Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 05:59 PM UTC

PDB ID	:	8YEC / pdb_00008yec
Title	:	Crystal structure of L-ribulose 3-epimerase in complex with D-allulose
Authors	:	Watanabe, M.; Nakamichi, Y.; Mine, S.
Deposited on	:	2024-02-22
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

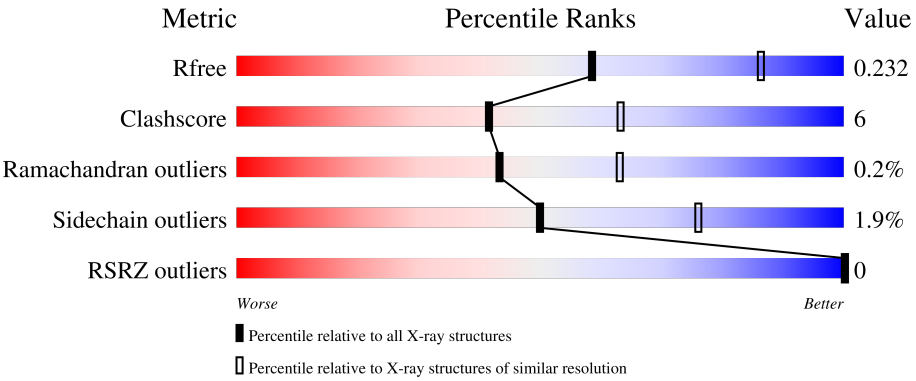
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	297	89% 10%
1	B	297	86% 10%
1	C	297	81% 17%
1	D	297	87% 10%
1	E	297	78% 21%

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Mol	Chain	Length	Quality of chain
1	F	297	81% 15%
1	G	297	82% 17%
1	H	297	83% 14%
1	I	297	81% 17%
1	J	297	79% 17%
1	K	297	85% 13%
1	L	297	84% 13%
1	M	297	84% 15%
1	N	297	84% 13%
1	O	297	83% 16%
1	P	297	78% 19%

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
6	PEG	C	305	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36802 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 Ketose 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	295	Total	C	N	O	S	0	0	0
			2258	1427	384	438	9			
1	F	289	Total	C	N	O	S	0	0	0
			2212	1395	377	431	9			
1	A	296	Total	C	N	O	S	0	0	0
			2267	1432	385	441	9			
1	B	288	Total	C	N	O	S	0	0	0
			2201	1389	374	429	9			
1	C	297	Total	C	N	O	S	0	0	0
			2275	1438	386	442	9			
1	D	289	Total	C	N	O	S	0	0	0
			2212	1395	377	431	9			
1	G	296	Total	C	N	O	S	0	0	0
			2267	1432	385	441	9			
1	H	289	Total	C	N	O	S	0	0	0
			2212	1395	377	431	9			
1	I	296	Total	C	N	O	S	0	0	0
			2267	1432	385	441	9			
1	J	289	Total	C	N	O	S	0	0	0
			2211	1395	377	430	9			
1	K	297	Total	C	N	O	S	0	0	0
			2275	1438	386	442	9			
1	L	288	Total	C	N	O	S	0	0	0
			2201	1389	374	429	9			
1	M	296	Total	C	N	O	S	0	0	0
			2267	1432	385	441	9			
1	N	288	Total	C	N	O	S	0	0	0
			2201	1389	374	429	9			
1	O	296	Total	C	N	O	S	0	0	0
			2267	1432	385	441	9			
1	P	289	Total	C	N	O	S	0	0	0
			2212	1395	377	431	9			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	LEU	-	expression tag	UNP A0A1L7NQ96
E	-6	GLU	-	expression tag	UNP A0A1L7NQ96
E	-5	VAL	-	expression tag	UNP A0A1L7NQ96
E	-4	LEU	-	expression tag	UNP A0A1L7NQ96
E	-3	PHE	-	expression tag	UNP A0A1L7NQ96
E	-2	GLN	-	expression tag	UNP A0A1L7NQ96
E	-1	GLY	-	expression tag	UNP A0A1L7NQ96
E	0	PRO	-	expression tag	UNP A0A1L7NQ96
F	-7	LEU	-	expression tag	UNP A0A1L7NQ96
F	-6	GLU	-	expression tag	UNP A0A1L7NQ96
F	-5	VAL	-	expression tag	UNP A0A1L7NQ96
F	-4	LEU	-	expression tag	UNP A0A1L7NQ96
F	-3	PHE	-	expression tag	UNP A0A1L7NQ96
F	-2	GLN	-	expression tag	UNP A0A1L7NQ96
F	-1	GLY	-	expression tag	UNP A0A1L7NQ96
F	0	PRO	-	expression tag	UNP A0A1L7NQ96
A	-7	LEU	-	expression tag	UNP A0A1L7NQ96
A	-6	GLU	-	expression tag	UNP A0A1L7NQ96
A	-5	VAL	-	expression tag	UNP A0A1L7NQ96
A	-4	LEU	-	expression tag	UNP A0A1L7NQ96
A	-3	PHE	-	expression tag	UNP A0A1L7NQ96
A	-2	GLN	-	expression tag	UNP A0A1L7NQ96
A	-1	GLY	-	expression tag	UNP A0A1L7NQ96
A	0	PRO	-	expression tag	UNP A0A1L7NQ96
B	-7	LEU	-	expression tag	UNP A0A1L7NQ96
B	-6	GLU	-	expression tag	UNP A0A1L7NQ96
B	-5	VAL	-	expression tag	UNP A0A1L7NQ96
B	-4	LEU	-	expression tag	UNP A0A1L7NQ96
B	-3	PHE	-	expression tag	UNP A0A1L7NQ96
B	-2	GLN	-	expression tag	UNP A0A1L7NQ96
B	-1	GLY	-	expression tag	UNP A0A1L7NQ96
B	0	PRO	-	expression tag	UNP A0A1L7NQ96
C	-7	LEU	-	expression tag	UNP A0A1L7NQ96
C	-6	GLU	-	expression tag	UNP A0A1L7NQ96
C	-5	VAL	-	expression tag	UNP A0A1L7NQ96
C	-4	LEU	-	expression tag	UNP A0A1L7NQ96
C	-3	PHE	-	expression tag	UNP A0A1L7NQ96
C	-2	GLN	-	expression tag	UNP A0A1L7NQ96
C	-1	GLY	-	expression tag	UNP A0A1L7NQ96
C	0	PRO	-	expression tag	UNP A0A1L7NQ96
D	-7	LEU	-	expression tag	UNP A0A1L7NQ96
D	-6	GLU	-	expression tag	UNP A0A1L7NQ96

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP A0A1L7NQ96
D	-4	LEU	-	expression tag	UNP A0A1L7NQ96
D	-3	PHE	-	expression tag	UNP A0A1L7NQ96
D	-2	GLN	-	expression tag	UNP A0A1L7NQ96
D	-1	GLY	-	expression tag	UNP A0A1L7NQ96
D	0	PRO	-	expression tag	UNP A0A1L7NQ96
G	-7	LEU	-	expression tag	UNP A0A1L7NQ96
G	-6	GLU	-	expression tag	UNP A0A1L7NQ96
G	-5	VAL	-	expression tag	UNP A0A1L7NQ96
G	-4	LEU	-	expression tag	UNP A0A1L7NQ96
G	-3	PHE	-	expression tag	UNP A0A1L7NQ96
G	-2	GLN	-	expression tag	UNP A0A1L7NQ96
G	-1	GLY	-	expression tag	UNP A0A1L7NQ96
G	0	PRO	-	expression tag	UNP A0A1L7NQ96
H	-7	LEU	-	expression tag	UNP A0A1L7NQ96
H	-6	GLU	-	expression tag	UNP A0A1L7NQ96
H	-5	VAL	-	expression tag	UNP A0A1L7NQ96
H	-4	LEU	-	expression tag	UNP A0A1L7NQ96
H	-3	PHE	-	expression tag	UNP A0A1L7NQ96
H	-2	GLN	-	expression tag	UNP A0A1L7NQ96
H	-1	GLY	-	expression tag	UNP A0A1L7NQ96
H	0	PRO	-	expression tag	UNP A0A1L7NQ96
I	-7	LEU	-	expression tag	UNP A0A1L7NQ96
I	-6	GLU	-	expression tag	UNP A0A1L7NQ96
I	-5	VAL	-	expression tag	UNP A0A1L7NQ96
I	-4	LEU	-	expression tag	UNP A0A1L7NQ96
I	-3	PHE	-	expression tag	UNP A0A1L7NQ96
I	-2	GLN	-	expression tag	UNP A0A1L7NQ96
I	-1	GLY	-	expression tag	UNP A0A1L7NQ96
I	0	PRO	-	expression tag	UNP A0A1L7NQ96
J	-7	LEU	-	expression tag	UNP A0A1L7NQ96
J	-6	GLU	-	expression tag	UNP A0A1L7NQ96
J	-5	VAL	-	expression tag	UNP A0A1L7NQ96
J	-4	LEU	-	expression tag	UNP A0A1L7NQ96
J	-3	PHE	-	expression tag	UNP A0A1L7NQ96
J	-2	GLN	-	expression tag	UNP A0A1L7NQ96
J	-1	GLY	-	expression tag	UNP A0A1L7NQ96
J	0	PRO	-	expression tag	UNP A0A1L7NQ96
K	-7	LEU	-	expression tag	UNP A0A1L7NQ96
K	-6	GLU	-	expression tag	UNP A0A1L7NQ96
K	-5	VAL	-	expression tag	UNP A0A1L7NQ96
K	-4	LEU	-	expression tag	UNP A0A1L7NQ96

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	PHE	-	expression tag	UNP A0A1L7NQ96
K	-2	GLN	-	expression tag	UNP A0A1L7NQ96
K	-1	GLY	-	expression tag	UNP A0A1L7NQ96
K	0	PRO	-	expression tag	UNP A0A1L7NQ96
L	-7	LEU	-	expression tag	UNP A0A1L7NQ96
L	-6	GLU	-	expression tag	UNP A0A1L7NQ96
L	-5	VAL	-	expression tag	UNP A0A1L7NQ96
L	-4	LEU	-	expression tag	UNP A0A1L7NQ96
L	-3	PHE	-	expression tag	UNP A0A1L7NQ96
L	-2	GLN	-	expression tag	UNP A0A1L7NQ96
L	-1	GLY	-	expression tag	UNP A0A1L7NQ96
L	0	PRO	-	expression tag	UNP A0A1L7NQ96
M	-7	LEU	-	expression tag	UNP A0A1L7NQ96
M	-6	GLU	-	expression tag	UNP A0A1L7NQ96
M	-5	VAL	-	expression tag	UNP A0A1L7NQ96
M	-4	LEU	-	expression tag	UNP A0A1L7NQ96
M	-3	PHE	-	expression tag	UNP A0A1L7NQ96
M	-2	GLN	-	expression tag	UNP A0A1L7NQ96
M	-1	GLY	-	expression tag	UNP A0A1L7NQ96
M	0	PRO	-	expression tag	UNP A0A1L7NQ96
N	-7	LEU	-	expression tag	UNP A0A1L7NQ96
N	-6	GLU	-	expression tag	UNP A0A1L7NQ96
N	-5	VAL	-	expression tag	UNP A0A1L7NQ96
N	-4	LEU	-	expression tag	UNP A0A1L7NQ96
N	-3	PHE	-	expression tag	UNP A0A1L7NQ96
N	-2	GLN	-	expression tag	UNP A0A1L7NQ96
N	-1	GLY	-	expression tag	UNP A0A1L7NQ96
N	0	PRO	-	expression tag	UNP A0A1L7NQ96
O	-7	LEU	-	expression tag	UNP A0A1L7NQ96
O	-6	GLU	-	expression tag	UNP A0A1L7NQ96
O	-5	VAL	-	expression tag	UNP A0A1L7NQ96
O	-4	LEU	-	expression tag	UNP A0A1L7NQ96
O	-3	PHE	-	expression tag	UNP A0A1L7NQ96
O	-2	GLN	-	expression tag	UNP A0A1L7NQ96
O	-1	GLY	-	expression tag	UNP A0A1L7NQ96
O	0	PRO	-	expression tag	UNP A0A1L7NQ96
P	-7	LEU	-	expression tag	UNP A0A1L7NQ96
P	-6	GLU	-	expression tag	UNP A0A1L7NQ96
P	-5	VAL	-	expression tag	UNP A0A1L7NQ96
P	-4	LEU	-	expression tag	UNP A0A1L7NQ96
P	-3	PHE	-	expression tag	UNP A0A1L7NQ96
P	-2	GLN	-	expression tag	UNP A0A1L7NQ96

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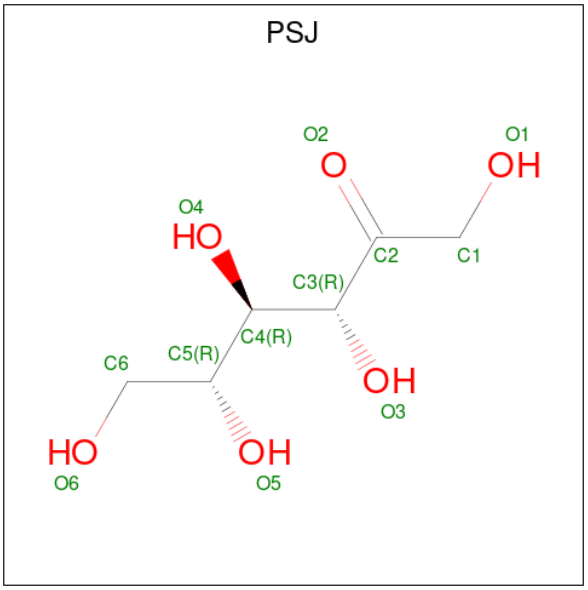
Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	GLY	-	expression tag	UNP A0A1L7NQ96
P	0	PRO	-	expression tag	UNP A0A1L7NQ96

- Molecule 2 is D-psicose (CCD ID: PSJ) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 12 6 6	0	1
2	F	1	Total C O 12 6 6	0	1
2	A	1	Total C O 12 6 6	0	1
2	B	1	Total C O 12 6 6	0	1
2	C	1	Total C O 12 6 6	0	1
2	D	1	Total C O 12 6 6	0	1
2	G	1	Total C O 12 6 6	0	1
2	H	1	Total C O 12 6 6	0	1
2	I	1	Total C O 12 6 6	0	1
2	J	1	Total C O 12 6 6	0	1

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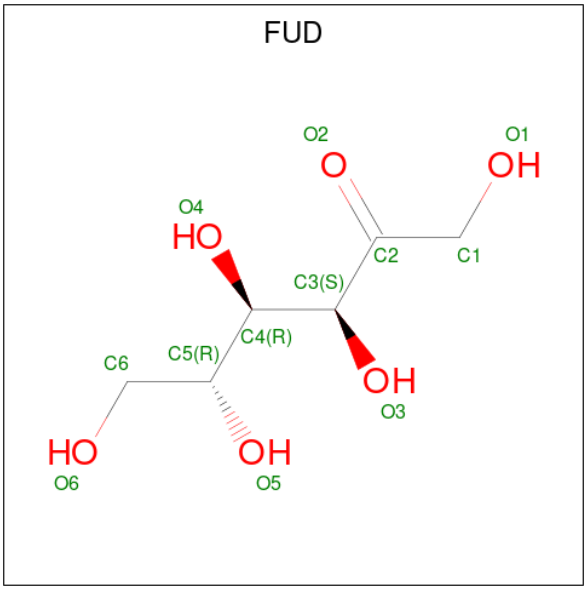
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total C O 12 6 6	0	1
2	L	1	Total C O 12 6 6	0	1
2	M	1	Total C O 12 6 6	0	1
2	N	1	Total C O 12 6 6	0	1
2	O	1	Total C O 12 6 6	0	1
2	P	1	Total C O 12 6 6	0	1

- Molecule 3 is D-fructose (CCD ID: FUD) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 12 6 6	0	1
3	F	1	Total C O 12 6 6	0	1
3	A	1	Total C O 12 6 6	0	1
3	B	1	Total C O 12 6 6	0	1
3	C	1	Total C O 12 6 6	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 12 6 6	0	1
3	G	1	Total C O 12 6 6	0	1
3	H	1	Total C O 12 6 6	0	1
3	I	1	Total C O 12 6 6	0	1
3	J	1	Total C O 12 6 6	0	1
3	K	1	Total C O 12 6 6	0	1
3	L	1	Total C O 12 6 6	0	1
3	M	1	Total C O 12 6 6	0	1
3	N	1	Total C O 12 6 6	0	1
3	O	1	Total C O 12 6 6	0	1
3	P	1	Total C O 12 6 6	0	1

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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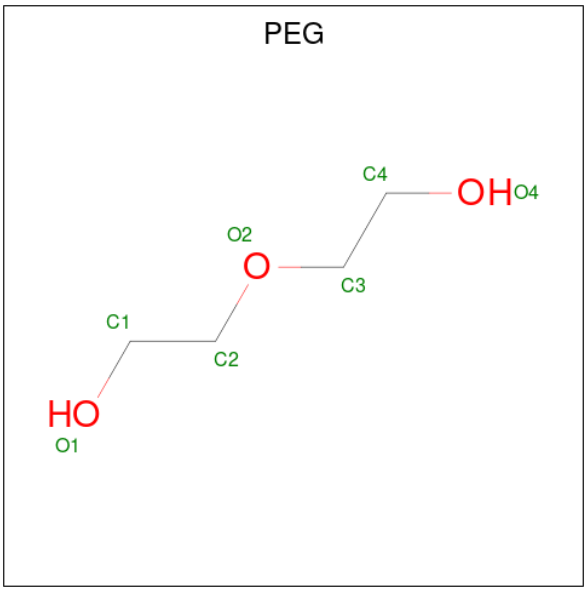
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0
4	N	1	Total Mg 1 1	0	0
4	O	1	Total Mg 1 1	0	0
4	P	1	Total Mg 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0
5	J	1	Total Na 1 1	0	0
5	K	1	Total Na 1 1	0	0
5	N	1	Total Na 1 1	0	0
5	O	1	Total Na 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	26	Total O 26 26	0	0
7	F	29	Total O 29 29	0	0
7	A	57	Total O 57 57	0	0
7	B	31	Total O 31 31	0	0
7	C	33	Total O 33 33	0	0
7	D	39	Total O 39 39	0	0
7	G	42	Total O 42 42	0	0
7	H	39	Total O 39 39	0	0
7	I	31	Total O 31 31	0	0
7	J	26	Total O 26 26	0	0
7	K	49	Total O 49 49	0	0

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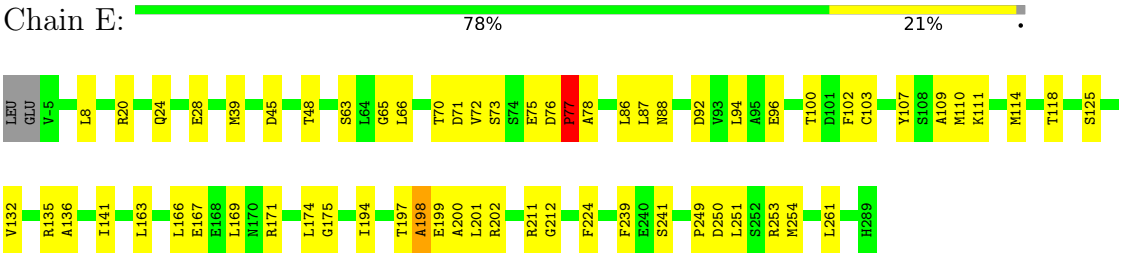
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	33	Total O 33 33	0	0
7	M	38	Total O 38 38	0	0
7	N	37	Total O 37 37	0	0
7	O	32	Total O 32 32	0	0
7	P	40	Total O 40 40	0	0

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.

