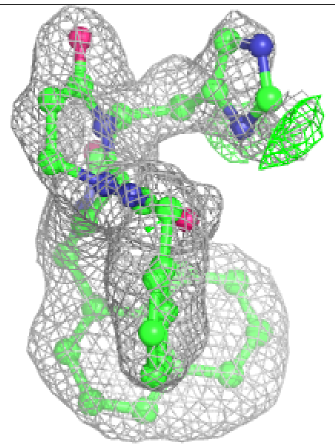


Electron density around A1EEF E 301:

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

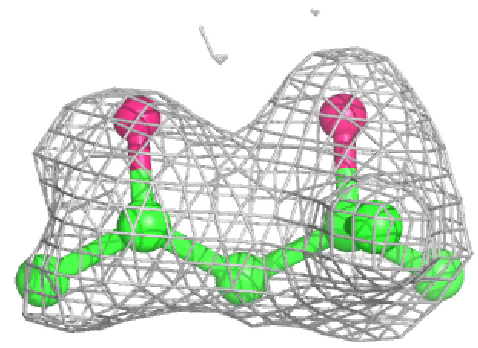


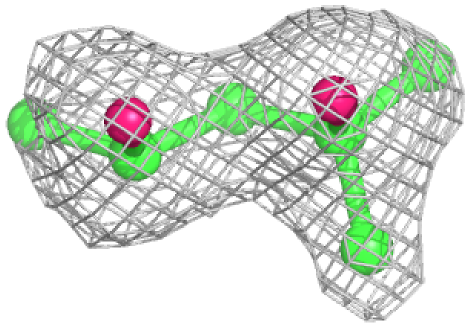


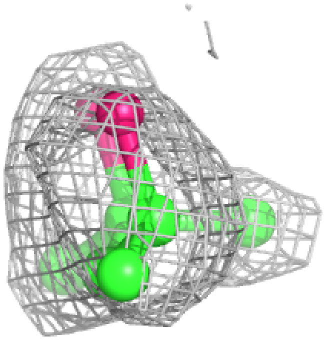


Electron density around MPD L 303:

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

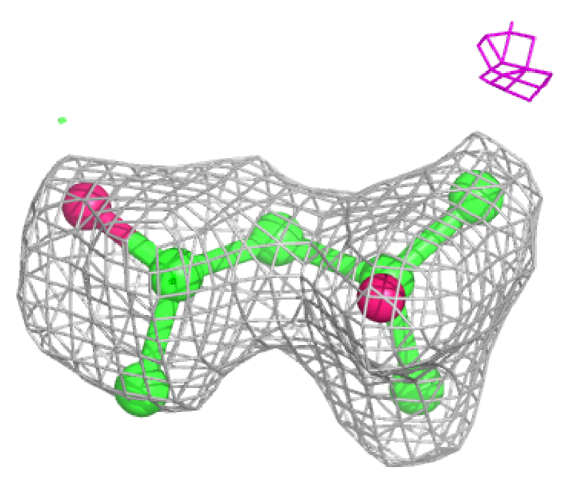


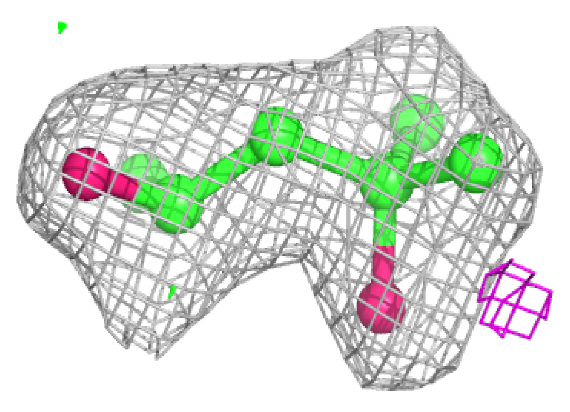


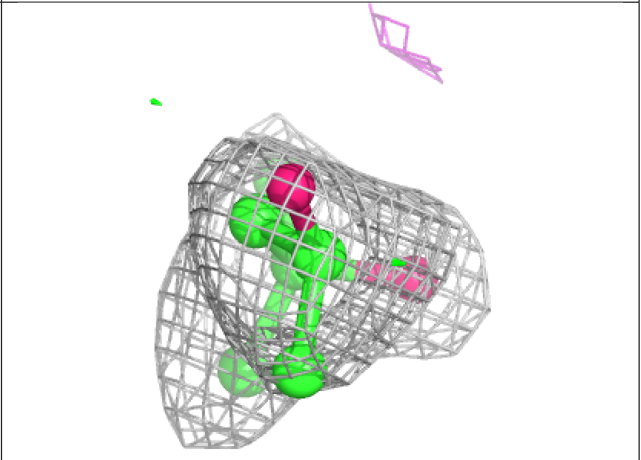


Electron density around MPD F 303:

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

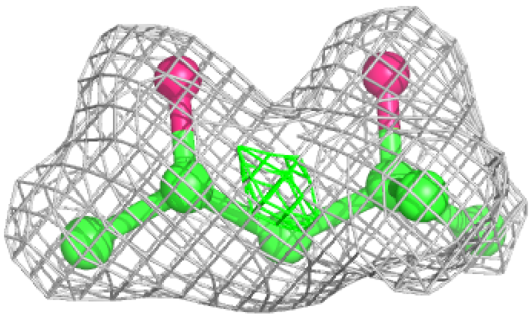


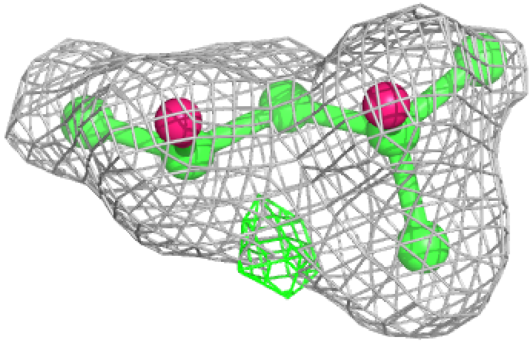


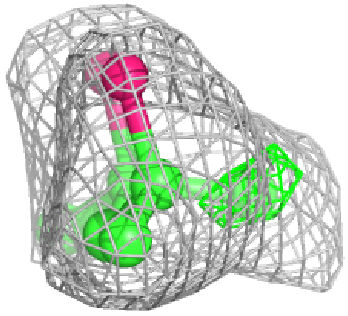


Electron density around MPD J 303:

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

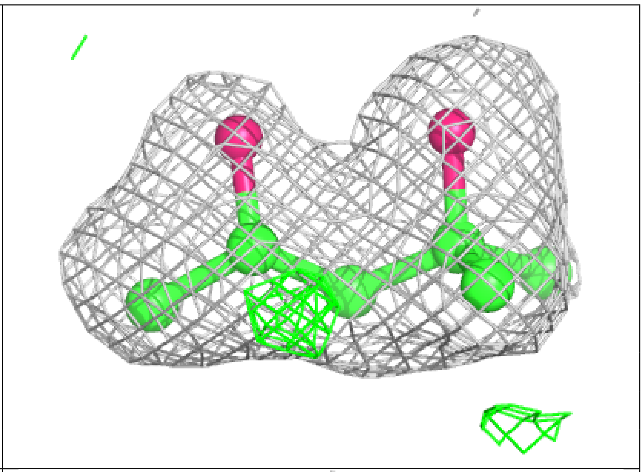


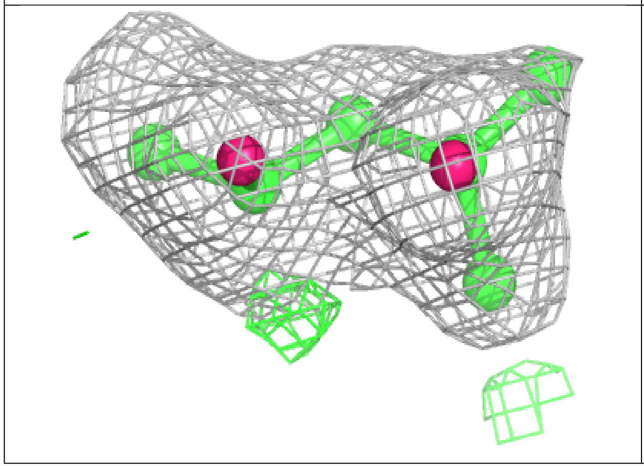


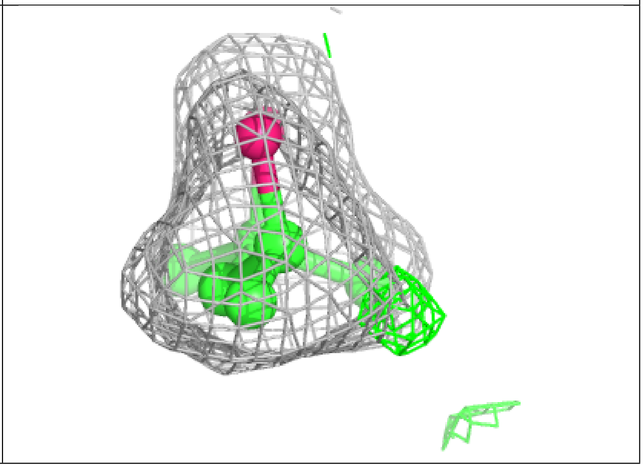


Electron density around MPD C 303:

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

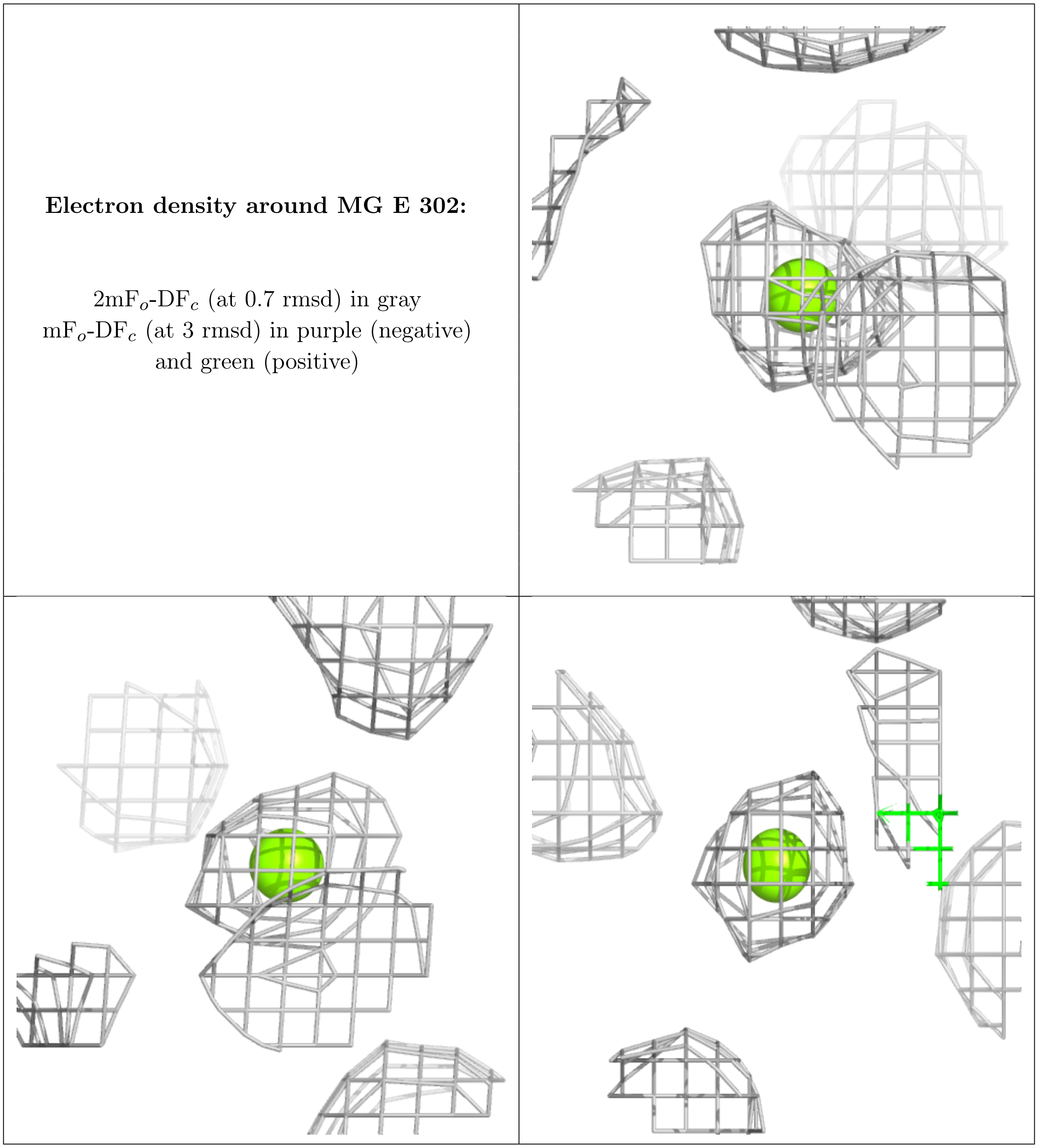


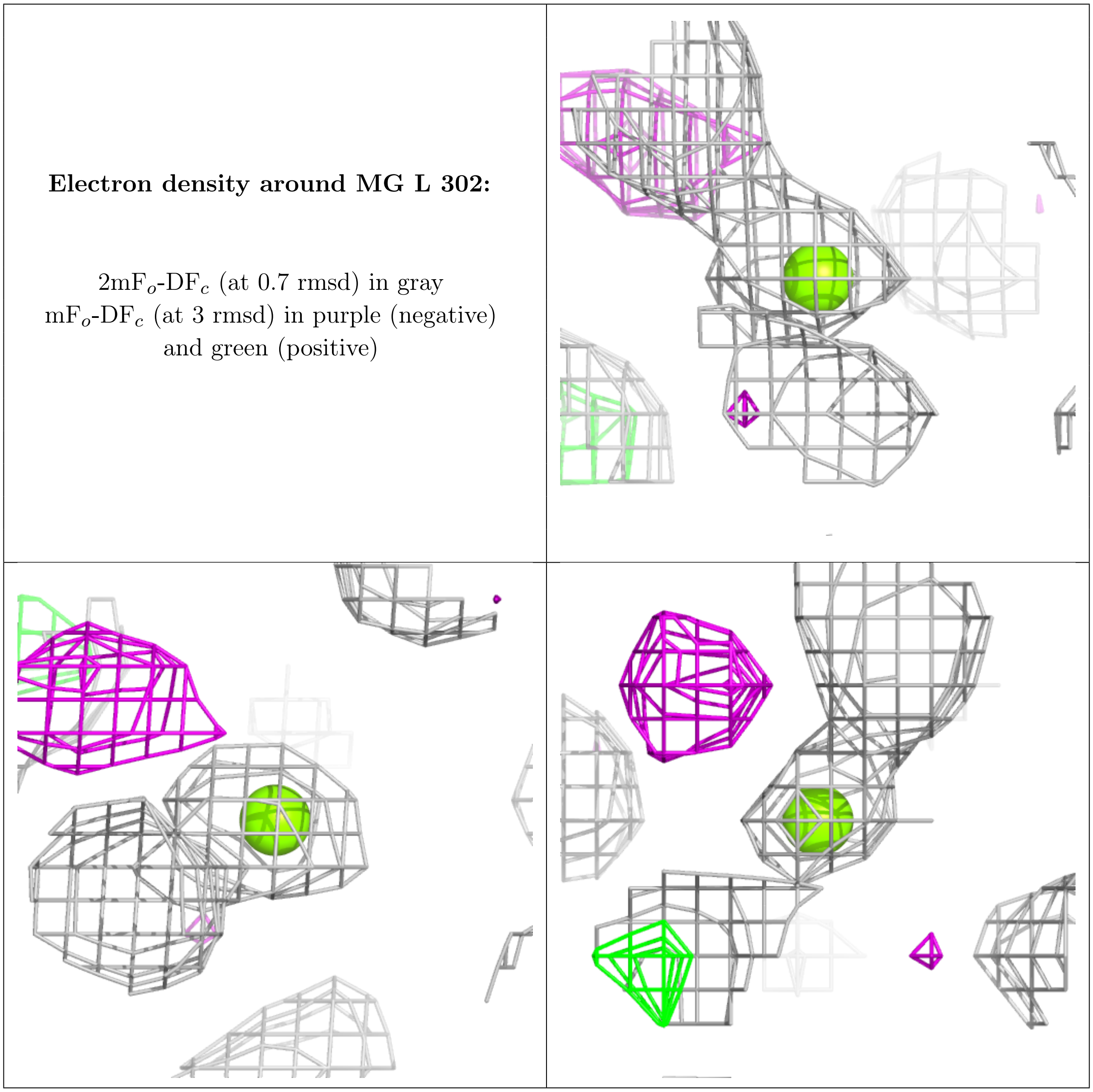




Electron density around MG E 302:

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



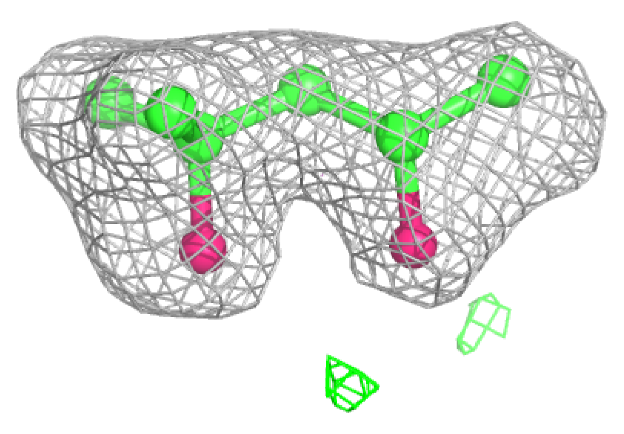


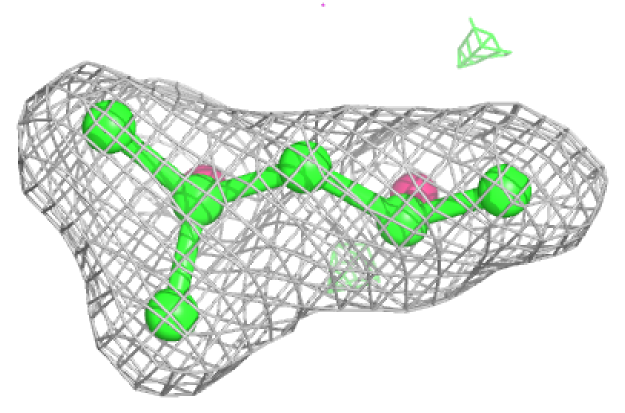
Electron density around MG L 302:

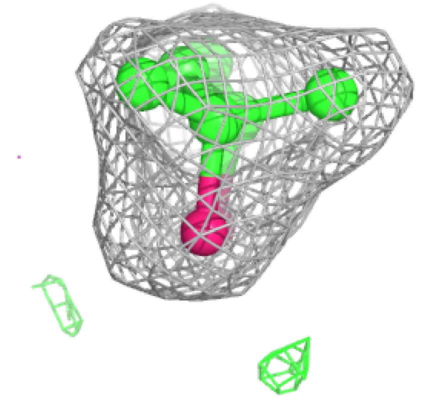
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MPD 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)

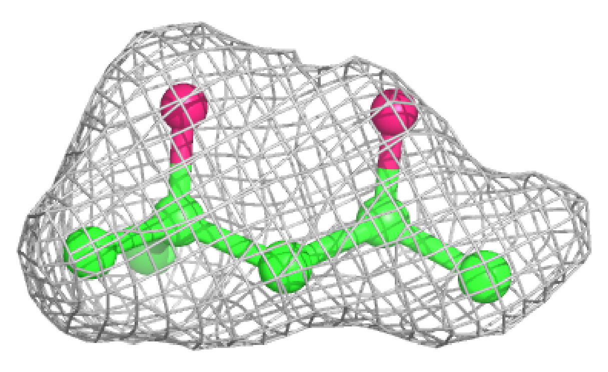


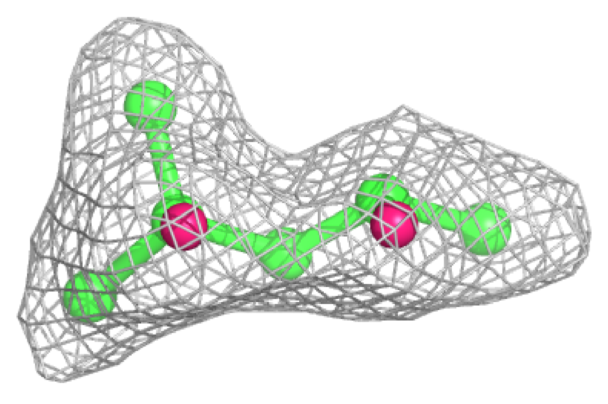


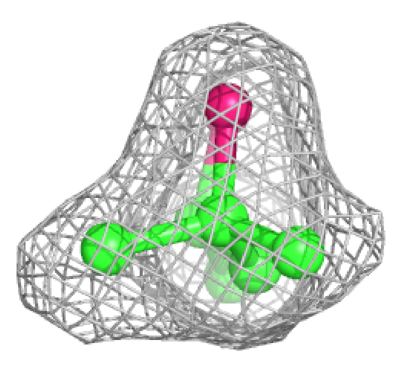


Electron density around MPD N 303:

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

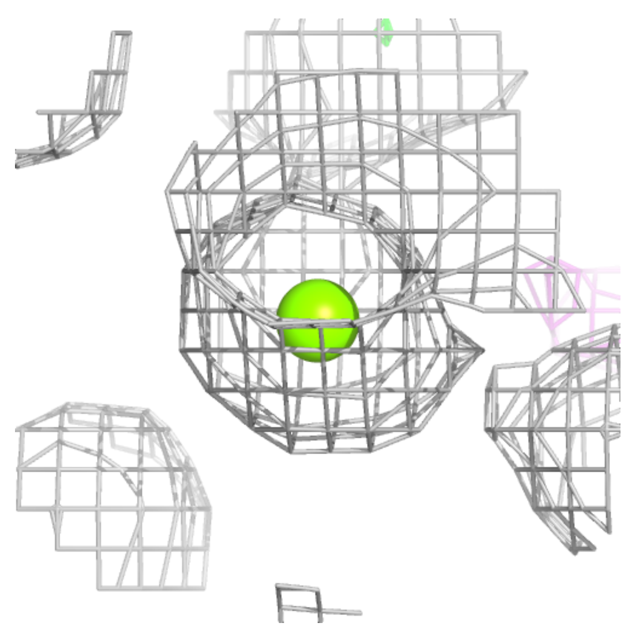


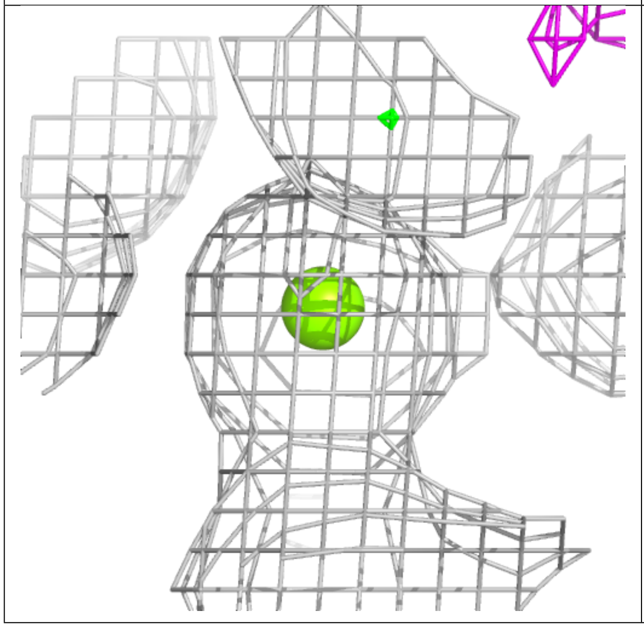




Electron density around MG F 302:

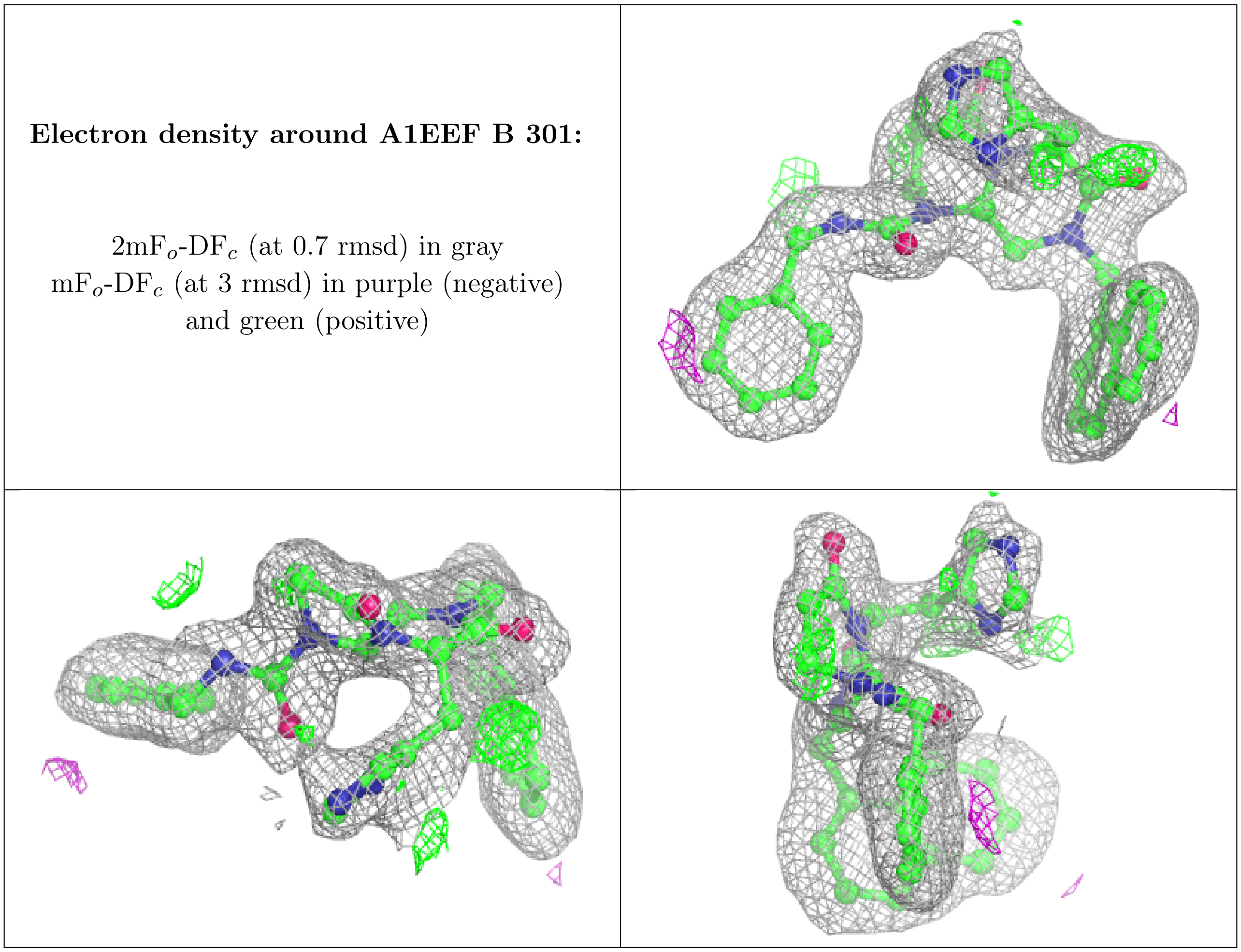
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