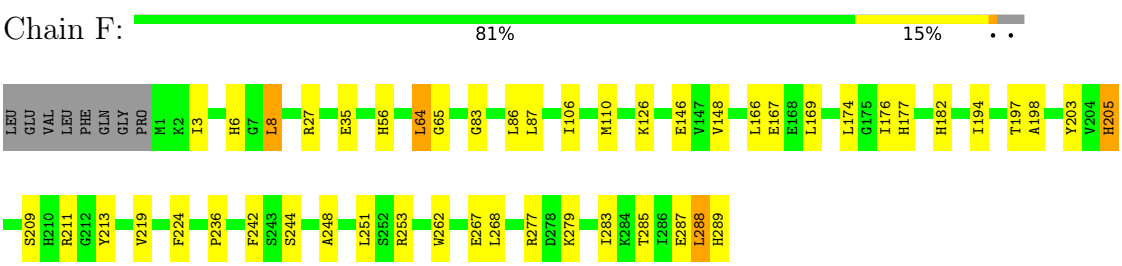
• Molecule 1: Ketose 3-epimerase

Chain E:



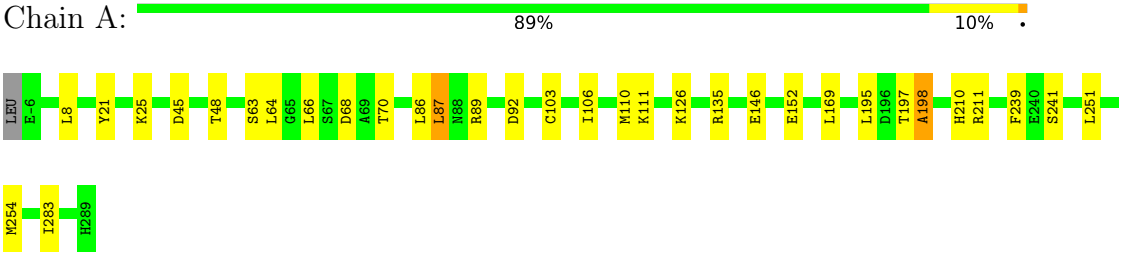
• Molecule 1: Ketose 3-epimerase

Chain F:



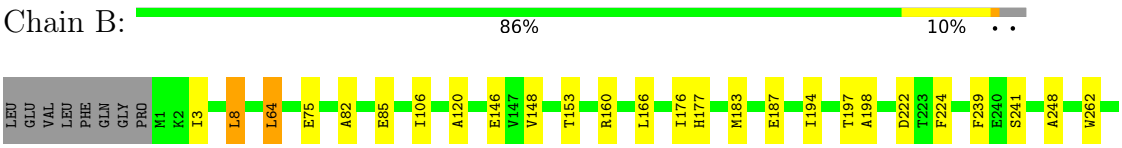
• Molecule 1: Ketose 3-epimerase

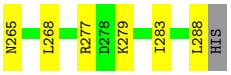
Chain A:



• Molecule 1: Ketose 3-epimerase

Chain B:

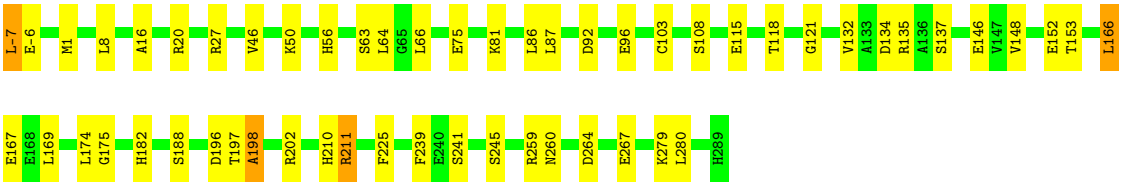




• Molecule 1: Ketose 3-epimerase

Chain C:

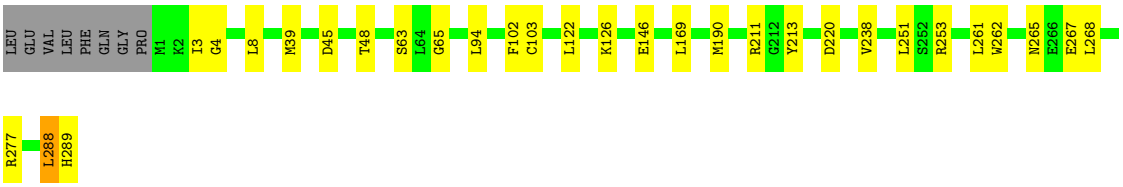




• Molecule 1: Ketose 3-epimerase

Chain D:

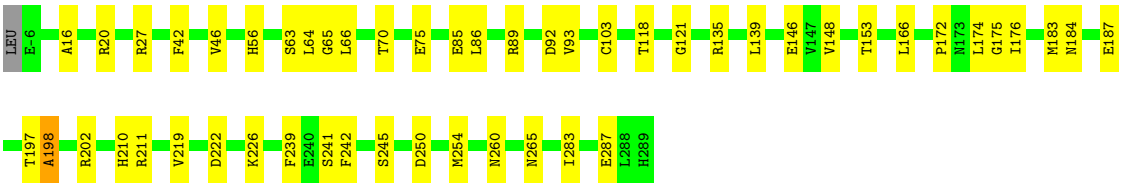




• Molecule 1: Ketose 3-epimerase

Chain G:

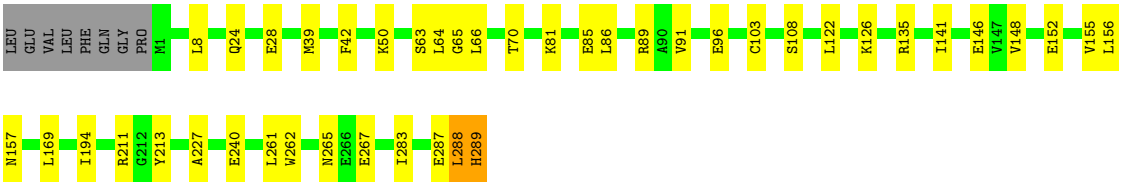




• Molecule 1: Ketose 3-epimerase

Chain H:

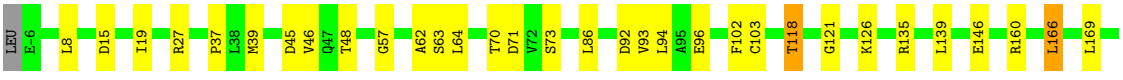


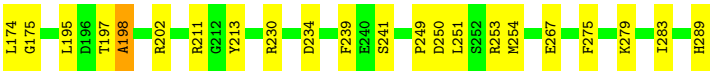


• Molecule 1: Ketose 3-epimerase

Chain I:



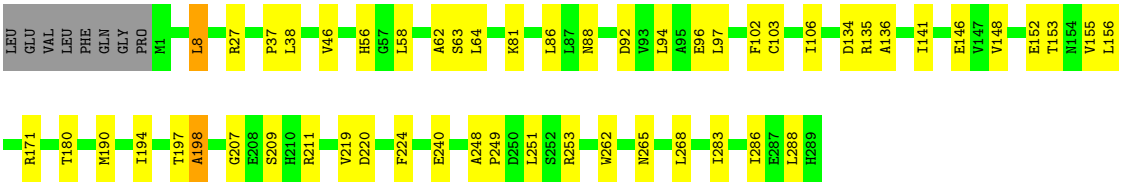




• Molecule 1: Ketose 3-epimerase

Chain J:

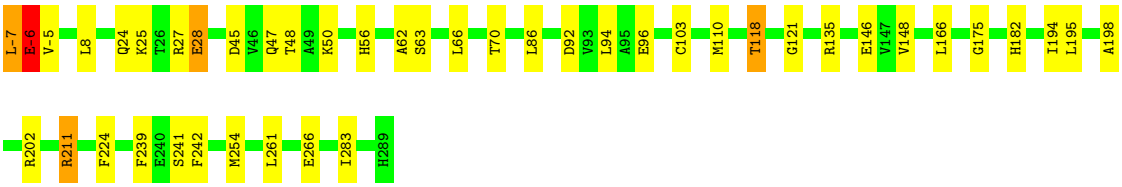




• Molecule 1: Ketose 3-epimerase

Chain K:

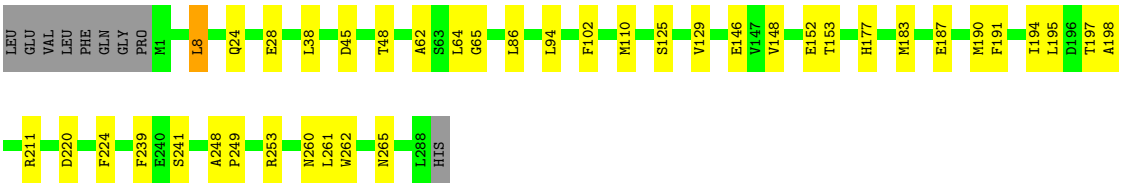




• Molecule 1: Ketose 3-epimerase

Chain L:

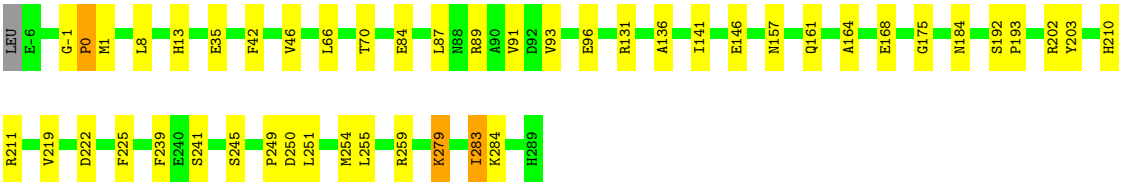




• Molecule 1: Ketose 3-epimerase

Chain M:





• Molecule 1: Ketose 3-epimerase

Chain N:







• Molecule 1: Ketose 3-epimerase

Chain O:



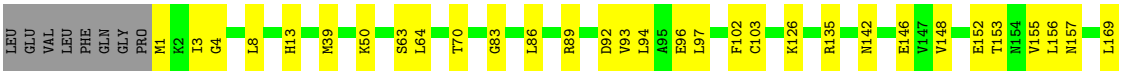


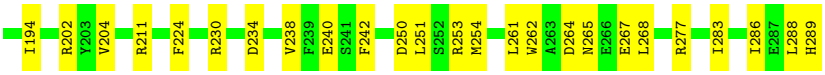


• Molecule 1: Ketose 3-epimerase

Chain P:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.43Å 135.13Å 151.13Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.50) 98.2 (30.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.207 , 0.255 (Not available) , 0.232	Depositor DCC
R_{free} test set	8921 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 16.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l 0.014 for k,h,-l 0.457 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36802	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0602e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PSJ, PEG, FUD, NA, MG

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	0.51	0/2313	0.73	0/3136
1	B	0.51	0/2244	0.72	0/3043
1	C	0.49	0/2321	0.71	0/3147
1	D	0.52	0/2256	0.72	0/3058
1	E	0.48	0/2304	0.73	1/3124 (0.0%)
1	F	0.49	0/2256	0.71	0/3058
1	G	0.51	0/2313	0.73	0/3136
1	H	0.50	0/2256	0.71	0/3058
1	I	0.48	0/2313	0.73	1/3136 (0.0%)
1	J	0.49	0/2255	0.72	0/3058
1	K	0.50	0/2321	0.74	0/3147
1	L	0.51	0/2244	0.73	0/3043
1	M	0.51	0/2313	0.78	2/3136 (0.1%)
1	N	0.51	0/2244	0.72	0/3043
1	O	0.49	0/2313	0.71	0/3136
1	P	0.52	0/2256	0.72	0/3058
All	All	0.50	0/36522	0.73	4/49517 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	0	PRO	N-CD-CG	-12.03	85.16	103.20
1	M	0	PRO	CA-CB-CG	-7.99	89.32	104.50
1	E	77	PRO	N-CD-CG	-5.82	94.47	103.20
1	I	234	ASP	CA-CB-CG	5.27	117.87	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	211	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2205	20	0
1	B	2201	0	2145	19	0
1	C	2275	0	2216	37	0
1	D	2212	0	2152	18	0
1	E	2258	0	2199	38	0
1	F	2212	0	2152	31	0
1	G	2267	0	2205	30	0
1	H	2212	0	2152	28	0
1	I	2267	0	2205	38	0
1	J	2211	0	2152	34	0
1	K	2275	0	2216	27	0
1	L	2201	0	2145	22	0
1	M	2267	0	2205	28	0
1	N	2201	0	2145	24	0
1	O	2267	0	2205	27	0
1	P	2212	0	2152	35	0
2	A	12	0	12	1	0
2	B	12	0	11	1	0
2	C	12	0	12	1	0
2	D	12	0	11	1	0
2	E	12	0	12	0	0
2	F	12	0	11	2	0
2	G	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	12	0	12	1	0
2	I	12	0	11	1	0
2	J	12	0	12	1	0
2	K	12	0	12	1	0
2	L	12	0	11	1	0
2	M	12	0	12	3	0
2	N	12	0	12	2	0
2	O	12	0	12	2	0
2	P	12	0	11	2	0
3	A	12	0	11	1	0
3	B	12	0	11	0	0
3	C	12	0	11	1	0
3	D	12	0	11	0	0
3	E	12	0	12	1	0
3	F	12	0	11	1	0
3	G	12	0	12	0	0
3	H	12	0	12	2	0
3	I	12	0	11	0	0
3	J	12	0	11	2	0
3	K	12	0	12	0	0
3	L	12	0	11	1	0
3	M	12	0	12	1	0
3	N	12	0	11	1	0
3	O	12	0	12	1	0
3	P	12	0	11	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
6	C	7	0	10	5	0
7	A	57	0	0	1	0
7	B	31	0	0	0	0
7	C	33	0	0	0	0
7	D	39	0	0	1	0
7	E	26	0	0	1	0
7	F	29	0	0	0	0
7	G	42	0	0	3	0
7	H	39	0	0	1	0
7	I	31	0	0	2	0
7	J	26	0	0	0	0
7	K	49	0	0	3	0
7	L	33	0	0	0	0
7	M	38	0	0	2	0
7	N	37	0	0	1	0
7	O	32	0	0	1	0
7	P	40	0	0	1	0
All	All	36802	0	35229	454	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 6.

All (454) 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:C:188:SER:H	6:C:305:PEG:H11	1.22	1.02
1:H:39:MET:HE1	1:H:65:GLY:H	1.26	0.96
1:D:213:TYR:OH	1:D:267:GLU:OE1	1.92	0.87
1:I:213:TYR:OH	1:I:267:GLU:OE1	1.95	0.85
1:K:28:GLU:OE2	7:K:401:HOH:O	1.94	0.84
1:D:288:LEU:HD12	1:D:289:HIS:H	1.48	0.77
1:N:152:GLU:OE1	3:N:303[B]:FUD:O1	2.00	0.77
1:C:118:THR:HG23	1:C:121:GLY:H	1.49	0.76
1:M:211:ARG:NH2	2:M:301[A]:PSJ:O1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:GLY:HA3	1:G:202:ARG:HD2	1.69	0.75
1:P:39:MET:HE2	1:P:251:LEU:HD13	1.68	0.75
1:I:92:ASP:OD2	1:I:135:ARG:NH2	2.20	0.74
1:H:287:GLU:HB3	1:H:288:LEU:HD13	1.70	0.73
1:H:126:LYS:HB3	1:H:169:LEU:HD11	1.69	0.73
1:K:-7:LEU:O	1:K:-6:GLU:HB2	1.90	0.70
1:A:92:ASP:OD1	1:A:135:ARG:NH2	2.24	0.70
1:K:92:ASP:OD2	1:K:135:ARG:NH2	2.24	0.70
1:N:199:GLU:N	1:N:199:GLU:OE1	2.24	0.70
1:K:-7:LEU:HA	1:K:56:HIS:HA	1.73	0.69
1:N:126:LYS:HB3	1:N:169:LEU:HD11	1.73	0.69
1:G:70:THR:HG21	1:G:86:LEU:HD12	1.74	0.69
1:C:1:MET:HE3	1:C:280:LEU:HD13	1.75	0.68
1:D:146:GLU:OE1	2:D:301[A]:PSJ:H3	1.93	0.68
1:K:50:LYS:NZ	1:K:96:GLU:O	2.27	0.68
1:D:8:LEU:HD22	1:D:251:LEU:HD23	1.75	0.67
1:E:72:VAL:HG12	1:E:125:SER:HA	1.77	0.67
1:G:287:GLU:OE1	7:G:401:HOH:O	2.12	0.66
1:F:244:SER:HB3	1:P:13:HIS:NE2	2.11	0.66
1:J:27:ARG:HD2	1:J:58:LEU:HD13	1.76	0.66
1:I:249:PRO:O	1:I:253:ARG:HD3	1.95	0.66
1:H:146:GLU:OE1	2:H:301[A]:PSJ:H3	1.95	0.66
1:P:146:GLU:OE1	2:P:301[A]:PSJ:H3	1.96	0.66
1:O:87:LEU:HD23	1:O:132:VAL:HG21	1.78	0.65
1:F:8:LEU:HD13	1:F:251:LEU:HD23	1.79	0.64
1:P:50:LYS:HG3	1:P:97:LEU:HD23	1.79	0.64
1:I:126:LYS:HB3	1:I:169:LEU:HD21	1.80	0.64
1:C:225:PHE:CD2	1:C:279:LYS:HG2	2.33	0.63
1:K:47:GLN:NE2	7:K:402:HOH:O	2.31	0.63
1:H:39:MET:HE2	1:H:39:MET:HA	1.79	0.63
1:C:152:GLU:OE1	3:C:302[B]:FUD:O1	2.17	0.63
1:O:211:ARG:NH2	3:O:302[B]:FUD:O1	2.30	0.62
1:N:146:GLU:OE1	2:N:302[A]:PSJ:H3	1.99	0.62
1:K:25:LYS:NZ	7:K:403:HOH:O	2.33	0.62
1:M:0:PRO:HG2	1:M:1:MET:N	2.13	0.62
1:O:50:LYS:HE3	1:O:96:GLU:O	2.00	0.62
1:I:8:LEU:HD23	1:I:37:PRO:HG3	1.82	0.61
1:E:197:THR:HG22	1:E:201:LEU:HB2	1.82	0.61
1:O:126:LYS:HB3	1:O:169:LEU:HD21	1.81	0.61
1:P:142:ASN:OD1	1:P:202:ARG:NH2	2.22	0.61
1:E:92:ASP:CG	1:E:135:ARG:HH21	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:MET:HE2	1:I:254:MET:HE1	1.83	0.60
1:I:135:ARG:O	1:I:139:LEU:HD13	2.01	0.60
1:L:152:GLU:OE1	3:L:302[B]:FUD:O1	2.05	0.60
1:M:87:LEU:O	1:M:91:VAL:HG23	2.03	0.59
1:D:3:ILE:HD12	1:D:277:ARG:HG2	1.83	0.59
1:H:24:GLN:O	1:H:28:GLU:HG3	2.02	0.59
1:G:118:THR:HG23	1:G:121:GLY:H	1.66	0.59
1:A:110:MET:HE2	1:A:254:MET:HE2	1.83	0.59
1:O:146:GLU:OE1	2:O:301[A]:PSJ:H3	2.01	0.59
1:P:283:ILE:HA	1:P:286:ILE:HD12	1.83	0.59
1:G:166:LEU:HD22	1:G:174:LEU:HG	1.84	0.59
1:J:64:LEU:HD22	1:J:106:ILE:HG22	1.85	0.59
1:I:92:ASP:CG	1:I:135:ARG:HH21	2.11	0.58
1:L:24:GLN:O	1:L:28:GLU:HG3	2.03	0.58
1:G:146:GLU:OE1	2:G:301[A]:PSJ:H3	2.04	0.58
1:M:146:GLU:OE1	2:M:301[A]:PSJ:H3	2.04	0.58
1:J:8:LEU:HD12	1:J:37:PRO:HG3	1.85	0.57
1:J:8:LEU:HD21	1:J:248:ALA:HB2	1.85	0.57
1:F:166:LEU:HD11	1:F:176:ILE:HG13	1.87	0.57
1:H:39:MET:HE1	1:H:65:GLY:N	2.09	0.57
1:E:88:ASN:ND2	1:E:132:VAL:HG22	2.20	0.56
1:O:20:ARG:HD2	1:O:48:THR:HG23	1.87	0.56
1:C:135:ARG:HH11	1:C:135:ARG:HG2	1.71	0.56
1:J:283:ILE:HA	1:J:286:ILE:HD12	1.87	0.56
1:I:118:THR:HG23	1:I:121:GLY:H	1.69	0.56
1:J:27:ARG:HD3	1:J:56:HIS:O	2.05	0.56
1:K:70:THR:HG21	1:K:86:LEU:HD12	1.87	0.56
1:I:230:ARG:HH11	1:I:230:ARG:HG2	1.70	0.56
1:G:183:MET:HG2	1:G:187:GLU:HG3	1.87	0.56
1:B:148:VAL:HG23	1:B:153:THR:HG22	1.86	0.56
1:C:146:GLU:OE1	2:C:301[A]:PSJ:H3	2.06	0.56
1:E:39:MET:HE1	1:E:65:GLY:O	2.06	0.55
1:F:213:TYR:OH	1:F:267:GLU:HG2	2.06	0.55
1:G:16:ALA:O	1:G:20:ARG:HG3	2.06	0.55
1:E:92:ASP:OD1	1:E:135:ARG:NH2	2.36	0.55
1:B:64:LEU:HD22	1:B:106:ILE:HG22	1.87	0.55
1:C:87:LEU:HD23	1:C:132:VAL:HG21	1.88	0.55
1:A:146:GLU:OE1	2:A:301[A]:PSJ:H3	2.07	0.55
1:G:27:ARG:HD3	1:G:56:HIS:O	2.06	0.55
1:D:262:TRP:CZ3	1:D:265:ASN:HB3	2.42	0.55
1:C:188:SER:H	6:C:305:PEG:C1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:GLU:OE2	1:N:131:ARG:NE	2.38	0.55
1:C:259:ARG:HD3	7:D:433:HOH:O	2.06	0.54
1:K:118:THR:HG23	1:K:121:GLY:H	1.71	0.54
1:O:183:MET:HG2	1:O:187:GLU:HG3	1.89	0.54
1:H:213:TYR:OH	1:H:267:GLU:HG2	2.07	0.54
1:K:45:ASP:OD2	1:K:48:THR:OG1	2.25	0.54
1:E:75:GLU:O	1:E:77:PRO:HD2	2.07	0.54
1:G:63:SER:HA	1:G:103:CYS:O	2.08	0.54
1:P:251:LEU:HD21	2:P:301[A]:PSJ:H6	1.89	0.54
1:E:249:PRO:O	1:E:253:ARG:HD3	2.08	0.54
1:H:152:GLU:OE1	3:H:302[B]:FUD:O1	2.19	0.54
1:M:175:GLY:HA3	1:M:202:ARG:HG3	1.90	0.54
1:J:38:LEU:HG	1:J:62:ALA:HB1	1.91	0.53
1:A:8:LEU:HD22	1:A:251:LEU:HD23	1.89	0.53
1:B:239:PHE:CZ	1:B:241:SER:HB2	2.44	0.53
1:L:262:TRP:CZ3	1:L:265:ASN:HB3	2.44	0.53
1:I:63:SER:HA	1:I:103:CYS:O	2.09	0.53
1:L:146:GLU:OE1	2:L:301[A]:PSJ:H3	2.09	0.53
1:B:3:ILE:HD12	1:B:277:ARG:NH1	2.24	0.53
1:C:46:VAL:HG11	1:C:96:GLU:HB3	1.91	0.53
1:J:249:PRO:O	1:J:253:ARG:HD3	2.09	0.53
1:L:239:PHE:CZ	1:L:241:SER:HB2	2.44	0.53
1:P:262:TRP:CZ3	1:P:265:ASN:HB3	2.44	0.53
1:F:64:LEU:HD22	1:F:106:ILE:HG22	1.90	0.53
1:F:194:ILE:HD11	1:F:224:PHE:CE1	2.44	0.53
1:H:155:VAL:HG12	1:H:156:LEU:HG	1.91	0.52
1:G:172:PRO:HB3	7:G:441:HOH:O	2.09	0.52
1:L:249:PRO:O	1:L:253:ARG:HD3	2.10	0.52
1:E:70:THR:HG21	1:E:86:LEU:CD2	2.40	0.52
1:B:194:ILE:HD11	1:B:224:PHE:CE1	2.45	0.52
1:L:64:LEU:HD11	1:L:86:LEU:CD2	2.40	0.52
1:E:63:SER:HA	1:E:103:CYS:O	2.10	0.52
1:K:211:ARG:HD2	1:K:242:PHE:HD2	1.75	0.52
1:L:183:MET:HG2	1:L:187:GLU:HG3	1.91	0.52
1:F:83:GLY:O	1:F:87:LEU:HG	2.10	0.51
1:L:260:ASN:O	1:L:261:LEU:HD23	2.10	0.51
1:E:166:LEU:HD22	1:E:174:LEU:CD2	2.40	0.51
1:P:126:LYS:HB3	1:P:169:LEU:HD11	1.92	0.51
1:F:8:LEU:HD21	1:F:248:ALA:HB2	1.93	0.51
1:L:65:GLY:HA3	1:L:110:MET:HE2	1.91	0.51
1:F:262:TRP:CE2	1:F:268:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:HD11	1:B:224:PHE:CD1	2.46	0.51
1:C:63:SER:HA	1:C:103:CYS:O	2.11	0.51
1:O:115:GLU:OE2	1:P:253:ARG:HD2	2.11	0.51
1:K:25:LYS:HE3	1:K:266:GLU:OE1	2.11	0.51
1:L:190:MET:HG3	1:L:220:ASP:HB3	1.92	0.51
1:I:239:PHE:CZ	1:I:241:SER:HB2	2.46	0.51
1:E:70:THR:HG21	1:E:86:LEU:HD23	1.94	0.50
1:E:109:ALA:HB3	1:E:111:LYS:HD3	1.93	0.50
1:O:134:ASP:O	1:O:137:SER:HB3	2.12	0.50
1:P:267:GLU:HG2	7:P:421:HOH:O	2.10	0.50
1:I:175:GLY:HA3	1:I:202:ARG:HG3	1.93	0.50
1:I:118:THR:CG2	1:I:121:GLY:H	2.24	0.50
1:C:92:ASP:CG	1:C:135:ARG:HH22	2.20	0.50
1:L:8:LEU:HD21	1:L:248:ALA:HB2	1.94	0.50
1:M:46:VAL:HG22	1:M:93:VAL:HG13	1.92	0.50
1:P:63:SER:HA	1:P:103:CYS:O	2.12	0.50
1:H:262:TRP:CZ3	1:H:265:ASN:HB3	2.47	0.49
1:K:110:MET:HE2	1:K:254:MET:HE2	1.93	0.49
1:L:45:ASP:OD2	1:L:48:THR:OG1	2.28	0.49
1:A:110:MET:CE	1:A:254:MET:HE2	2.42	0.49
1:P:148:VAL:HG23	1:P:153:THR:HG22	1.94	0.49
1:C:64:LEU:HD11	1:C:86:LEU:CD1	2.42	0.49
1:A:66:LEU:HD22	1:A:70:THR:HB	1.94	0.49
1:H:70:THR:HG21	1:H:86:LEU:HD13	1.95	0.49
1:H:288:LEU:HB2	1:H:289:HIS:CE1	2.48	0.49
1:N:64:LEU:HD11	1:N:86:LEU:HD21	1.94	0.49
1:N:92:ASP:OD2	1:N:135:ARG:NH2	2.46	0.49
1:F:211:ARG:HD2	1:F:242:PHE:HD2	1.78	0.49
1:H:240:GLU:OE2	3:H:302[B]:FUD:H3	2.12	0.49
1:M:0:PRO:HG2	1:M:1:MET:H	1.77	0.49
1:K:118:THR:CG2	1:K:121:GLY:H	2.26	0.49
1:F:194:ILE:HD11	1:F:224:PHE:CD1	2.48	0.48
1:G:75:GLU:CD	1:G:118:THR:HG21	2.37	0.48
1:O:24:GLN:NE2	1:O:28:GLU:OE2	2.46	0.48
1:B:82:ALA:O	1:B:85:GLU:HG2	2.13	0.48
1:C:245:SER:OG	1:C:260:ASN:OD1	2.30	0.48
1:K:63:SER:HA	1:K:103:CYS:O	2.12	0.48
1:N:262:TRP:CZ3	1:N:265:ASN:HB3	2.48	0.48
1:G:239:PHE:CZ	1:G:241:SER:HB2	2.49	0.48
1:I:70:THR:HG21	1:I:86:LEU:HD12	1.95	0.48
1:D:39:MET:HE1	1:D:65:GLY:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ARG:HB2	7:I:415:HOH:O	2.14	0.48
1:E:211:ARG:HB2	7:E:415:HOH:O	2.12	0.48
1:F:146:GLU:OE1	2:F:301[A]:PSJ:H3	2.13	0.48
1:D:39:MET:HE1	1:D:65:GLY:N	2.29	0.48
1:A:66:LEU:HD21	1:A:87:LEU:CD1	2.43	0.48
1:B:75:GLU:OE1	1:B:120:ALA:HB3	2.14	0.48
1:M:35:GLU:OE1	1:M:203:TYR:OH	2.24	0.48
1:D:262:TRP:CE2	1:D:268:LEU:HD22	2.48	0.48
1:G:176:ILE:HD12	1:G:197:THR:HG23	1.96	0.48
1:G:118:THR:CG2	1:G:121:GLY:H	2.27	0.48
1:I:160:ARG:HG3	1:I:160:ARG:HH11	1.78	0.48
1:F:64:LEU:HD11	1:F:86:LEU:CD2	2.44	0.48
1:P:264:ASP:OD1	1:P:267:GLU:HB2	2.14	0.48
1:C:188:SER:N	6:C:305:PEG:H11	2.07	0.48
1:J:262:TRP:CE2	1:J:268:LEU:HD22	2.48	0.48
1:L:194:ILE:HD11	1:L:224:PHE:CD1	2.48	0.48
1:M:136:ALA:HB1	1:M:141:ILE:HB	1.96	0.48
1:K:146:GLU:OE1	2:K:301[A]:PSJ:H3	2.14	0.47
1:L:94:LEU:CD1	1:L:102:PHE:HB2	2.44	0.47
1:F:203:TYR:CD2	1:F:236:PRO:HG2	2.49	0.47
1:C:115:GLU:OE2	1:D:253:ARG:HD2	2.13	0.47
1:D:63:SER:HA	1:D:103:CYS:O	2.13	0.47
1:D:94:LEU:CD1	1:D:102:PHE:HB2	2.44	0.47
1:D:288:LEU:HD12	1:D:289:HIS:N	2.25	0.47
1:I:146:GLU:OE1	2:I:301[A]:PSJ:H3	2.14	0.47
1:A:210:HIS:O	1:A:211:ARG:HB2	2.15	0.47
1:G:64:LEU:HD23	1:G:65:GLY:N	2.29	0.47
1:G:66:LEU:HD22	1:G:70:THR:HB	1.95	0.47
1:K:175:GLY:HA3	1:K:202:ARG:HG3	1.96	0.47
1:L:148:VAL:HG23	1:L:153:THR:HG22	1.96	0.47
1:N:50:LYS:HD3	1:N:96:GLU:O	2.15	0.47
1:N:211:ARG:NH2	2:N:302[A]:PSJ:O1	2.45	0.47
1:C:135:ARG:HG2	1:C:135:ARG:NH1	2.28	0.47
1:G:226:LYS:HG3	1:G:283:ILE:CD1	2.44	0.47
1:I:15:ASP:O	1:I:19:ILE:HG13	2.14	0.47
1:M:84:GLU:OE2	1:M:131:ARG:NE	2.44	0.47
1:J:92:ASP:O	1:J:96:GLU:HG3	2.15	0.47
1:M:239:PHE:CZ	1:M:241:SER:HB2	2.50	0.47
1:F:126:LYS:HB3	1:F:169:LEU:HD11	1.96	0.47
1:C:27:ARG:HD3	1:C:56:HIS:O	2.15	0.47
1:G:148:VAL:HG23	1:G:153:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:THR:O	1:L:198:ALA:C	2.58	0.47
1:E:163:LEU:O	1:E:167:GLU:HG2	2.15	0.47
1:C:134:ASP:O	1:C:137:SER:HB3	2.15	0.47
1:L:194:ILE:HD11	1:L:224:PHE:CE1	2.50	0.47
1:M:-1:GLY:HA3	7:M:438:HOH:O	2.15	0.47
1:M:225:PHE:CD2	1:M:279:LYS:HG2	2.50	0.47
1:A:63:SER:HA	1:A:103:CYS:O	2.14	0.47
1:I:62:ALA:CB	1:I:94:LEU:HD21	2.45	0.47
1:F:6:HIS:CE1	1:F:8:LEU:HD12	2.50	0.46
1:E:24:GLN:O	1:E:28:GLU:HG3	2.15	0.46
1:H:64:LEU:HD11	1:H:86:LEU:CD2	2.45	0.46
1:I:166:LEU:HD22	1:I:174:LEU:CD2	2.45	0.46
1:M:66:LEU:HD22	1:M:70:THR:HB	1.98	0.46
1:A:126:LYS:HB3	1:A:169:LEU:HD21	1.96	0.46
1:H:50:LYS:HD3	1:H:96:GLU:O	2.14	0.46
1:J:209:SER:HB3	1:J:219:VAL:HG23	1.97	0.46
1:P:8:LEU:HD22	1:P:251:LEU:HD23	1.97	0.46
1:M:164:ALA:O	1:M:168:GLU:HG3	2.15	0.46
1:P:1:MET:HE3	1:P:234:ASP:HA	1.95	0.46
1:C:75:GLU:CD	1:C:118:THR:HG21	2.41	0.46
1:E:20:ARG:CZ	1:E:48:THR:HG23	2.46	0.46
1:E:76:ASP:O	1:E:78:ALA:N	2.49	0.46
1:E:88:ASN:HD21	1:E:132:VAL:HG22	1.80	0.46
1:H:91:VAL:HG13	1:H:141:ILE:HD12	1.98	0.46
1:N:256:GLY:HA2	1:N:258:TRP:CZ2	2.51	0.46
1:P:70:THR:HB	1:P:83:GLY:HA2	1.98	0.46
1:F:3:ILE:HD12	1:F:277:ARG:NH1	2.30	0.46
1:C:-7:LEU:HB3	1:C:27:ARG:HG2	1.98	0.46
1:E:199:GLU:HG2	1:E:200:ALA:N	2.30	0.46
1:E:250:ASP:O	1:E:254:MET:HG3	2.16	0.46
1:A:211:ARG:HD3	7:A:430:HOH:O	2.16	0.46
1:C:175:GLY:HA3	1:C:202:ARG:HG3	1.98	0.46
1:J:240:GLU:OE2	3:J:303[B]:FUD:H3	2.16	0.46
1:E:107:TYR:O	1:E:125:SER:OG	2.28	0.45
1:J:262:TRP:CZ3	1:J:265:ASN:HB3	2.51	0.45
1:E:169:LEU:O	1:E:171:ARG:NH1	2.49	0.45
1:D:4:GLY:C	1:D:238:VAL:HG13	2.41	0.45
1:I:94:LEU:CD1	1:I:102:PHE:HB2	2.46	0.45
1:J:194:ILE:HD11	1:J:224:PHE:CD1	2.51	0.45
1:N:194:ILE:HD12	1:N:227:ALA:HB3	1.98	0.45
1:O:213:TYR:OH	1:O:267:GLU:OE1	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ARG:HD3	1:F:56:HIS:O	2.17	0.45
1:F:279:LYS:O	1:F:283:ILE:HD13	2.17	0.45
1:C:188:SER:OG	6:C:305:PEG:H22	2.17	0.45
1:J:152:GLU:OE1	3:J:303[B]:FUD:O1	2.25	0.45
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.82	0.45
1:I:250:ASP:O	1:I:254:MET:HG3	2.17	0.45
1:J:81:LYS:N	1:J:81:LYS:HD3	2.31	0.45
1:K:70:THR:HG21	1:K:86:LEU:CD1	2.46	0.45
1:K:239:PHE:CZ	1:K:241:SER:HB2	2.52	0.45
1:E:114:MET:O	1:F:253:ARG:HB3	2.16	0.45
1:C:16:ALA:HB1	1:C:20:ARG:NH1	2.32	0.45
1:O:25:LYS:HD3	1:O:25:LYS:HA	1.83	0.45
1:O:239:PHE:CZ	1:O:241:SER:HB2	2.52	0.45
1:P:92:ASP:OD2	1:P:135:ARG:NH2	2.50	0.45
1:P:262:TRP:CE2	1:P:268:LEU:HD22	2.51	0.45
1:B:8:LEU:HD21	1:B:248:ALA:HB2	1.98	0.45
1:H:63:SER:HA	1:H:103:CYS:O	2.16	0.45
1:H:81:LYS:HD2	1:H:81:LYS:HA	1.79	0.45
1:J:148:VAL:HG23	1:J:153:THR:HG22	1.98	0.45
1:B:197:THR:O	1:B:198:ALA:C	2.60	0.45
1:D:126:LYS:HB3	1:D:169:LEU:HD21	1.99	0.45
1:I:251:LEU:HD12	1:I:254:MET:HE3	1.99	0.45
1:N:64:LEU:HD11	1:N:86:LEU:CD2	2.46	0.45
1:I:166:LEU:HD22	1:I:174:LEU:HD23	1.99	0.44
1:J:136:ALA:HB1	1:J:141:ILE:HB	1.99	0.44
3:E:302[B]:FUD:H12	3:E:302[B]:FUD:H4	1.79	0.44
1:E:45:ASP:OD2	1:E:48:THR:OG1	2.31	0.44
1:J:146:GLU:OE1	2:J:302[A]:PSJ:H3	2.17	0.44
1:L:38:LEU:HD22	1:L:62:ALA:HB1	2.00	0.44
1:O:175:GLY:HA3	1:O:202:ARG:HG3	1.98	0.44
1:G:135:ARG:O	1:G:139:LEU:HD13	2.17	0.44
1:E:175:GLY:HA3	1:E:202:ARG:HG3	2.00	0.44
1:K:24:GLN:HG3	1:K:56:HIS:CE1	2.52	0.44
1:M:251:LEU:HD21	3:M:302[B]:FUD:O5	2.17	0.44
1:P:94:LEU:CD1	1:P:102:PHE:HB2	2.48	0.44
1:A:239:PHE:CZ	1:A:241:SER:HB2	2.52	0.44
1:C:225:PHE:CG	1:C:279:LYS:HG2	2.53	0.44
1:I:289:HIS:HD2	7:I:414:HOH:O	1.99	0.44
1:J:46:VAL:HG13	1:J:97:LEU:HD23	2.00	0.44
1:O:136:ALA:HB1	1:O:141:ILE:HB	2.00	0.44
1:O:211:ARG:HB2	7:O:404:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLY:HA3	1:F:110:MET:HE2	1.98	0.43
1:H:66:LEU:HB2	1:H:108:SER:O	2.17	0.43
1:J:8:LEU:HD13	1:J:251:LEU:HD23	1.99	0.43
1:O:13:HIS:HE1	1:O:249:PRO:HG3	1.83	0.43
1:E:239:PHE:CZ	1:E:241:SER:HB2	2.53	0.43
1:G:245:SER:OG	1:G:260:ASN:OD1	2.36	0.43
1:J:134:ASP:CG	1:J:171:ARG:HE	2.26	0.43
1:J:155:VAL:HG12	1:J:156:LEU:HG	2.00	0.43
2:M:301[A]:PSJ:H1	2:M:301[A]:PSJ:H4	1.96	0.43
1:P:8:LEU:CD2	1:P:251:LEU:HD23	2.48	0.43
1:C:148:VAL:HG23	1:C:153:THR:HG22	2.00	0.43
1:J:64:LEU:HD11	1:J:86:LEU:CD2	2.48	0.43
1:P:152:GLU:OE1	3:P:302[B]:FUD:O1	2.33	0.43
1:E:66:LEU:HD22	1:E:70:THR:HB	1.99	0.43
1:A:64:LEU:HD11	1:A:86:LEU:CD1	2.48	0.43
1:G:92:ASP:OD1	1:G:135:ARG:NH1	2.51	0.43
1:N:213:TYR:OH	1:N:267:GLU:OE1	2.25	0.43
1:O:184:ASN:HB2	1:O:219:VAL:HG22	2.00	0.43
1:I:70:THR:HG21	1:I:86:LEU:CD1	2.48	0.43
1:O:63:SER:HA	1:O:103:CYS:O	2.18	0.43
1:H:148:VAL:O	1:H:157:ASN:HA	2.19	0.43
1:J:46:VAL:HG13	1:J:97:LEU:CD2	2.47	0.43
1:J:63:SER:HA	1:J:103:CYS:O	2.18	0.43
1:P:4:GLY:C	1:P:238:VAL:HG13	2.44	0.43
1:C:166:LEU:CD2	1:C:174:LEU:HG	2.47	0.43
1:K:66:LEU:HD22	1:K:70:THR:HB	2.00	0.43
1:M:250:ASP:O	1:M:254:MET:HG3	2.19	0.43
1:N:283:ILE:HA	1:N:286:ILE:HD12	1.99	0.43
1:O:163:LEU:O	1:O:167:GLU:OE2	2.36	0.43
1:P:64:LEU:HD11	1:P:86:LEU:CD2	2.49	0.43
1:E:212:GLY:CA	1:E:261:LEU:HD23	2.49	0.43
1:A:21:TYR:O	1:A:25:LYS:HG2	2.19	0.43
1:I:92:ASP:O	1:I:96:GLU:HG3	2.18	0.43
1:M:255:LEU:HA	1:M:255:LEU:HD23	1.74	0.43
1:P:50:LYS:HD2	1:P:96:GLU:O	2.19	0.43
1:E:166:LEU:HD22	1:E:174:LEU:HD23	2.01	0.43
1:A:45:ASP:OD2	1:A:48:THR:OG1	2.32	0.43
1:I:27:ARG:NH1	1:I:57:GLY:O	2.51	0.43
1:O:225:PHE:CD2	1:O:279:LYS:HG2	2.54	0.43
2:O:301[A]:PSJ:H1	2:O:301[A]:PSJ:H4	1.88	0.43
1:F:197:THR:O	1:F:198:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:LEU:CD1	1:J:102:PHE:HB2	2.49	0.43
1:J:197:THR:O	1:J:198:ALA:C	2.60	0.43
1:H:261:LEU:HD22	7:H:421:HOH:O	2.19	0.42
1:I:71:ASP:OD1	1:I:73:SER:OG	2.34	0.42
1:K:62:ALA:CB	1:K:94:LEU:HD21	2.49	0.42
1:N:210:HIS:O	1:N:211:ARG:HB2	2.19	0.42
1:E:92:ASP:O	1:E:96:GLU:HG3	2.19	0.42
1:E:94:LEU:CD1	1:E:102:PHE:HB2	2.48	0.42
1:A:152:GLU:OE1	3:A:302[B]:FUD:O1	2.30	0.42
1:A:197:THR:O	1:A:198:ALA:C	2.61	0.42
1:B:146:GLU:OE1	2:B:301[A]:PSJ:H3	2.19	0.42
1:B:279:LYS:O	1:B:283:ILE:HD13	2.19	0.42
1:C:264:ASP:OD2	1:C:267:GLU:HB2	2.18	0.42
1:L:146:GLU:HA	1:L:177:HIS:HB3	2.01	0.42
1:M:46:VAL:HG11	1:M:96:GLU:HB3	2.01	0.42
1:D:45:ASP:OD2	1:D:48:THR:OG1	2.32	0.42
1:G:250:ASP:O	1:G:254:MET:HG3	2.19	0.42
1:J:64:LEU:HD11	1:J:86:LEU:HD22	2.01	0.42
1:J:190:MET:HG3	1:J:220:ASP:HB3	2.02	0.42
1:N:63:SER:HA	1:N:103:CYS:O	2.19	0.42
1:C:197:THR:O	1:C:198:ALA:C	2.62	0.42
1:M:192:SER:HB2	1:M:193:PRO:HD3	2.01	0.42
1:P:230:ARG:NH1	1:P:230:ARG:HG3	2.34	0.42
1:P:250:ASP:O	1:P:254:MET:HG3	2.18	0.42
1:F:244:SER:HB3	1:P:13:HIS:CD2	2.54	0.42
1:B:146:GLU:HA	1:B:177:HIS:HB3	2.01	0.42
1:H:288:LEU:HD22	1:H:288:LEU:H	1.85	0.42
1:J:88:ASN:ND2	1:J:135:ARG:HD3	2.35	0.42
1:C:239:PHE:CZ	1:C:241:SER:HB2	2.54	0.42
1:G:210:HIS:O	1:G:211:ARG:HB2	2.19	0.42
1:G:265:ASN:OD1	1:G:265:ASN:N	2.52	0.42
1:H:122:LEU:HD23	1:H:122:LEU:HA	1.82	0.42
1:I:45:ASP:OD2	1:I:48:THR:OG1	2.38	0.42
1:K:-6:GLU:HB3	1:K:-5:VAL:H	1.64	0.42
1:P:3:ILE:HD12	1:P:277:ARG:HG2	2.02	0.42
1:A:89:ARG:O	1:A:89:ARG:HD3	2.19	0.42
1:A:92:ASP:CG	1:A:135:ARG:HH21	2.25	0.42
1:N:66:LEU:HB2	1:N:108:SER:O	2.19	0.42
1:F:35:GLU:OE1	1:F:205:HIS:HE1	2.03	0.42
1:G:197:THR:O	1:G:198:ALA:C	2.62	0.42
1:I:160:ARG:HG3	1:I:160:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:-5:VAL:O	1:K:27:ARG:NH2	2.53	0.42
1:M:42:PHE:CD1	1:M:89:ARG:HG2	2.55	0.42
1:M:157:ASN:N	1:M:161:GLN:OE1	2.50	0.42
1:O:166:LEU:HD22	1:O:174:LEU:HG	2.01	0.42
1:E:110:MET:HE1	1:E:251:LEU:HD12	2.01	0.42
1:M:259:ARG:NH2	7:M:402:HOH:O	2.46	0.42
1:P:155:VAL:HG12	1:P:156:LEU:HG	2.01	0.42
1:C:66:LEU:HB2	1:C:108:SER:O	2.20	0.42
1:J:180:THR:HG1	1:J:207:GLY:H	1.68	0.42
1:E:66:LEU:HD11	1:E:87:LEU:HD11	2.01	0.41
1:D:190:MET:HG3	1:D:220:ASP:HB3	2.01	0.41
1:M:210:HIS:O	1:M:211:ARG:HB2	2.20	0.41
1:N:122:LEU:HD23	1:N:122:LEU:HA	1.77	0.41
1:O:42:PHE:CD1	1:O:89:ARG:HG2	2.55	0.41
1:E:197:THR:O	1:E:198:ALA:C	2.63	0.41
1:I:275:PHE:O	1:I:279:LYS:HB2	2.20	0.41
1:O:128:ALA:O	1:O:132:VAL:HG23	2.20	0.41
1:E:194:ILE:HD11	1:E:224:PHE:CE1	2.55	0.41
1:F:285:THR:HA	1:F:288:LEU:HD23	2.02	0.41
1:A:68:ASP:OD1	1:A:111:LYS:NZ	2.49	0.41
1:D:122:LEU:O	1:D:126:LYS:HG3	2.21	0.41
1:G:184:ASN:HB2	1:G:219:VAL:HG22	2.03	0.41
1:B:183:MET:HG2	1:B:187:GLU:HG3	2.02	0.41
1:N:183:MET:HG2	1:N:187:GLU:HG3	2.02	0.41
1:N:194:ILE:HD11	1:N:224:PHE:CD1	2.55	0.41
1:N:254:MET:HG2	7:N:416:HOH:O	2.20	0.41
1:B:222:ASP:OD1	1:B:279:LYS:HE3	2.20	0.41
1:H:194:ILE:HD12	1:H:227:ALA:HB3	2.02	0.41
1:I:64:LEU:HD13	1:I:102:PHE:HZ	1.85	0.41
1:M:279:LYS:HG3	1:M:283:ILE:HD13	2.02	0.41
1:N:155:VAL:HG12	1:N:156:LEU:HG	2.02	0.41
1:F:209:SER:HB3	1:F:219:VAL:HG23	2.01	0.41
1:F:211:ARG:NH2	2:F:301[A]:PSJ:O1	2.47	0.41
1:L:191:PHE:O	1:L:195:LEU:HG	2.20	0.41
1:P:89:ARG:O	1:P:93:VAL:HG23	2.20	0.41
1:P:211:ARG:HD2	1:P:242:PHE:HD2	1.86	0.41
1:M:184:ASN:HB2	1:M:219:VAL:HG22	2.02	0.41
1:F:148:VAL:HA	1:F:182:HIS:CG	2.55	0.41
1:C:148:VAL:HA	1:C:182:HIS:CG	2.56	0.41
1:I:62:ALA:HB2	1:I:94:LEU:HD21	2.03	0.41
1:J:27:ARG:HD2	1:J:58:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:284:LYS:HB3	1:O:284:LYS:HE3	1.81	0.41
1:P:148:VAL:O	1:P:157:ASN:HA	2.21	0.41
1:F:146:GLU:CD	1:F:177:HIS:CE1	2.99	0.41
1:F:166:LEU:HD22	1:F:174:LEU:HG	2.02	0.41
1:B:166:LEU:HD22	1:B:176:ILE:HG13	2.03	0.41
1:C:50:LYS:HB2	1:C:50:LYS:HE3	1.96	0.41
1:C:210:HIS:O	1:C:211:ARG:HB2	2.20	0.41
1:H:39:MET:CE	1:H:64:LEU:HA	2.50	0.41
1:H:42:PHE:CD1	1:H:89:ARG:HG2	2.56	0.41
1:H:135:ARG:HB3	1:H:135:ARG:NH1	2.36	0.41
1:K:148:VAL:HA	1:K:182:HIS:CG	2.55	0.41
1:N:146:GLU:HA	1:N:177:HIS:HB3	2.02	0.41
1:C:196:ASP:OD2	6:C:305:PEG:H32	2.21	0.41
1:L:125:SER:O	1:L:129:VAL:HG23	2.21	0.41
1:M:284:LYS:C	1:M:284:LYS:HD3	2.46	0.41
1:P:194:ILE:HD11	1:P:224:PHE:CE1	2.55	0.41
1:G:46:VAL:HG22	1:G:93:VAL:HG13	2.03	0.40
1:G:242:PHE:HA	7:G:428:HOH:O	2.21	0.40
1:I:197:THR:O	1:I:198:ALA:C	2.64	0.40
1:K:62:ALA:HB2	1:K:94:LEU:HD21	2.03	0.40
1:K:194:ILE:HD11	1:K:224:PHE:CE1	2.57	0.40
1:O:250:ASP:O	1:O:254:MET:HG3	2.21	0.40
1:I:39:MET:CE	1:I:254:MET:HE1	2.51	0.40
1:J:135:ARG:HG2	1:J:135:ARG:HH11	1.86	0.40
1:M:13:HIS:HE1	1:M:249:PRO:HG3	1.86	0.40
1:P:240:GLU:OE2	3:P:302[B]:FUD:H3	2.21	0.40
1:E:136:ALA:HB1	1:E:141:ILE:HB	2.04	0.40
1:F:211:ARG:HH22	3:F:302[B]:FUD:C1	2.33	0.40
1:B:262:TRP:CE2	1:B:268:LEU:HD22	2.56	0.40
1:B:262:TRP:CZ3	1:B:265:ASN:HB3	2.57	0.40
1:G:42:PHE:CD1	1:G:89:ARG:HG2	2.57	0.40
1:I:46:VAL:HG22	1:I:93:VAL:HG13	2.03	0.40
1:E:71:ASP:OD1	1:E:73:SER:OG	2.37	0.40
1:B:64:LEU:HD23	1:B:64:LEU:C	2.47	0.40
1:O:122:LEU:O	1:O:126:LYS:HG3	2.22	0.40