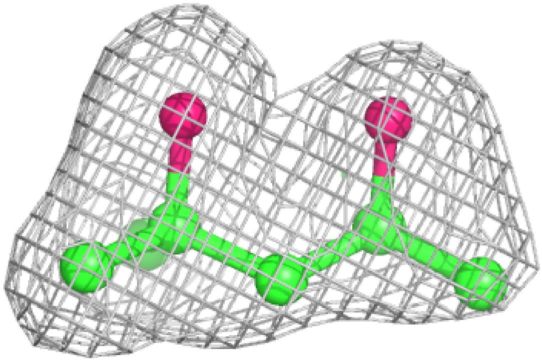
Electron density around A1EEF B 301:

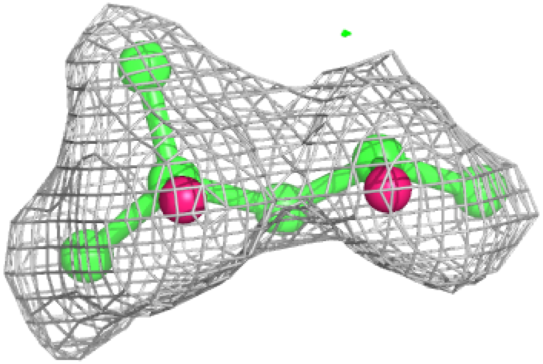
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

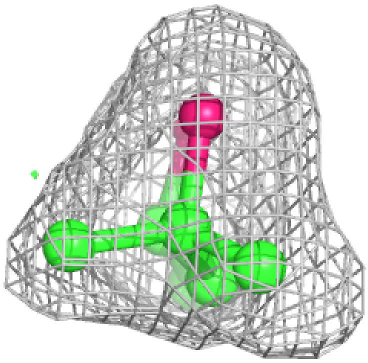


Electron density around MPD M 303:

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

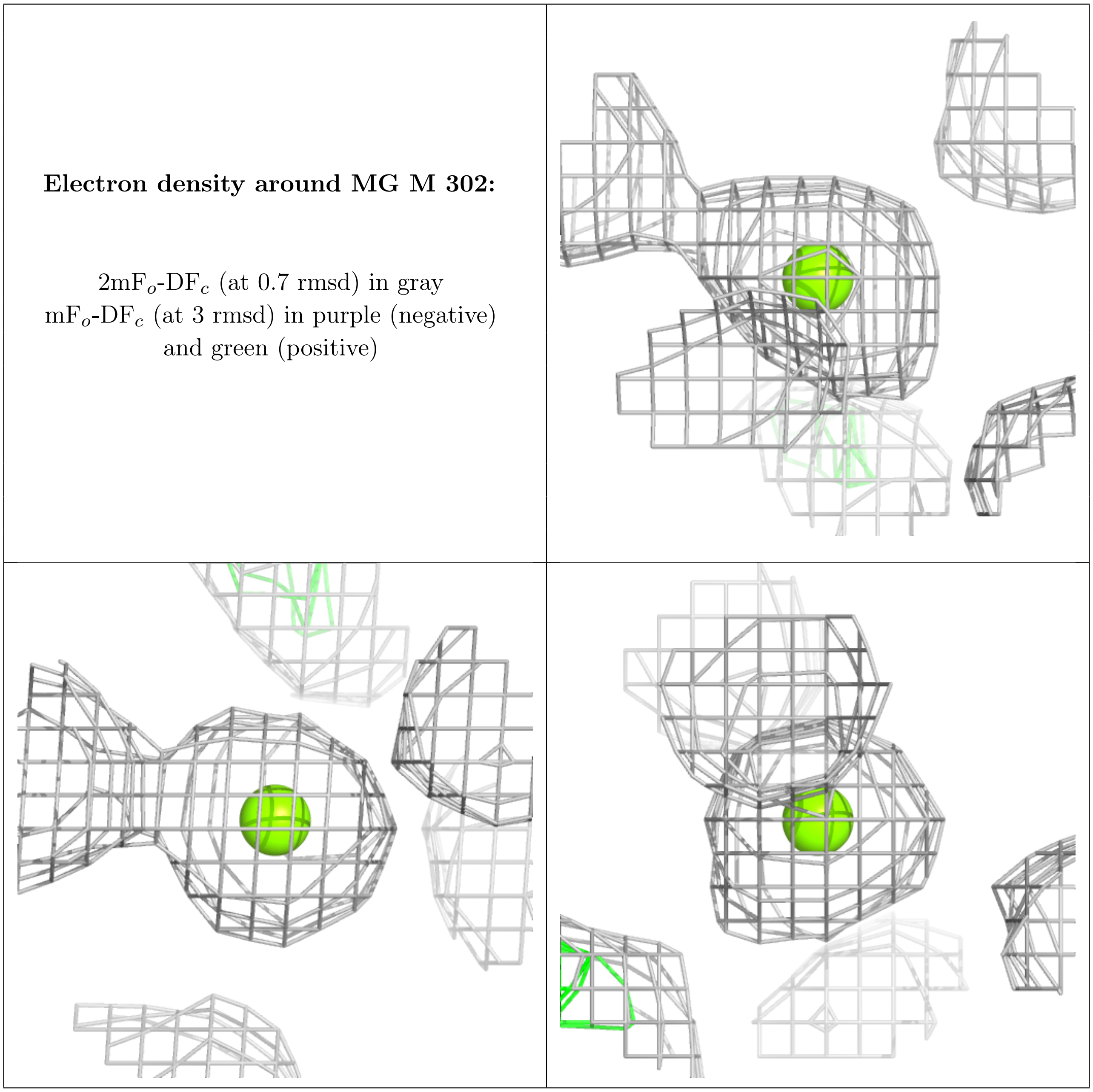






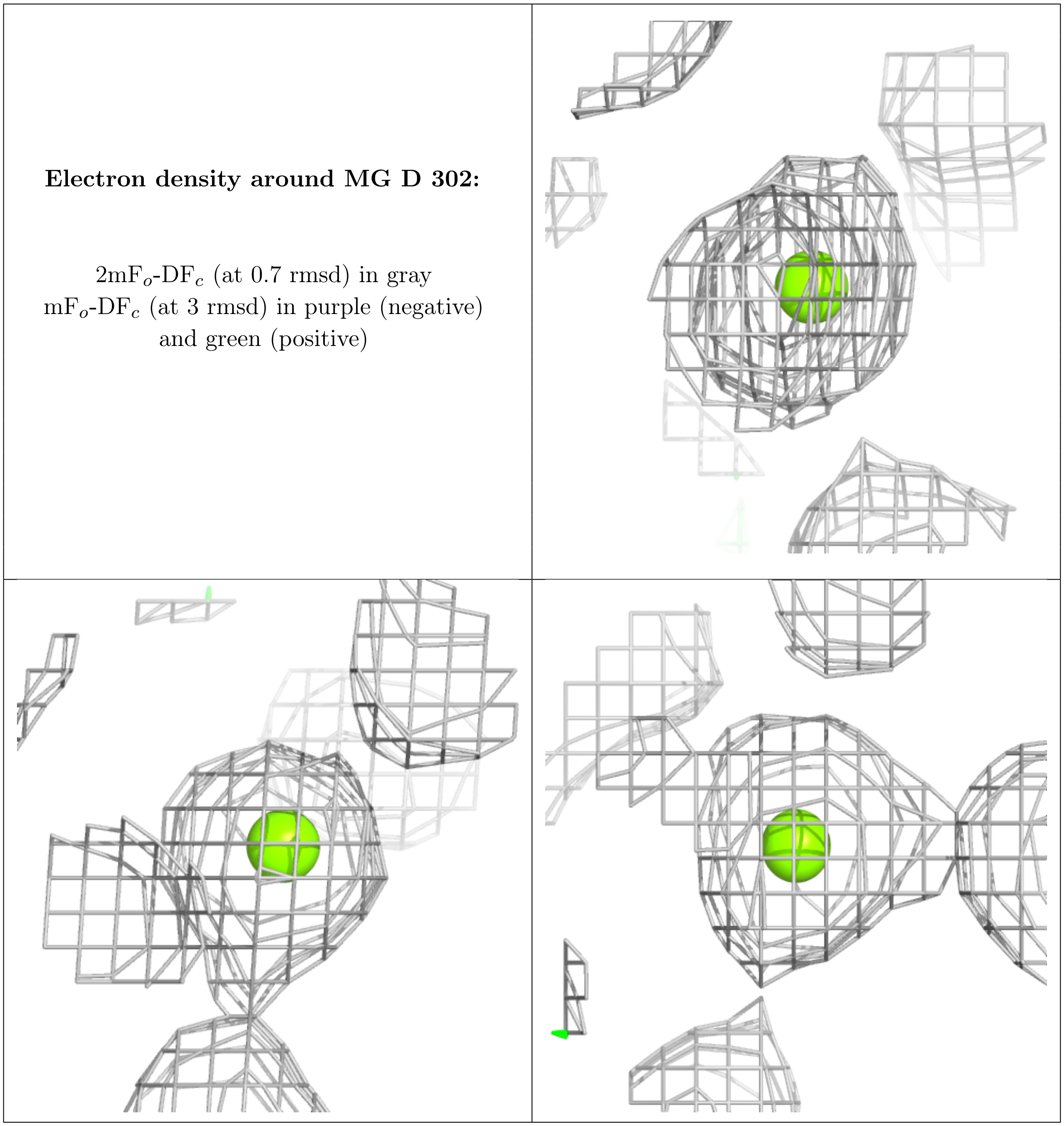
Electron density around MG M 302:

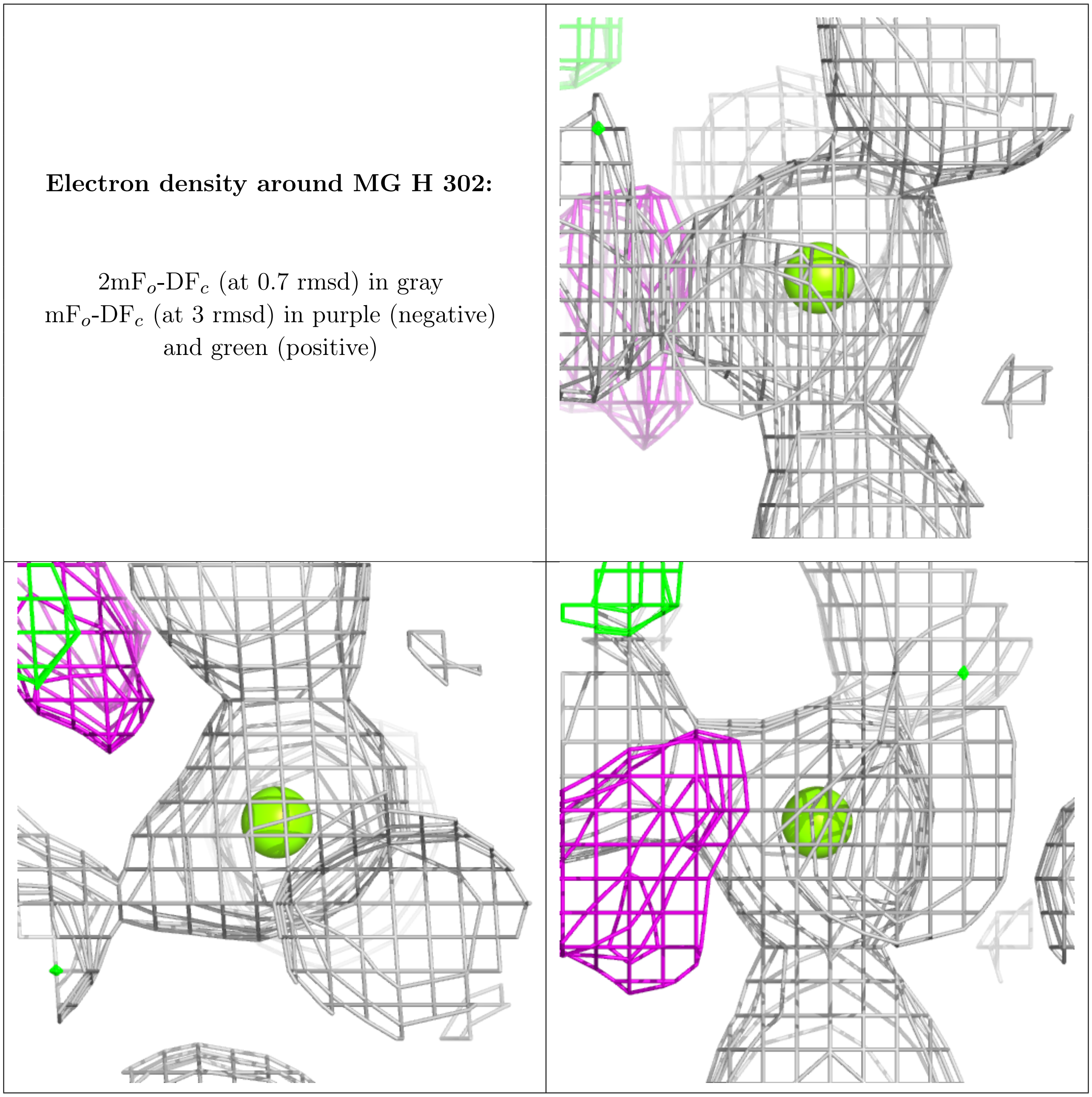
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)



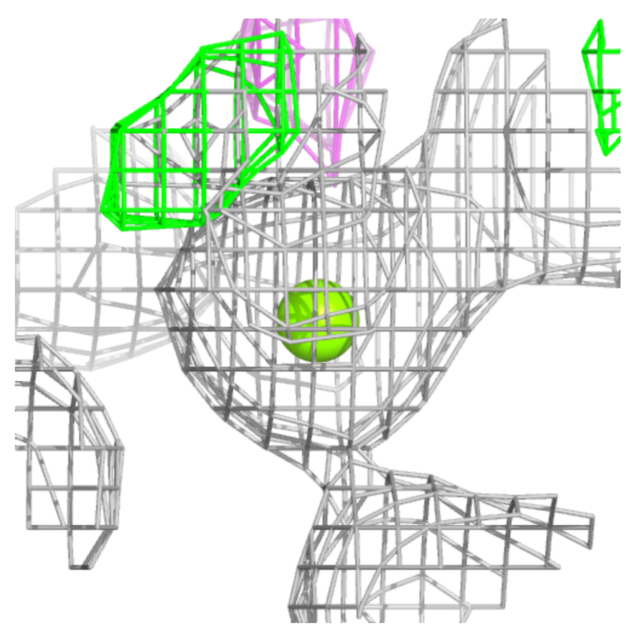


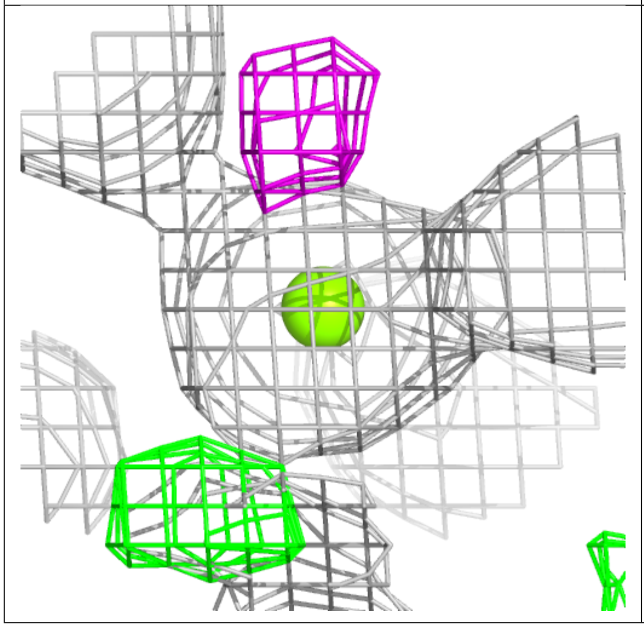
Electron density around MG H 302:

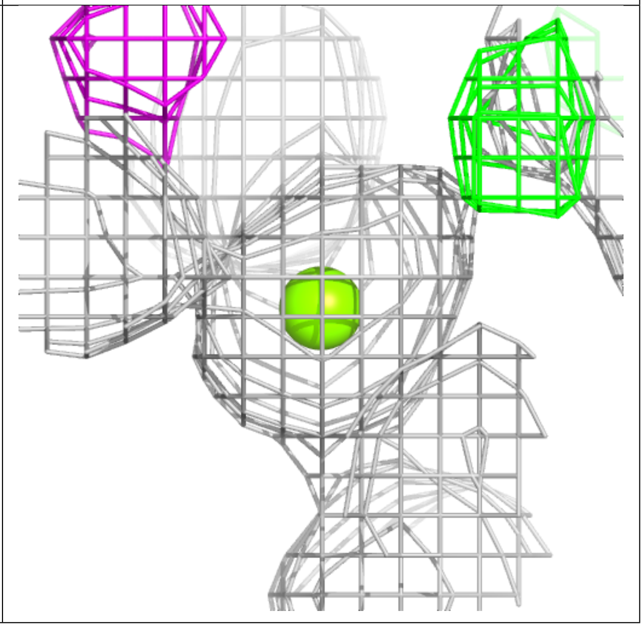
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG C 302:

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

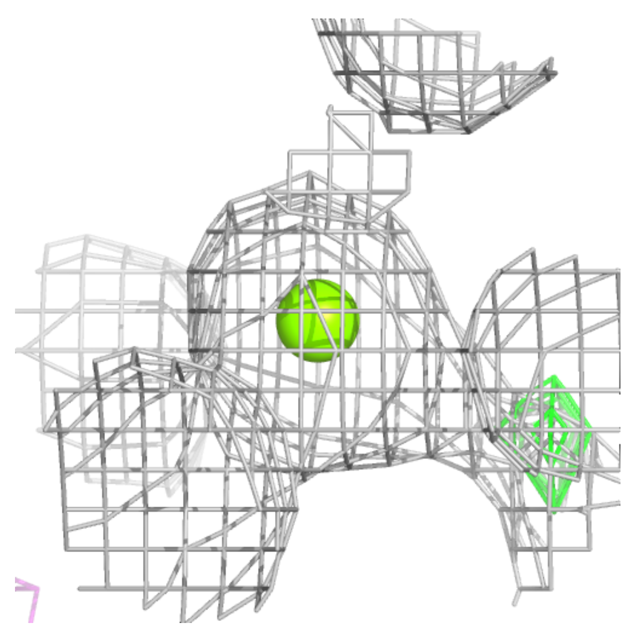


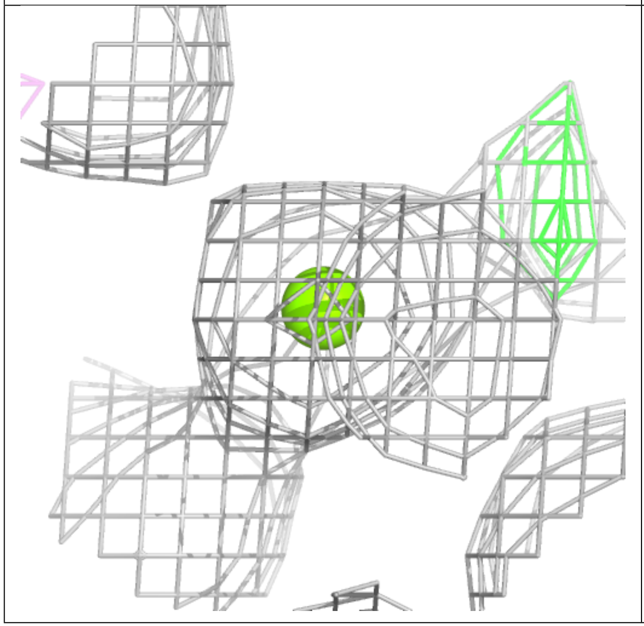


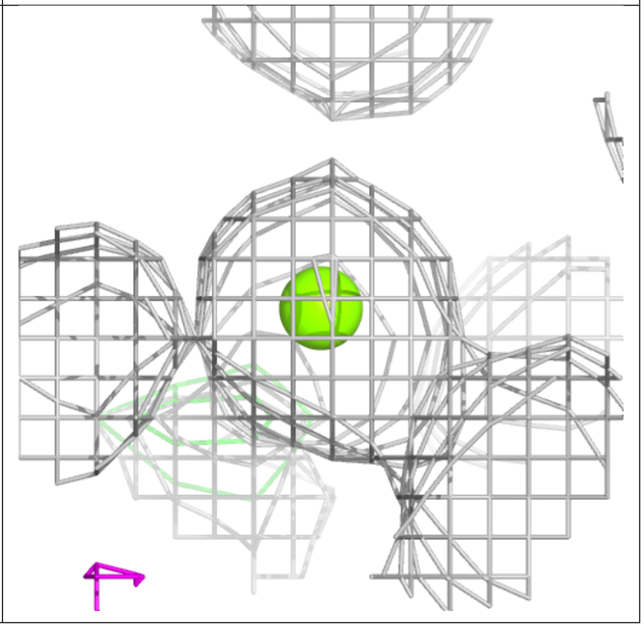


Electron density around MG N 302:

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

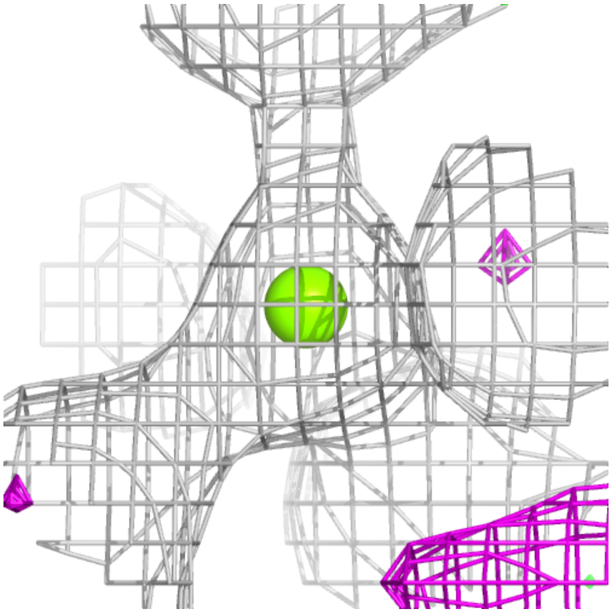


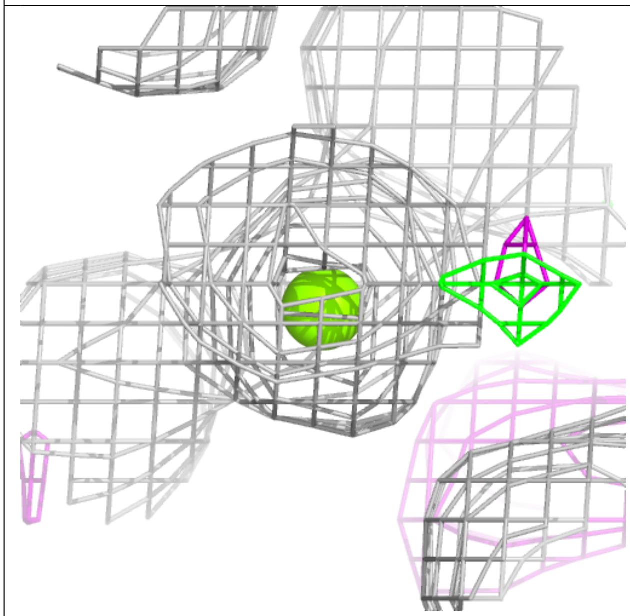


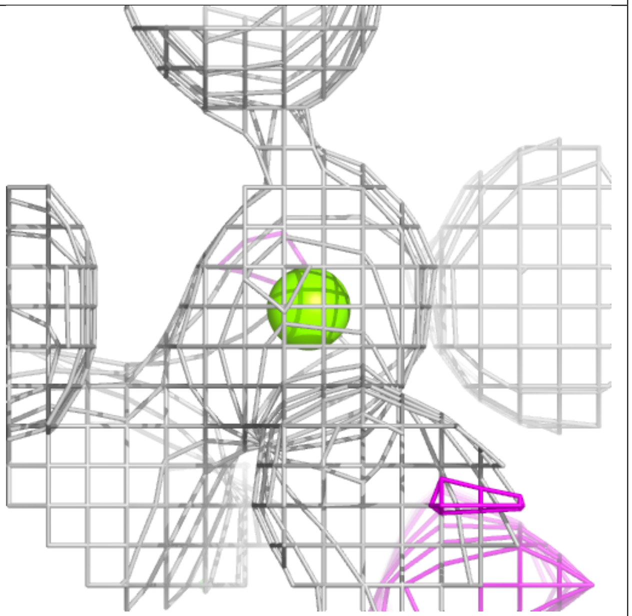


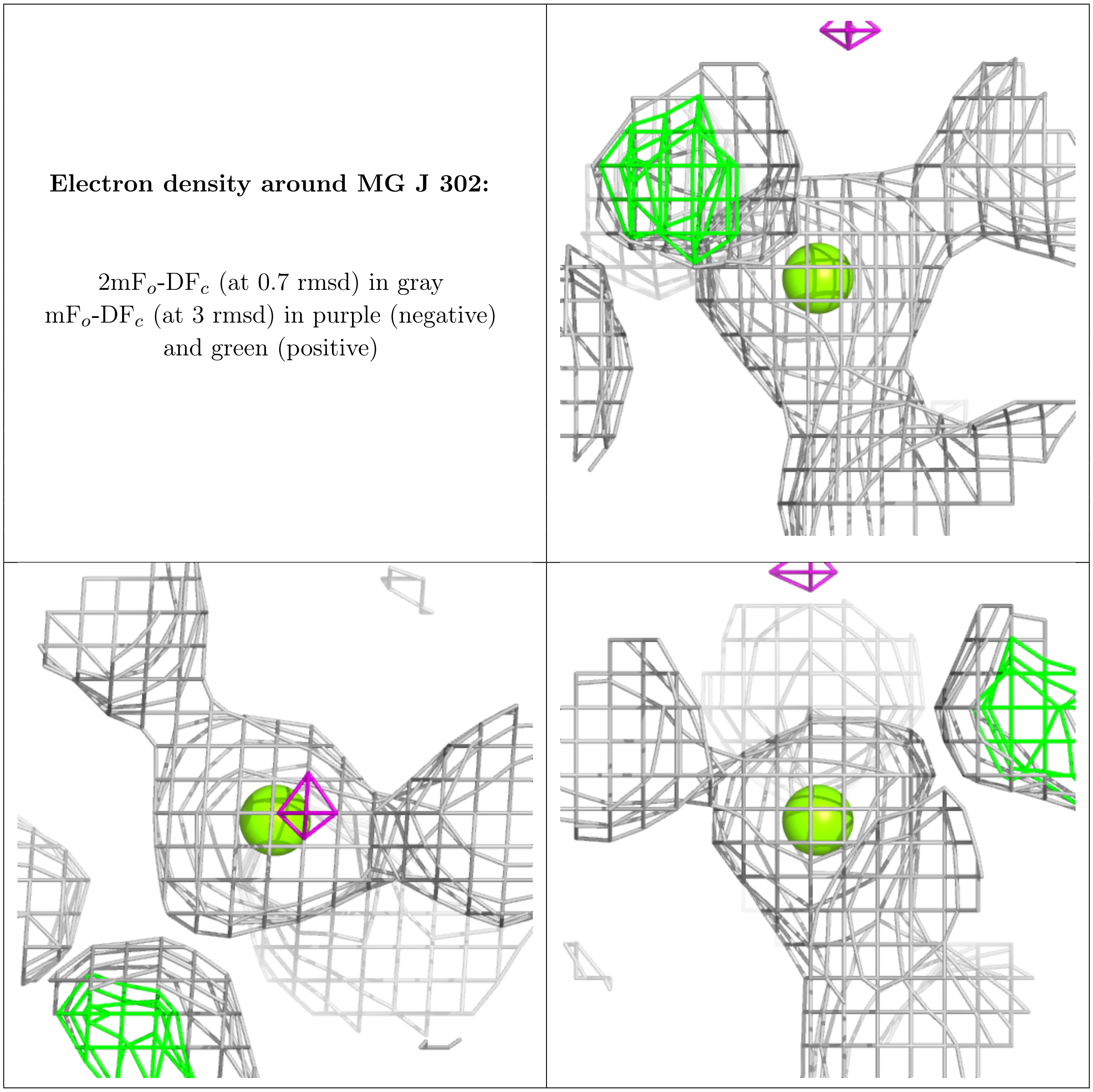
Electron density around MG B 302:

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







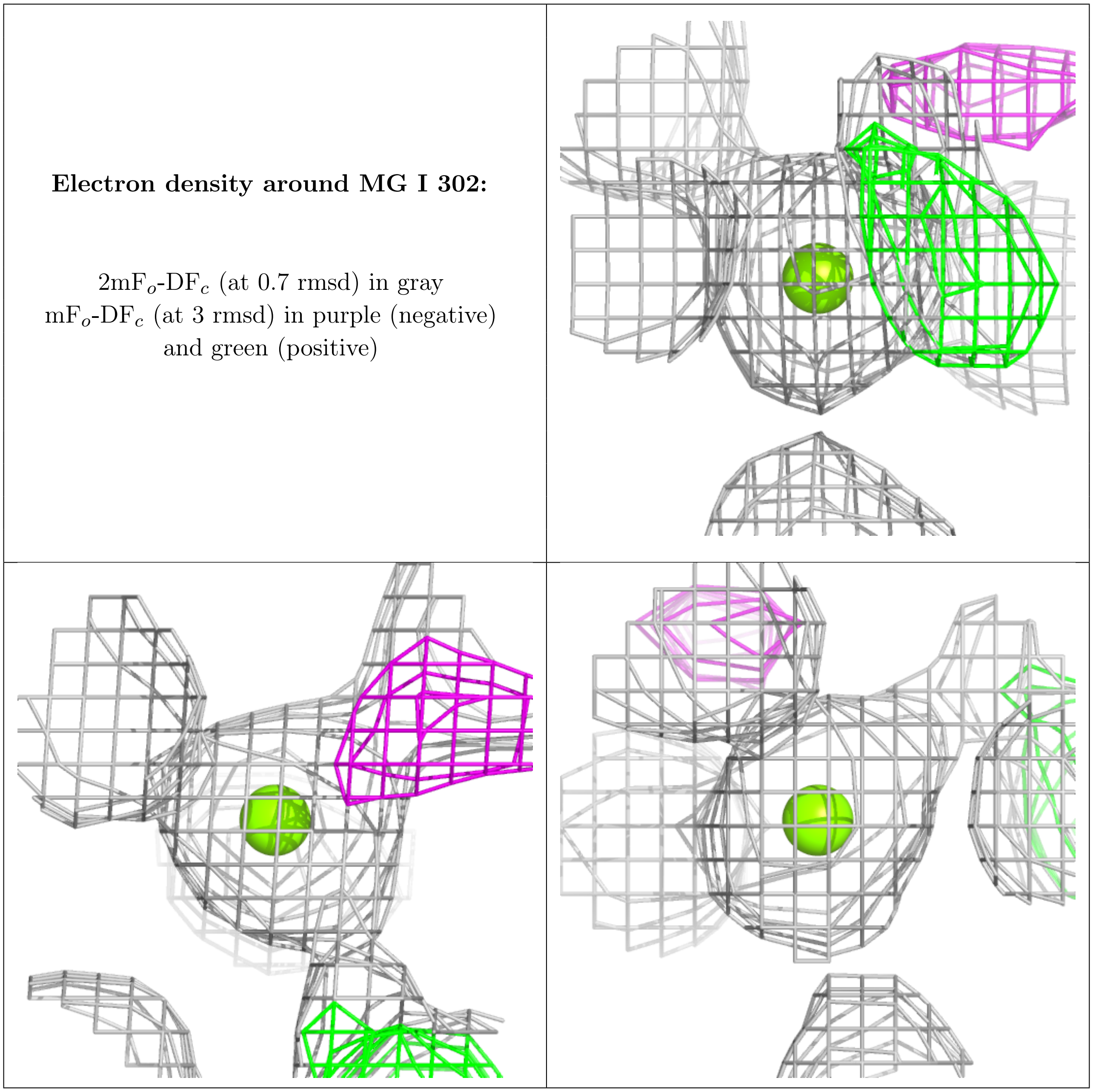


Electron density around MG J 302:

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

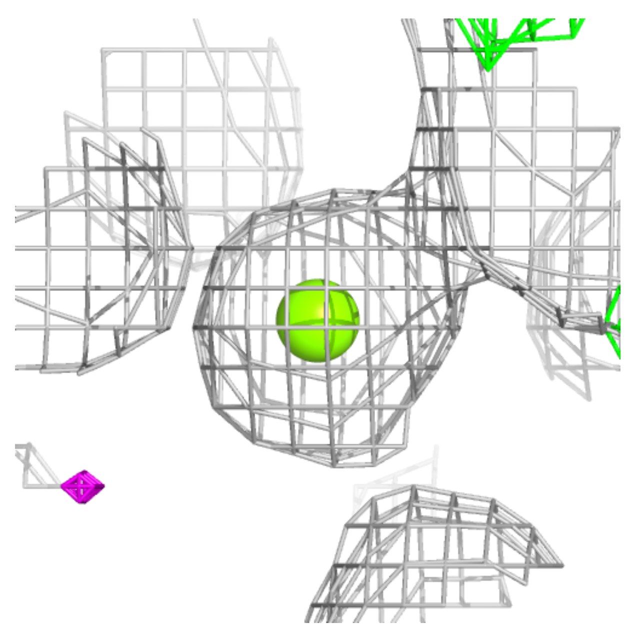
Electron density around MG I 302:

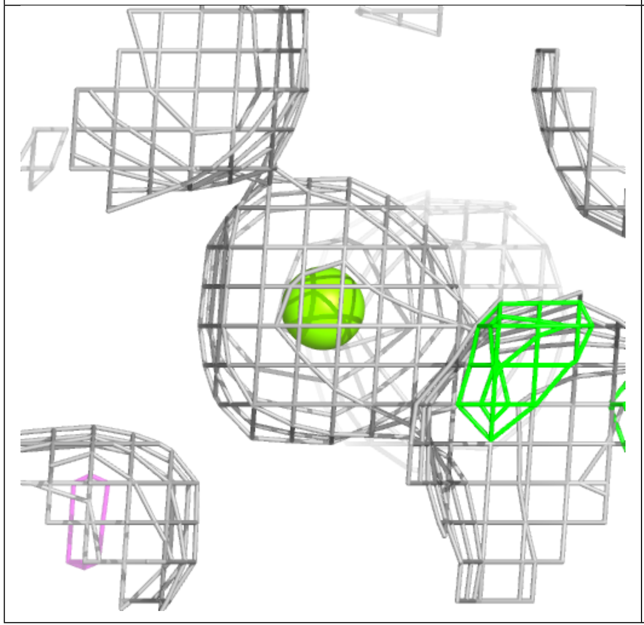
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