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	294/297 (99%)	280 (95%)	13 (4%)	1 (0%)	36	55
1	B	286/297 (96%)	276 (96%)	10 (4%)	0	100	100
1	C	295/297 (99%)	286 (97%)	8 (3%)	1 (0%)	36	55
1	D	287/297 (97%)	277 (96%)	10 (4%)	0	100	100
1	E	293/297 (99%)	276 (94%)	15 (5%)	2 (1%)	18	34
1	F	287/297 (97%)	278 (97%)	9 (3%)	0	100	100
1	G	294/297 (99%)	284 (97%)	9 (3%)	1 (0%)	36	55
1	H	287/297 (97%)	278 (97%)	9 (3%)	0	100	100
1	I	294/297 (99%)	282 (96%)	11 (4%)	1 (0%)	36	55
1	J	287/297 (97%)	275 (96%)	11 (4%)	1 (0%)	36	55
1	K	295/297 (99%)	280 (95%)	13 (4%)	2 (1%)	18	34
1	L	286/297 (96%)	273 (96%)	13 (4%)	0	100	100
1	M	294/297 (99%)	280 (95%)	14 (5%)	0	100	100
1	N	286/297 (96%)	276 (96%)	10 (4%)	0	100	100
1	O	294/297 (99%)	285 (97%)	8 (3%)	1 (0%)	36	55
1	P	287/297 (97%)	277 (96%)	10 (4%)	0	100	100
All	All	4646/4752 (98%)	4463 (96%)	173 (4%)	10 (0%)	43	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	77	PRO
1	E	198	ALA
1	A	198	ALA
1	C	198	ALA
1	I	198	ALA
1	K	-6	GLU