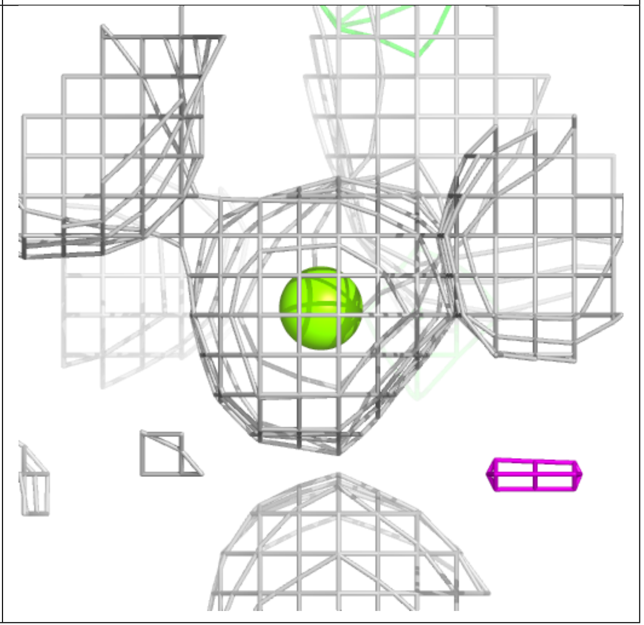


Electron density around MG G 302:

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

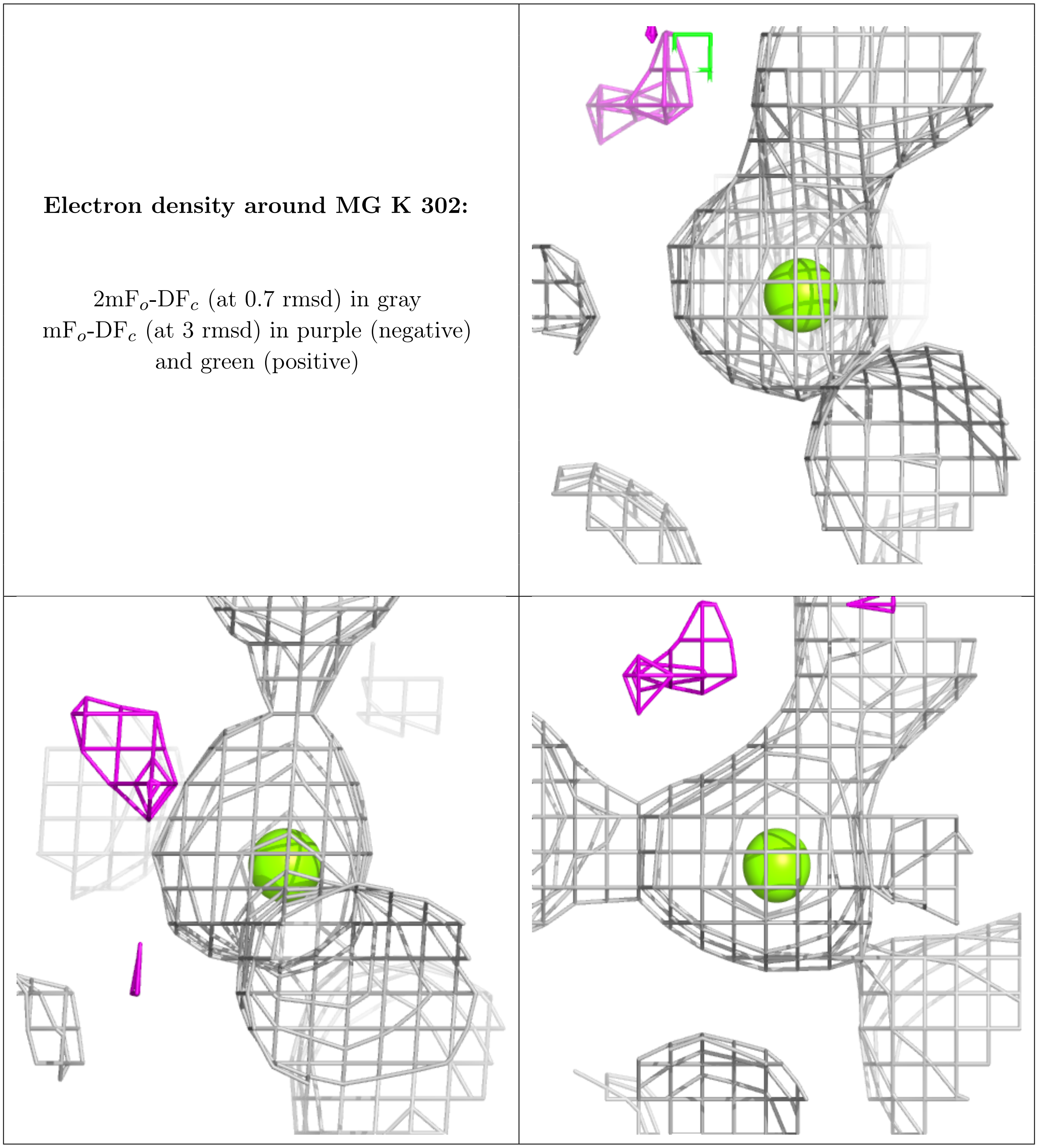


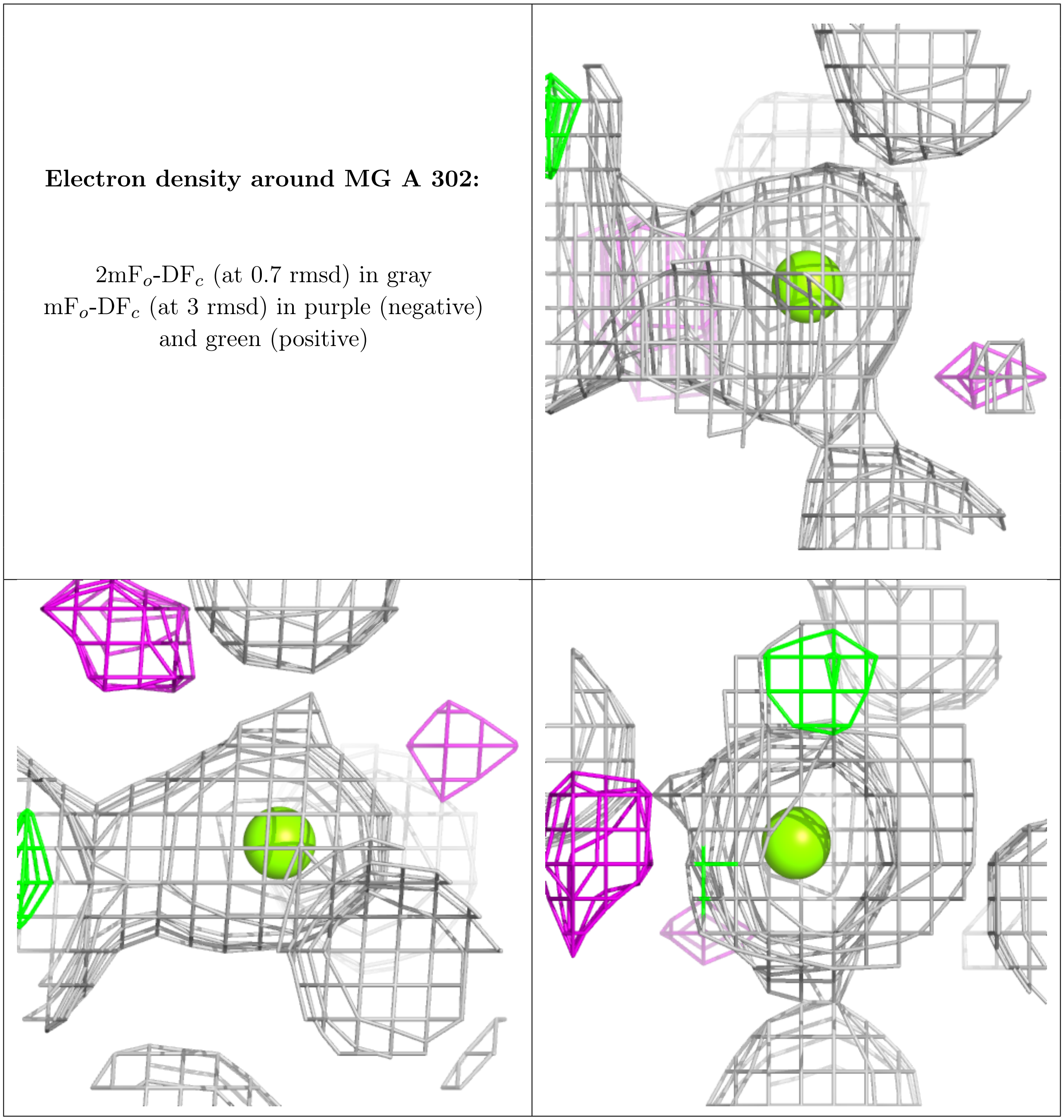




Electron density around MG K 302:

$2mF_o$-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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.