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Mol	Chain	Res	Type
1	K	198	ALA
1	O	198	ALA
1	G	198	ALA
1	J	198	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/238 (100%)	233 (98%)	4 (2%)	53	78
1	B	230/238 (97%)	226 (98%)	4 (2%)	53	78
1	C	238/238 (100%)	231 (97%)	7 (3%)	37	65
1	D	231/238 (97%)	228 (99%)	3 (1%)	61	82
1	E	236/238 (99%)	233 (99%)	3 (1%)	61	82
1	F	231/238 (97%)	224 (97%)	7 (3%)	36	64
1	G	237/238 (100%)	235 (99%)	2 (1%)	73	88
1	H	231/238 (97%)	225 (97%)	6 (3%)	40	68
1	I	237/238 (100%)	233 (98%)	4 (2%)	53	78
1	J	231/238 (97%)	228 (99%)	3 (1%)	61	82
1	K	238/238 (100%)	229 (96%)	9 (4%)	29	56
1	L	230/238 (97%)	228 (99%)	2 (1%)	70	87
1	M	237/238 (100%)	232 (98%)	5 (2%)	47	74
1	N	230/238 (97%)	229 (100%)	1 (0%)	84	93
1	O	237/238 (100%)	230 (97%)	7 (3%)	36	64
1	P	231/238 (97%)	227 (98%)	4 (2%)	53	78
All	All	3742/3808 (98%)	3671 (98%)	71 (2%)	50	76

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	LEU
1	E	100	THR
1	E	118	THR
1	F	8	LEU
1	F	64	LEU
1	F	167	GLU
1	F	205	HIS
1	F	287	GLU
1	F	288	LEU
1	F	289	HIS
1	A	87	LEU
1	A	106	ILE
1	A	195	LEU
1	A	283	ILE
1	B	8	LEU
1	B	64	LEU
1	B	160	ARG
1	B	288	LEU
1	C	-7	LEU
1	C	-6	GLU
1	C	8	LEU
1	C	81	LYS
1	C	166	LEU
1	C	167	GLU
1	C	211	ARG
1	D	211	ARG
1	D	261	LEU
1	D	288	LEU
1	G	85	GLU
1	G	222	ASP
1	H	8	LEU
1	H	85	GLU
1	H	211	ARG
1	H	283	ILE
1	H	288	LEU
1	H	289	HIS
1	I	118	THR
1	I	166	LEU
1	I	195	LEU
1	I	283	ILE
1	J	8	LEU
1	J	211	ARG
1	J	288	LEU

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Mol	Chain	Res	Type
1	K	-7	LEU
1	K	-6	GLU
1	K	8	LEU
1	K	28	GLU
1	K	118	THR
1	K	166	LEU
1	K	195	LEU
1	K	261	LEU
1	K	283	ILE
1	L	8	LEU
1	L	211	ARG
1	M	8	LEU
1	M	222	ASP
1	M	245	SER
1	M	279	LYS
1	M	283	ILE
1	N	8	LEU
1	O	8	LEU
1	O	87	LEU
1	O	91	VAL
1	O	167	GLU
1	O	195	LEU
1	O	211	ARG
1	O	245	SER
1	P	204	VAL
1	P	261	LEU
1	P	288	LEU
1	P	289	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	-2	GLN
1	E	88	ASN
1	E	260	ASN
1	F	142	ASN
1	F	205	HIS
1	A	289	HIS
1	B	24	GLN
1	B	142	ASN
1	B	205	HIS
1	C	13	HIS

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Mol	Chain	Res	Type
1	C	47	GLN
1	I	24	GLN
1	I	289	HIS
1	J	88	ASN
1	J	142	ASN
1	J	205	HIS
1	K	142	ASN
1	K	184	ASN
1	K	289	HIS
1	L	142	ASN
1	L	184	ASN
1	M	13	HIS
1	M	142	ASN
1	N	170	ASN
1	O	13	HIS
1	O	184	ASN
1	P	184	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 57 ligands modelled in this entry, 24 are monoatomic - leaving 33 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	$\#\|Z\|>2$
2	PSJ	M	301[A]	4	11,11,11	0.40	0	10,14,14	0.45	0
3	FUD	I	302[B]	4	11,11,11	0.47	0	10,14,14	0.61	0
3	FUD	H	302[B]	4	11,11,11	0.33	0	10,14,14	0.59	0
3	FUD	J	303[B]	4	11,11,11	0.33	0	10,14,14	0.56	0
2	PSJ	F	301[A]	4	11,11,11	0.25	0	10,14,14	0.72	0
2	PSJ	C	301[A]	4	11,11,11	0.46	0	10,14,14	0.73	0
3	FUD	M	302[B]	4	11,11,11	0.45	0	10,14,14	0.46	0
2	PSJ	L	301[A]	4	11,11,11	0.37	0	10,14,14	0.52	0
3	FUD	L	302[B]	4	11,11,11	0.39	0	10,14,14	0.91	0
2	PSJ	G	301[A]	4	11,11,11	0.37	0	10,14,14	0.58	0
2	PSJ	J	302[A]	4	11,11,11	0.29	0	10,14,14	0.60	0
3	FUD	G	302[B]	4	11,11,11	0.49	0	10,14,14	0.79	0
2	PSJ	H	301[A]	4	11,11,11	0.44	0	10,14,14	0.66	0
2	PSJ	K	301[A]	4	11,11,11	0.53	0	10,14,14	0.87	0
2	PSJ	B	301[A]	4	11,11,11	0.38	0	10,14,14	0.64	0
3	FUD	O	302[B]	4	11,11,11	0.53	0	10,14,14	1.02	0
2	PSJ	E	301[A]	4	11,11,11	0.44	0	10,14,14	0.64	0
3	FUD	A	302[B]	4	11,11,11	0.56	0	10,14,14	0.83	0
3	FUD	F	302[B]	4	11,11,11	0.29	0	10,14,14	0.39	0
3	FUD	K	302[B]	4	11,11,11	0.56	0	10,14,14	0.68	0
2	PSJ	O	301[A]	4	11,11,11	0.55	0	10,14,14	0.51	0
3	FUD	E	302[B]	4	11,11,11	0.42	0	10,14,14	0.63	0
2	PSJ	A	301[A]	4	11,11,11	0.51	0	10,14,14	0.73	0
2	PSJ	D	301[A]	4	11,11,11	0.39	0	10,14,14	0.50	0
3	FUD	B	302[B]	4	11,11,11	0.41	0	10,14,14	0.57	0
2	PSJ	N	302[A]	4	11,11,11	0.42	0	10,14,14	0.65	0
3	FUD	D	302[B]	4	11,11,11	0.37	0	10,14,14	0.52	0
3	FUD	P	302[B]	4	11,11,11	0.37	0	10,14,14	0.52	0
3	FUD	N	303[B]	4	11,11,11	0.42	0	10,14,14	0.96	0
2	PSJ	P	301[A]	4	11,11,11	0.42	0	10,14,14	0.55	0
2	PSJ	I	301[A]	4	11,11,11	0.48	0	10,14,14	0.83	1 (10%)
6	PEG	C	305	-	6,6,6	0.40	0	5,5,5	0.29	0
3	FUD	C	302[B]	4	11,11,11	0.41	0	10,14,14	0.59	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
2	PSJ	M	301[A]	4	-	10/16/16/16	-
3	FUD	I	302[B]	4	-	0/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUD	H	302[B]	4	-	4/16/16/16	-
3	FUD	J	303[B]	4	-	9/16/16/16	-
2	PSJ	F	301[A]	4	-	10/16/16/16	-
2	PSJ	C	301[A]	4	-	8/16/16/16	-
3	FUD	M	302[B]	4	-	4/16/16/16	-
2	PSJ	L	301[A]	4	-	10/16/16/16	-
3	FUD	L	302[B]	4	-	2/16/16/16	-
2	PSJ	G	301[A]	4	-	10/16/16/16	-
2	PSJ	J	302[A]	4	-	6/16/16/16	-
3	FUD	G	302[B]	4	-	4/16/16/16	-
2	PSJ	H	301[A]	4	-	10/16/16/16	-
2	PSJ	K	301[A]	4	-	8/16/16/16	-
2	PSJ	B	301[A]	4	-	7/16/16/16	-
3	FUD	O	302[B]	4	-	2/16/16/16	-
2	PSJ	E	301[A]	4	-	10/16/16/16	-
3	FUD	A	302[B]	4	-	4/16/16/16	-
3	FUD	F	302[B]	4	-	5/16/16/16	-
3	FUD	K	302[B]	4	-	0/16/16/16	-
2	PSJ	O	301[A]	4	-	10/16/16/16	-
3	FUD	E	302[B]	4	-	10/16/16/16	-
2	PSJ	A	301[A]	4	-	8/16/16/16	-
2	PSJ	D	301[A]	4	-	10/16/16/16	-
3	FUD	B	302[B]	4	-	5/16/16/16	-
2	PSJ	N	302[A]	4	-	10/16/16/16	-
3	FUD	D	302[B]	4	-	6/16/16/16	-
3	FUD	P	302[B]	4	-	6/16/16/16	-
3	FUD	N	303[B]	4	-	2/16/16/16	-
2	PSJ	P	301[A]	4	-	10/16/16/16	-
2	PSJ	I	301[A]	4	-	10/16/16/16	-
6	PEG	C	305	-	-	3/4/4/4	-
3	FUD	C	302[B]	4	-	4/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301[A]	PSJ	O1-C1-C2	-2.18	106.96	112.73

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301[A]	PSJ	C1-C2-C3-C4
2	E	301[A]	PSJ	O2-C2-C3-C4
2	E	301[A]	PSJ	C2-C3-C4-C5
2	E	301[A]	PSJ	O3-C3-C4-C5
2	E	301[A]	PSJ	C4-C5-C6-O6
2	E	301[A]	PSJ	O5-C5-C6-O6
2	F	301[A]	PSJ	C1-C2-C3-C4
2	F	301[A]	PSJ	O2-C2-C3-C4
2	F	301[A]	PSJ	C2-C3-C4-O4
2	F	301[A]	PSJ	C2-C3-C4-C5
2	F	301[A]	PSJ	O3-C3-C4-O4
2	F	301[A]	PSJ	O3-C3-C4-C5
2	A	301[A]	PSJ	C1-C2-C3-C4
2	A	301[A]	PSJ	O2-C2-C3-C4
2	A	301[A]	PSJ	C2-C3-C4-O4
2	A	301[A]	PSJ	C2-C3-C4-C5
2	A	301[A]	PSJ	O3-C3-C4-O4
2	A	301[A]	PSJ	O3-C3-C4-C5
2	B	301[A]	PSJ	C1-C2-C3-C4
2	B	301[A]	PSJ	O2-C2-C3-C4
2	B	301[A]	PSJ	C2-C3-C4-O4
2	B	301[A]	PSJ	C2-C3-C4-C5
2	B	301[A]	PSJ	O3-C3-C4-O4
2	B	301[A]	PSJ	O3-C3-C4-C5
2	C	301[A]	PSJ	C1-C2-C3-C4
2	C	301[A]	PSJ	O2-C2-C3-C4
2	C	301[A]	PSJ	C2-C3-C4-O4
2	C	301[A]	PSJ	C2-C3-C4-C5
2	C	301[A]	PSJ	O3-C3-C4-O4
2	C	301[A]	PSJ	O3-C3-C4-C5
2	D	301[A]	PSJ	C1-C2-C3-C4
2	D	301[A]	PSJ	O2-C2-C3-C4
2	D	301[A]	PSJ	C2-C3-C4-O4
2	D	301[A]	PSJ	C2-C3-C4-C5
2	D	301[A]	PSJ	O3-C3-C4-O4
2	D	301[A]	PSJ	O3-C3-C4-C5
2	D	301[A]	PSJ	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	301[A]	PSJ	O5-C5-C6-O6
2	G	301[A]	PSJ	C1-C2-C3-C4
2	G	301[A]	PSJ	O2-C2-C3-C4
2	G	301[A]	PSJ	C2-C3-C4-O4
2	G	301[A]	PSJ	C2-C3-C4-C5
2	G	301[A]	PSJ	O3-C3-C4-O4
2	G	301[A]	PSJ	O3-C3-C4-C5
2	G	301[A]	PSJ	O4-C4-C5-C6
2	H	301[A]	PSJ	C1-C2-C3-C4
2	H	301[A]	PSJ	O2-C2-C3-C4
2	H	301[A]	PSJ	C2-C3-C4-O4
2	H	301[A]	PSJ	C2-C3-C4-C5
2	H	301[A]	PSJ	O3-C3-C4-O4
2	H	301[A]	PSJ	O3-C3-C4-C5
2	H	301[A]	PSJ	C4-C5-C6-O6
2	H	301[A]	PSJ	O5-C5-C6-O6
2	I	301[A]	PSJ	O1-C1-C2-C3
2	I	301[A]	PSJ	C1-C2-C3-C4
2	I	301[A]	PSJ	O2-C2-C3-C4
2	I	301[A]	PSJ	C2-C3-C4-O4
2	I	301[A]	PSJ	C2-C3-C4-C5
2	I	301[A]	PSJ	O3-C3-C4-O4
2	I	301[A]	PSJ	O3-C3-C4-C5
2	J	302[A]	PSJ	C1-C2-C3-C4
2	J	302[A]	PSJ	O2-C2-C3-C4
2	J	302[A]	PSJ	C2-C3-C4-O4
2	J	302[A]	PSJ	C2-C3-C4-C5
2	J	302[A]	PSJ	O3-C3-C4-O4
2	J	302[A]	PSJ	O3-C3-C4-C5
2	K	301[A]	PSJ	O2-C2-C3-C4
2	K	301[A]	PSJ	C2-C3-C4-O4
2	K	301[A]	PSJ	C2-C3-C4-C5
2	K	301[A]	PSJ	O3-C3-C4-O4
2	K	301[A]	PSJ	O3-C3-C4-C5
2	L	301[A]	PSJ	C1-C2-C3-C4
2	L	301[A]	PSJ	O2-C2-C3-C4
2	L	301[A]	PSJ	C2-C3-C4-O4
2	L	301[A]	PSJ	C2-C3-C4-C5
2	L	301[A]	PSJ	O3-C3-C4-O4
2	L	301[A]	PSJ	O3-C3-C4-C5
2	M	301[A]	PSJ	C1-C2-C3-C4
2	M	301[A]	PSJ	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	M	301[A]	PSJ	C2-C3-C4-O4
2	M	301[A]	PSJ	C2-C3-C4-C5
2	M	301[A]	PSJ	O3-C3-C4-O4
2	M	301[A]	PSJ	O3-C3-C4-C5
2	N	302[A]	PSJ	C1-C2-C3-O3
2	N	302[A]	PSJ	C1-C2-C3-C4
2	N	302[A]	PSJ	O2-C2-C3-C4
2	N	302[A]	PSJ	C2-C3-C4-O4
2	N	302[A]	PSJ	C2-C3-C4-C5
2	N	302[A]	PSJ	O3-C3-C4-O4
2	N	302[A]	PSJ	O3-C3-C4-C5
2	N	302[A]	PSJ	C4-C5-C6-O6
2	N	302[A]	PSJ	O5-C5-C6-O6
2	O	301[A]	PSJ	C1-C2-C3-C4
2	O	301[A]	PSJ	O2-C2-C3-C4
2	O	301[A]	PSJ	C2-C3-C4-O4
2	O	301[A]	PSJ	C2-C3-C4-C5
2	O	301[A]	PSJ	O3-C3-C4-O4
2	O	301[A]	PSJ	O3-C3-C4-C5
2	P	301[A]	PSJ	C1-C2-C3-C4
2	P	301[A]	PSJ	O2-C2-C3-C4
2	P	301[A]	PSJ	C2-C3-C4-O4
2	P	301[A]	PSJ	C2-C3-C4-C5
2	P	301[A]	PSJ	O3-C3-C4-O4
2	P	301[A]	PSJ	O3-C3-C4-C5
2	P	301[A]	PSJ	C4-C5-C6-O6
2	P	301[A]	PSJ	O5-C5-C6-O6
3	E	302[B]	FUD	C1-C2-C3-C4
3	E	302[B]	FUD	O2-C2-C3-C4
3	E	302[B]	FUD	O2-C2-C3-O3
3	F	302[B]	FUD	C1-C2-C3-C4
3	F	302[B]	FUD	O2-C2-C3-C4
3	A	302[B]	FUD	C1-C2-C3-C4
3	A	302[B]	FUD	O2-C2-C3-C4
3	C	302[B]	FUD	C1-C2-C3-C4
3	C	302[B]	FUD	O2-C2-C3-C4
3	D	302[B]	FUD	C2-C3-C4-C5
3	D	302[B]	FUD	C2-C3-C4-O4
3	D	302[B]	FUD	O3-C3-C4-C5
3	D	302[B]	FUD	O3-C3-C4-O4
3	G	302[B]	FUD	C1-C2-C3-C4
3	G	302[B]	FUD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	G	302[B]	FUD	O2-C2-C3-O3
3	H	302[B]	FUD	C1-C2-C3-C4
3	H	302[B]	FUD	O2-C2-C3-C4
3	H	302[B]	FUD	O2-C2-C3-O3
3	J	303[B]	FUD	C1-C2-C3-C4
3	J	303[B]	FUD	O2-C2-C3-C4
3	L	302[B]	FUD	C1-C2-C3-C4
3	L	302[B]	FUD	O2-C2-C3-C4
3	M	302[B]	FUD	C1-C2-C3-C4
3	M	302[B]	FUD	O2-C2-C3-C4
3	N	303[B]	FUD	O2-C2-C3-C4
3	O	302[B]	FUD	O1-C1-C2-O2
3	P	302[B]	FUD	O1-C1-C2-O2
3	P	302[B]	FUD	C1-C2-C3-C4
3	P	302[B]	FUD	O2-C2-C3-C4
3	B	302[B]	FUD	C3-C4-C5-O5
3	B	302[B]	FUD	O4-C4-C5-C6
2	G	301[A]	PSJ	O4-C4-C5-O5
3	B	302[B]	FUD	O4-C4-C5-O5
2	G	301[A]	PSJ	C3-C4-C5-O5
2	M	301[A]	PSJ	C3-C4-C5-O5
3	J	303[B]	FUD	O4-C4-C5-C6
2	G	301[A]	PSJ	C3-C4-C5-C6
2	M	301[A]	PSJ	C3-C4-C5-C6
2	O	301[A]	PSJ	C3-C4-C5-C6
3	B	302[B]	FUD	C3-C4-C5-C6
3	J	303[B]	FUD	C3-C4-C5-C6
3	J	303[B]	FUD	O4-C4-C5-O5
2	E	301[A]	PSJ	O3-C3-C4-O4
3	E	302[B]	FUD	O3-C3-C4-C5
2	M	301[A]	PSJ	O4-C4-C5-C6
2	O	301[A]	PSJ	O4-C4-C5-C6
2	M	301[A]	PSJ	O4-C4-C5-O5
2	O	301[A]	PSJ	C3-C4-C5-O5
2	I	301[A]	PSJ	O1-C1-C2-O2
6	C	305	PEG	O1-C1-C2-O2
2	O	301[A]	PSJ	O4-C4-C5-O5
2	L	301[A]	PSJ	O4-C4-C5-C6
3	J	303[B]	FUD	C3-C4-C5-O5
2	E	301[A]	PSJ	C2-C3-C4-O4
2	L	301[A]	PSJ	C3-C4-C5-C6
2	E	301[A]	PSJ	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	F	301[A]	PSJ	O4-C4-C5-C6
3	E	302[B]	FUD	O3-C3-C4-O4
3	J	303[B]	FUD	O3-C3-C4-O4
2	L	301[A]	PSJ	O4-C4-C5-O5
2	H	301[A]	PSJ	C1-C2-C3-O3
2	P	301[A]	PSJ	C1-C2-C3-O3
3	F	302[B]	FUD	C1-C2-C3-O3
3	A	302[B]	FUD	C1-C2-C3-O3
3	C	302[B]	FUD	C1-C2-C3-O3
3	G	302[B]	FUD	C1-C2-C3-O3
3	H	302[B]	FUD	C1-C2-C3-O3
3	J	303[B]	FUD	C1-C2-C3-O3
3	M	302[B]	FUD	C1-C2-C3-O3
3	P	302[B]	FUD	C1-C2-C3-O3
2	L	301[A]	PSJ	C3-C4-C5-O5
2	C	301[A]	PSJ	O2-C2-C3-O3
2	D	301[A]	PSJ	O2-C2-C3-O3
2	H	301[A]	PSJ	O2-C2-C3-O3
2	I	301[A]	PSJ	O2-C2-C3-O3
2	N	302[A]	PSJ	O2-C2-C3-O3
2	P	301[A]	PSJ	O2-C2-C3-O3
3	F	302[B]	FUD	O2-C2-C3-O3
3	A	302[B]	FUD	O2-C2-C3-O3
3	C	302[B]	FUD	O2-C2-C3-O3
3	J	303[B]	FUD	O2-C2-C3-O3
3	M	302[B]	FUD	O2-C2-C3-O3
3	P	302[B]	FUD	O2-C2-C3-O3
2	F	301[A]	PSJ	C3-C4-C5-C6
2	K	301[A]	PSJ	C1-C2-C3-C4
3	N	303[B]	FUD	C1-C2-C3-C4
3	D	302[B]	FUD	O5-C5-C6-O6
2	F	301[A]	PSJ	O4-C4-C5-O5
2	F	301[A]	PSJ	C3-C4-C5-O5
2	A	301[A]	PSJ	O1-C1-C2-O2
2	K	301[A]	PSJ	O1-C1-C2-O2
2	E	301[A]	PSJ	O1-C1-C2-C3
2	A	301[A]	PSJ	O1-C1-C2-C3
2	K	301[A]	PSJ	O1-C1-C2-C3
3	O	302[B]	FUD	O1-C1-C2-C3
3	P	302[B]	FUD	O1-C1-C2-C3
3	E	302[B]	FUD	C2-C3-C4-O4
3	E	302[B]	FUD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	302[B]	FUD	O5-C5-C6-O6
2	C	301[A]	PSJ	O4-C4-C5-C6
3	F	302[B]	FUD	C3-C4-C5-O5
2	D	301[A]	PSJ	C1-C2-C3-O3
2	I	301[A]	PSJ	C1-C2-C3-O3
3	E	302[B]	FUD	C1-C2-C3-O3
6	C	305	PEG	C1-C2-O2-C3
6	C	305	PEG	O2-C3-C4-O4
3	E	302[B]	FUD	C4-C5-C6-O6
2	B	301[A]	PSJ	O4-C4-C5-C6
3	D	302[B]	FUD	O2-C2-C3-C4
3	E	302[B]	FUD	O5-C5-C6-O6

There are no ring outliers.

27 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301[A]	PSJ	3	0
3	H	302[B]	FUD	2	0
3	J	303[B]	FUD	2	0
2	F	301[A]	PSJ	2	0
2	C	301[A]	PSJ	1	0
3	M	302[B]	FUD	1	0
2	L	301[A]	PSJ	1	0
3	L	302[B]	FUD	1	0
2	G	301[A]	PSJ	1	0
2	J	302[A]	PSJ	1	0
2	H	301[A]	PSJ	1	0
2	K	301[A]	PSJ	1	0
2	B	301[A]	PSJ	1	0
3	O	302[B]	FUD	1	0
3	A	302[B]	FUD	1	0
3	F	302[B]	FUD	1	0
2	O	301[A]	PSJ	2	0
3	E	302[B]	FUD	1	0
2	A	301[A]	PSJ	1	0
2	D	301[A]	PSJ	1	0
2	N	302[A]	PSJ	2	0
3	P	302[B]	FUD	2	0
3	N	303[B]	FUD	1	0
2	P	301[A]	PSJ	2	0
2	I	301[A]	PSJ	1	0

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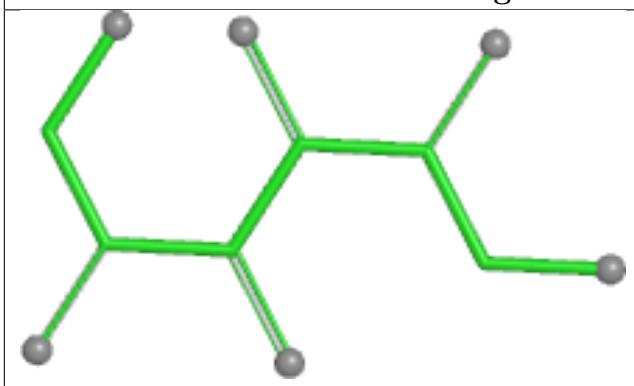
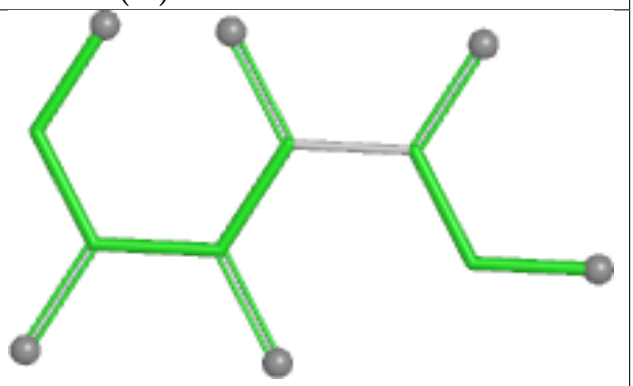
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	305	PEG	5	0
3	C	302[B]	FUD	1	0

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.

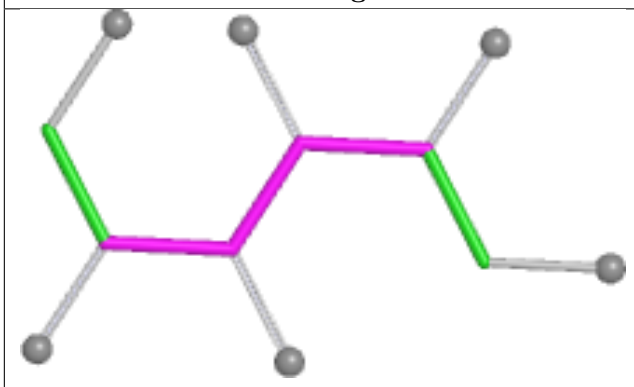
Ligand PSJ M 301 (A)



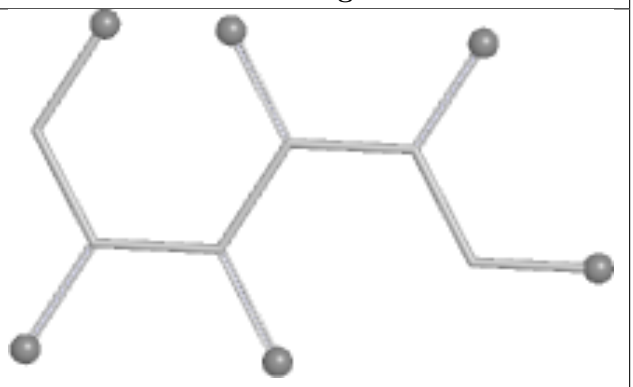
Bond lengths



Bond angles

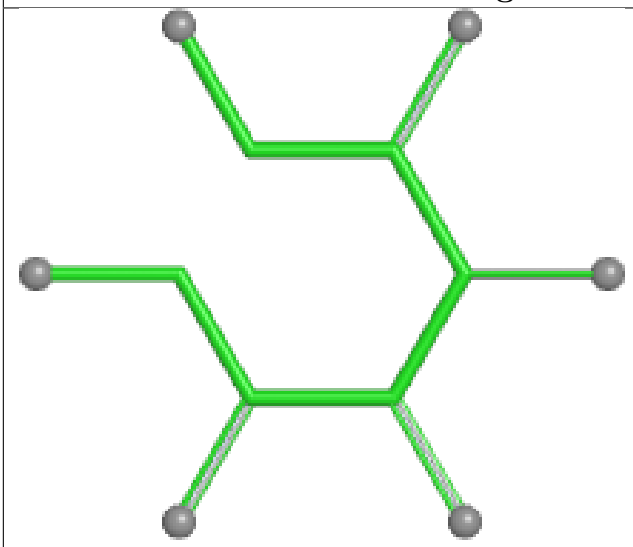


Torsions

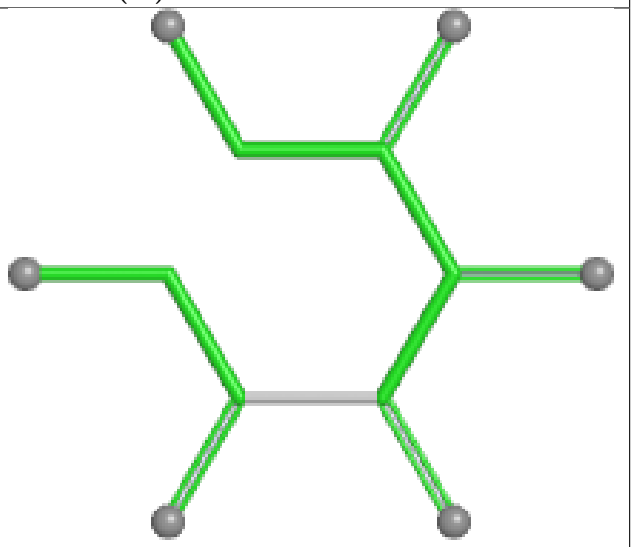


Rings

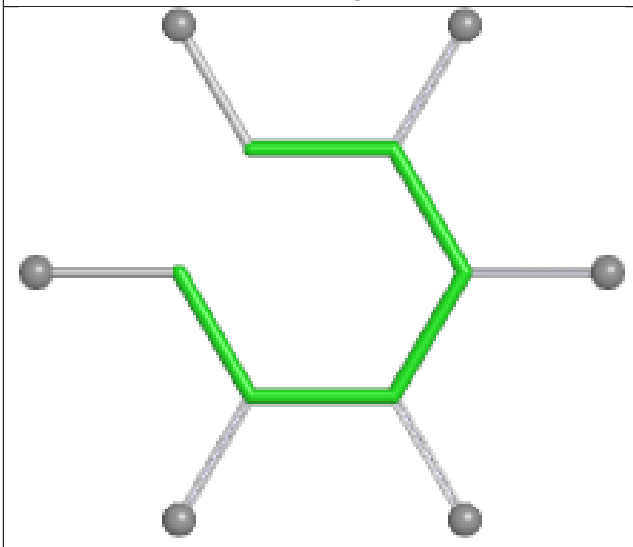
Ligand FUD I 302 (B)



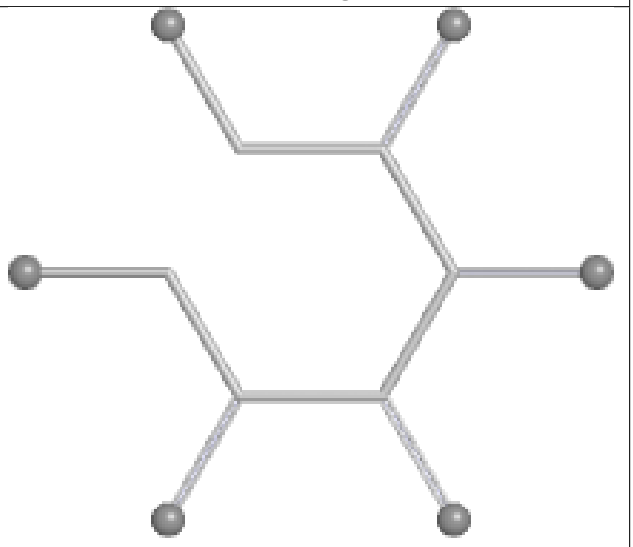
Bond lengths



Bond angles

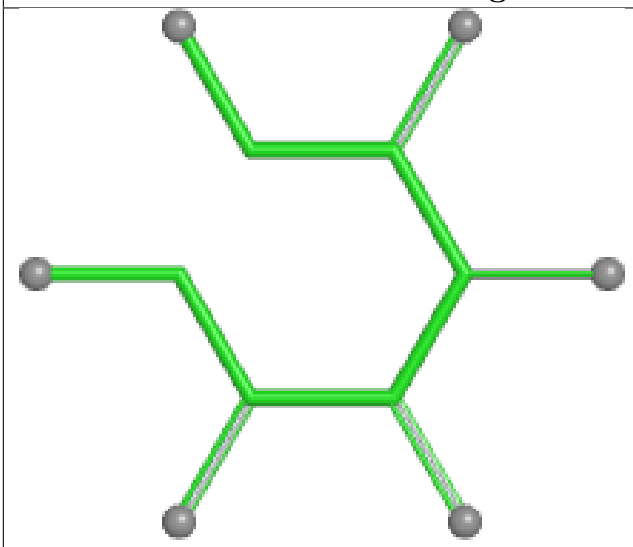


Torsions

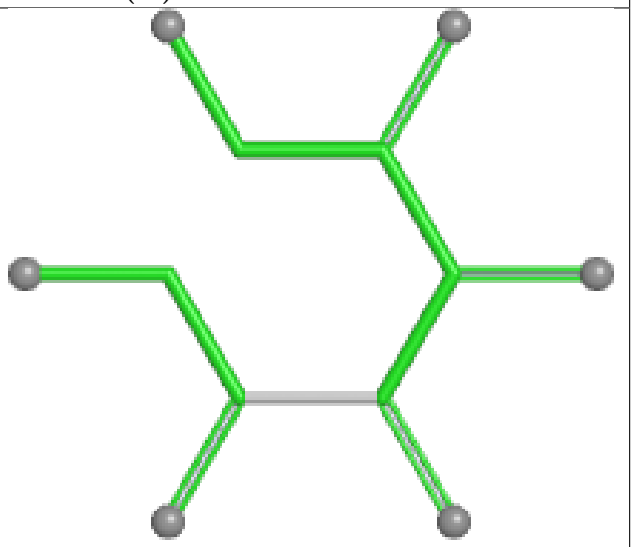


Rings

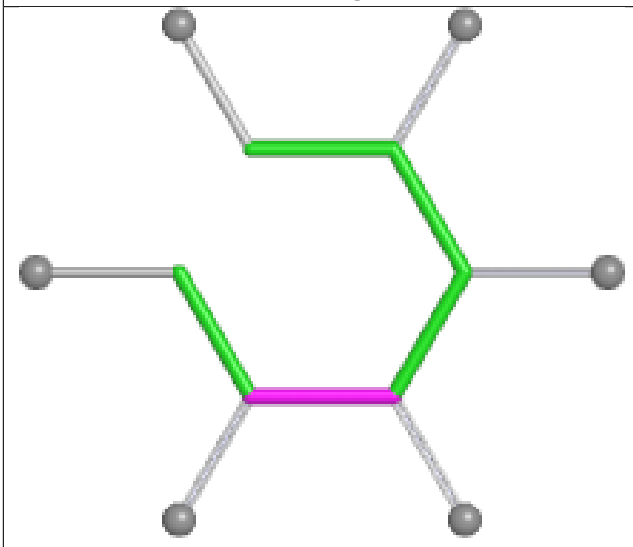
Ligand FUD H 302 (B)



Bond lengths



Bond angles



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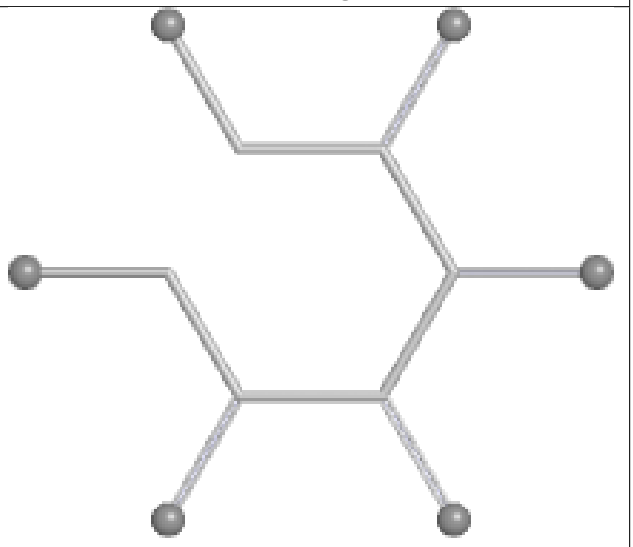
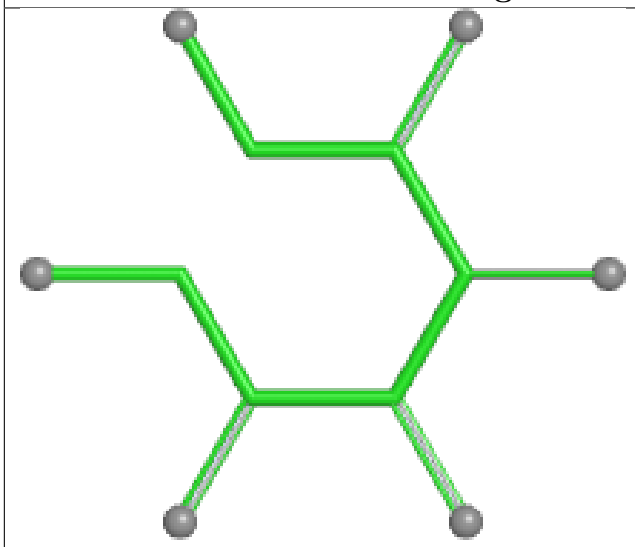


Rings

Ligand FUD J 303 (B)



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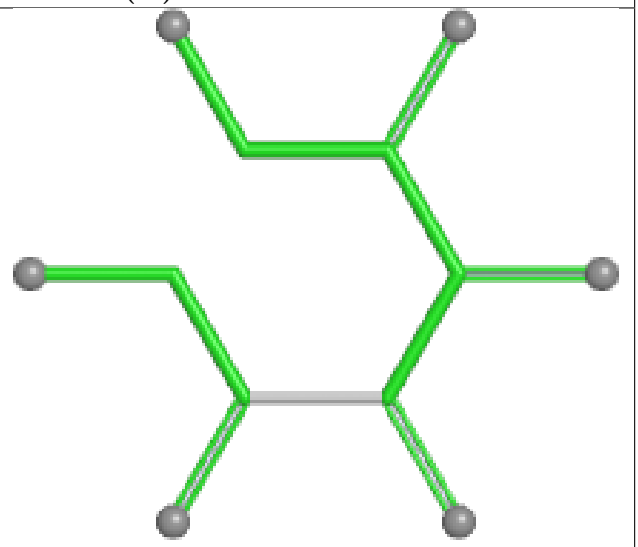
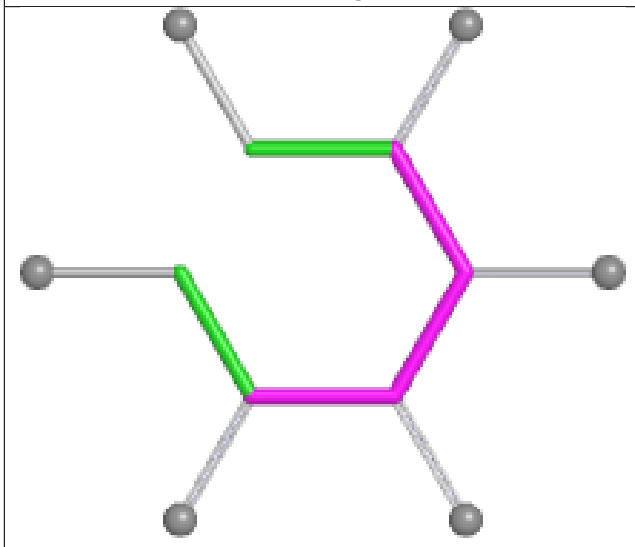


Bond angles



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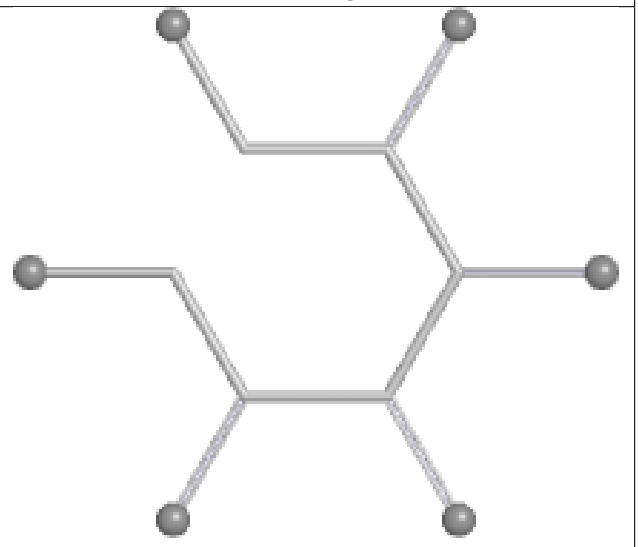
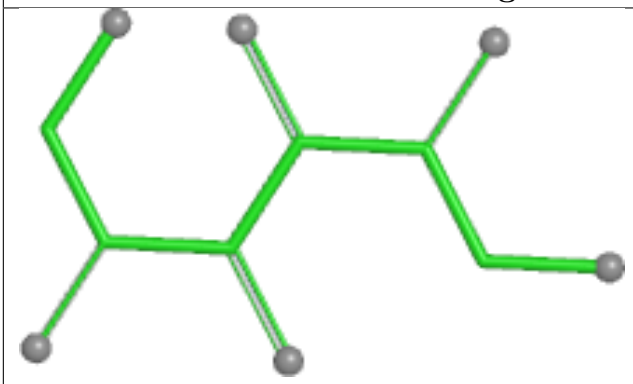


Rings

Ligand PSJ F 301 (A)



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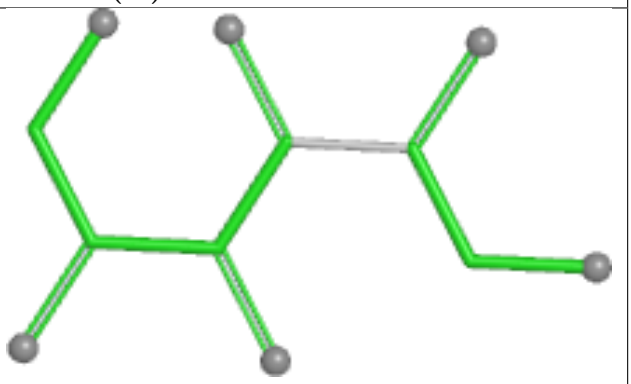
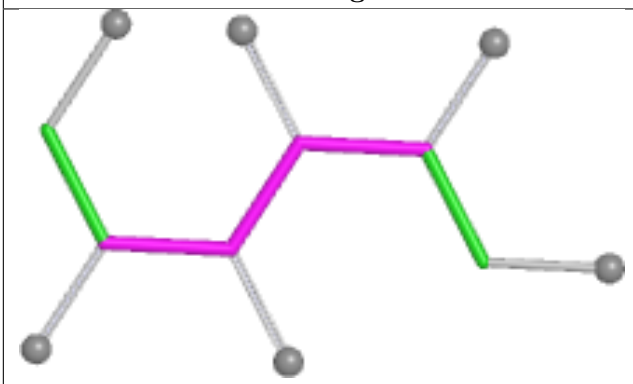


Bond angles



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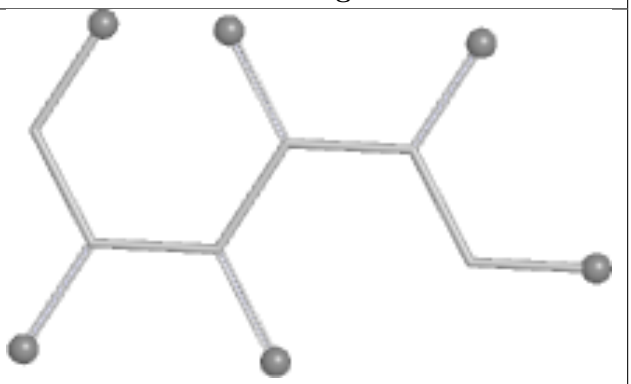
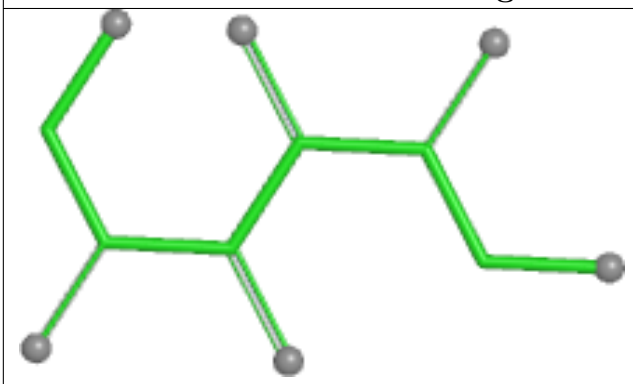


Rings

Ligand PSJ C 301 (A)



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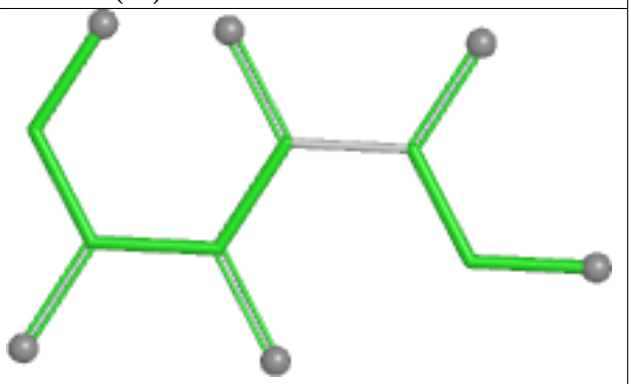
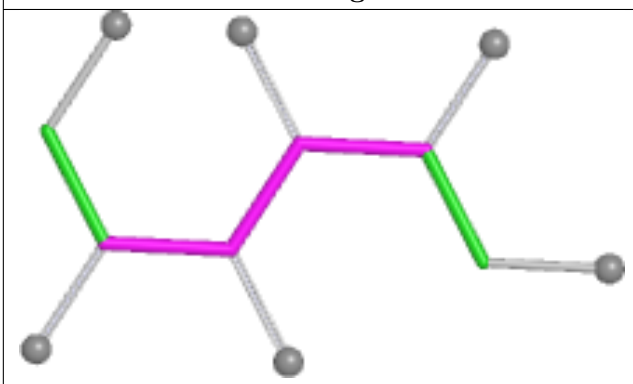


Bond angles



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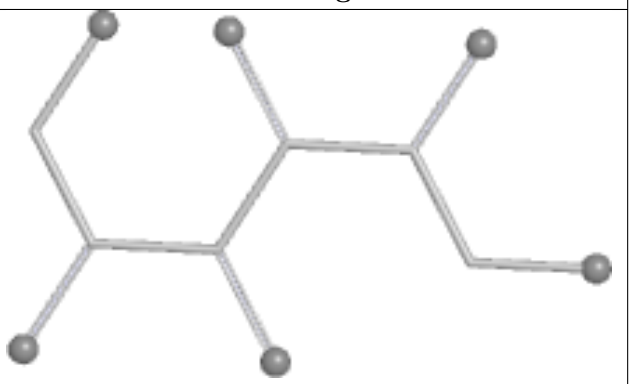
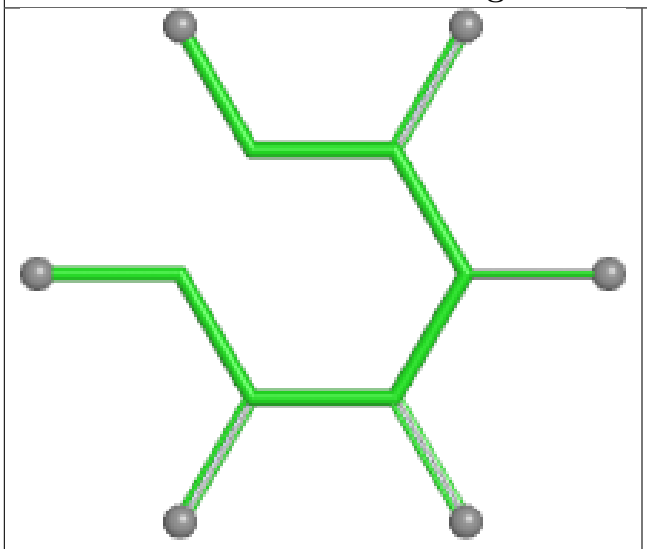


Rings

Ligand FUD M 302 (B)



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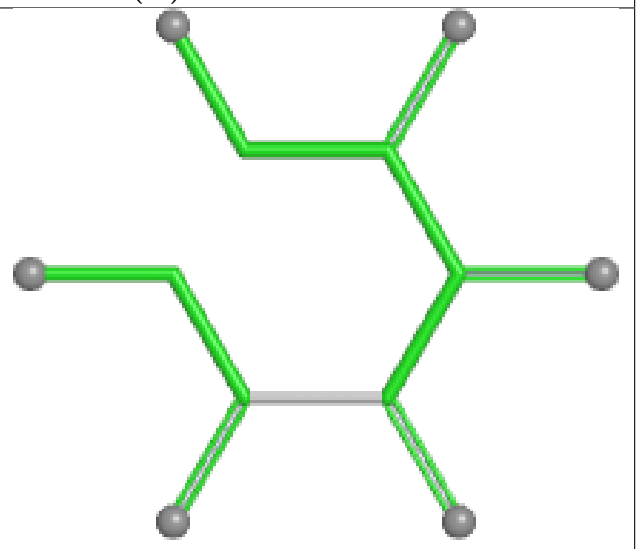
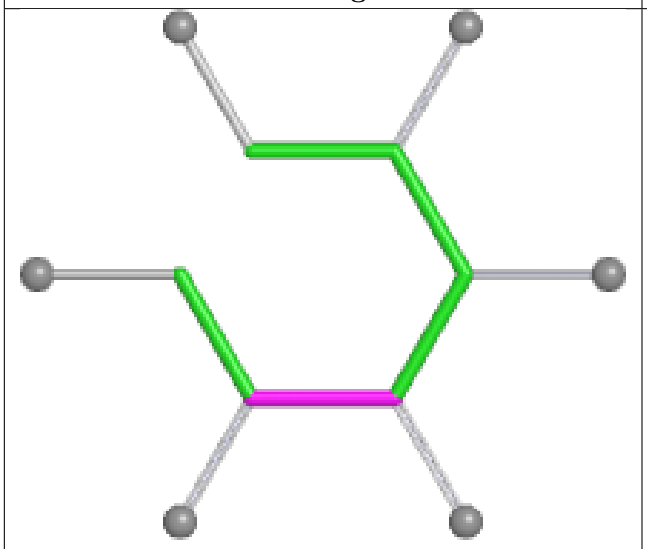


Bond angles



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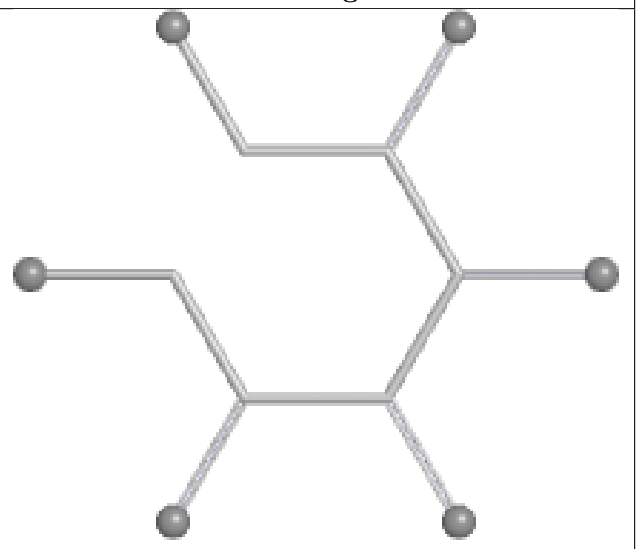
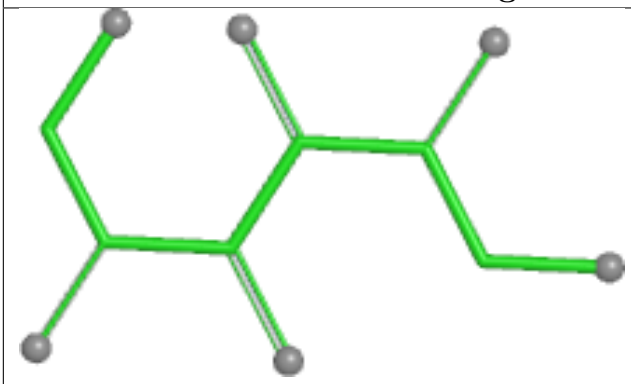


Rings

Ligand PSJ L 301 (A)



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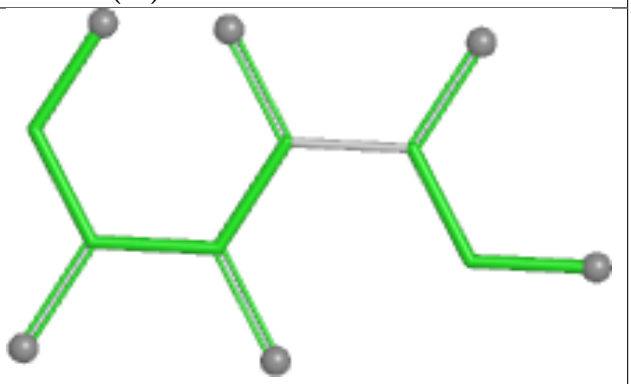
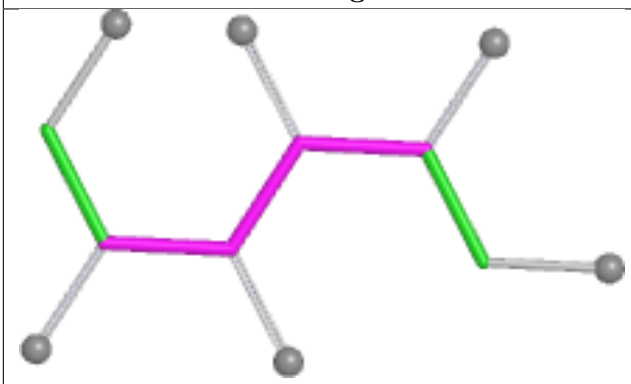


Bond angles



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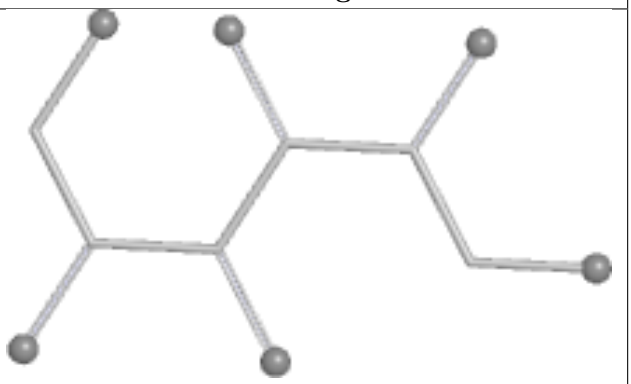
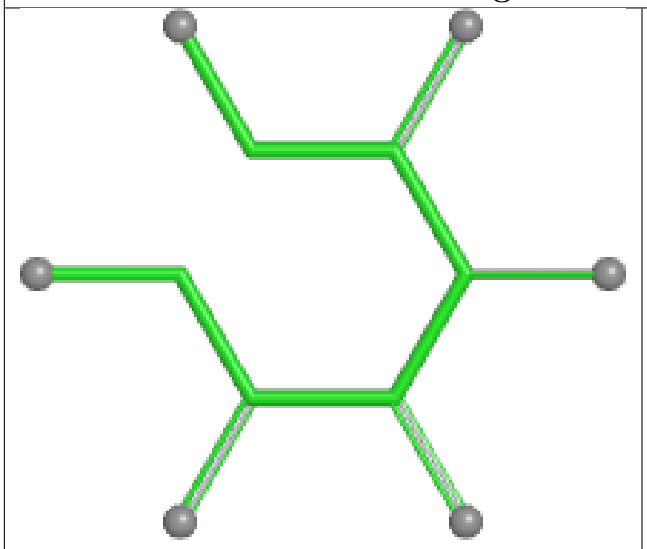


Rings

Ligand FUD L 302 (B)



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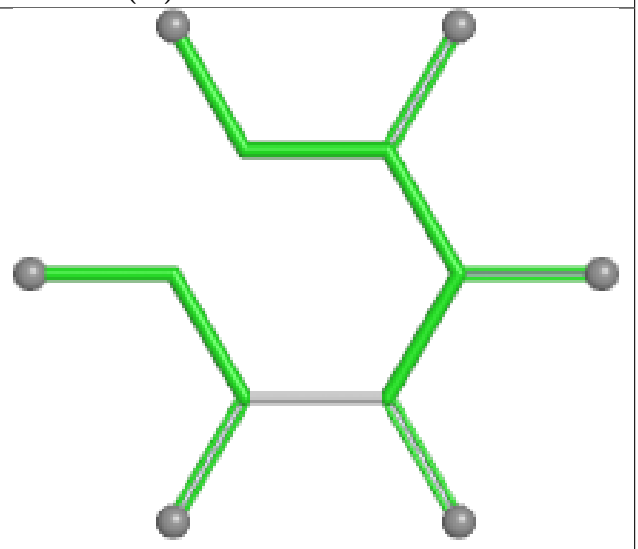
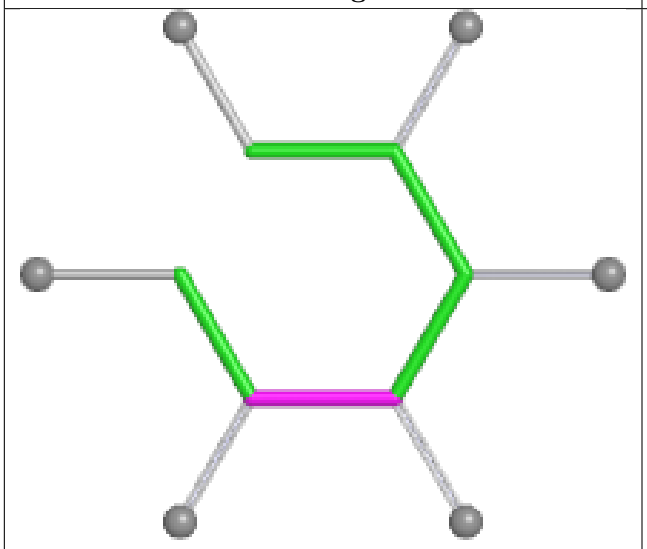


Bond angles



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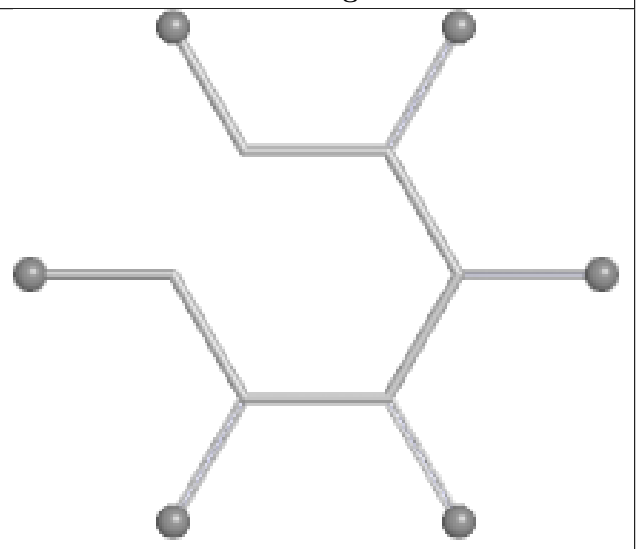
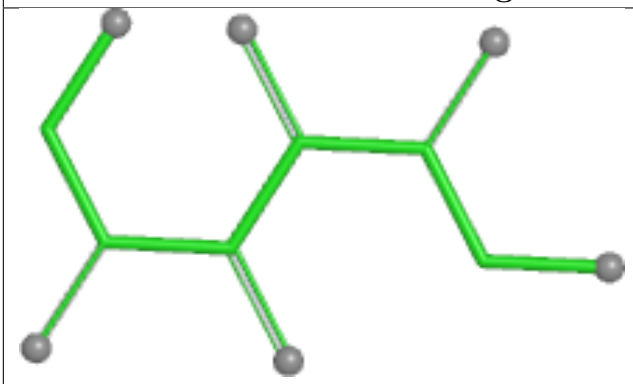


Rings

Ligand PSJ G 301 (A)



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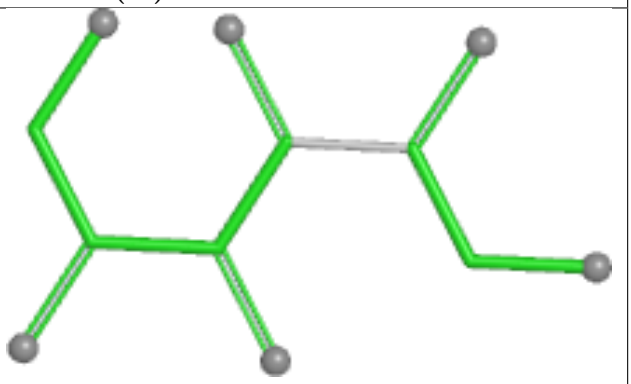
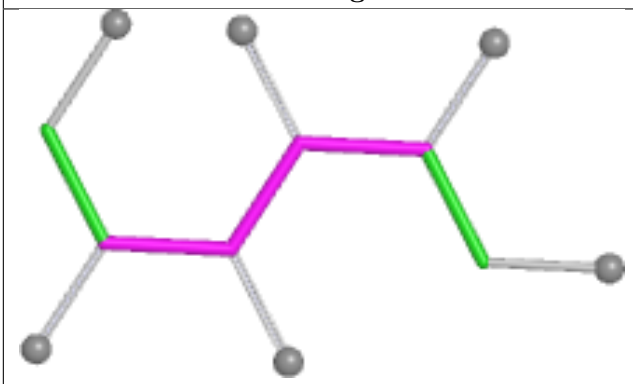


Bond angles



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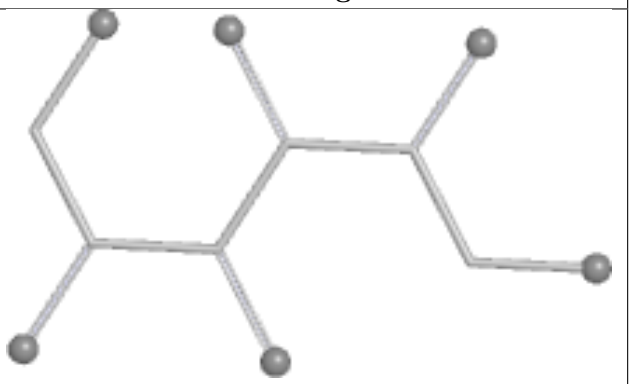
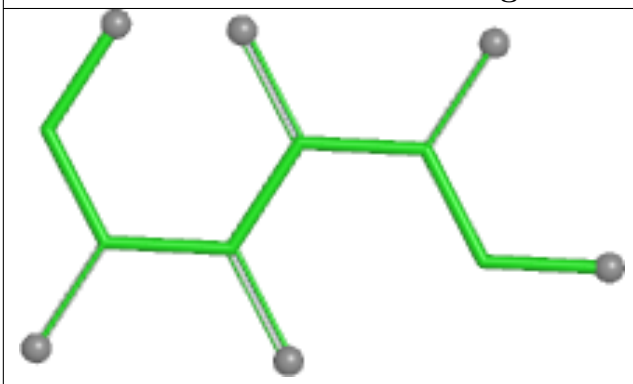


Rings

Ligand PSJ J 302 (A)



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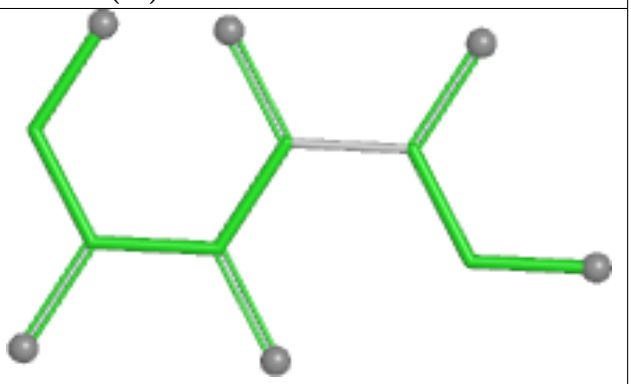
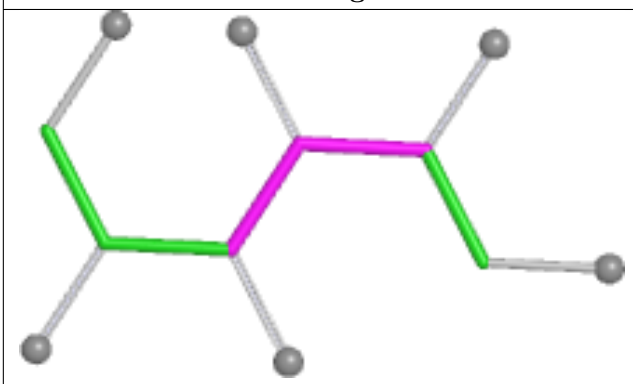


Bond angles



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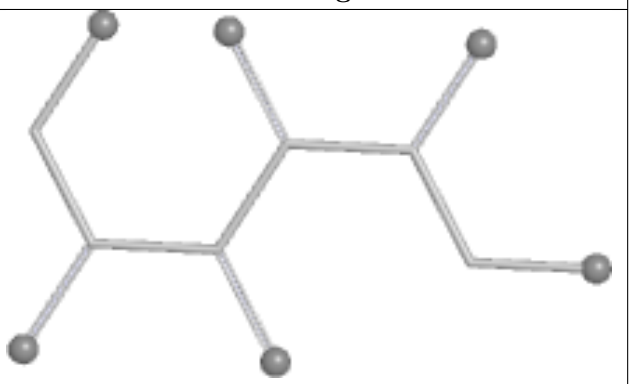
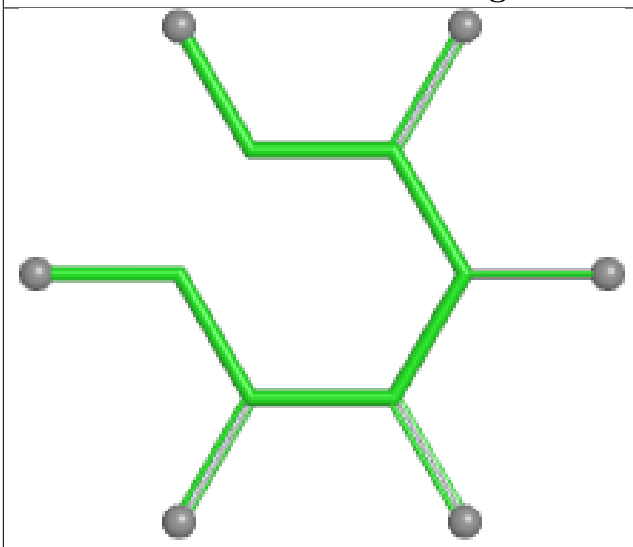


Rings

Ligand FUD G 302 (B)



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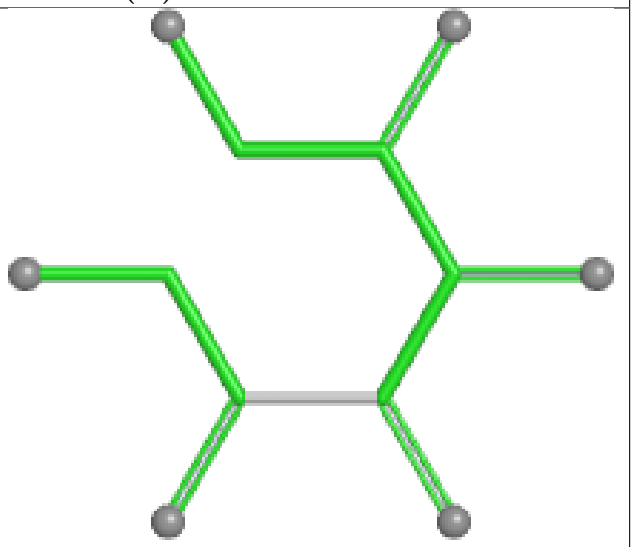
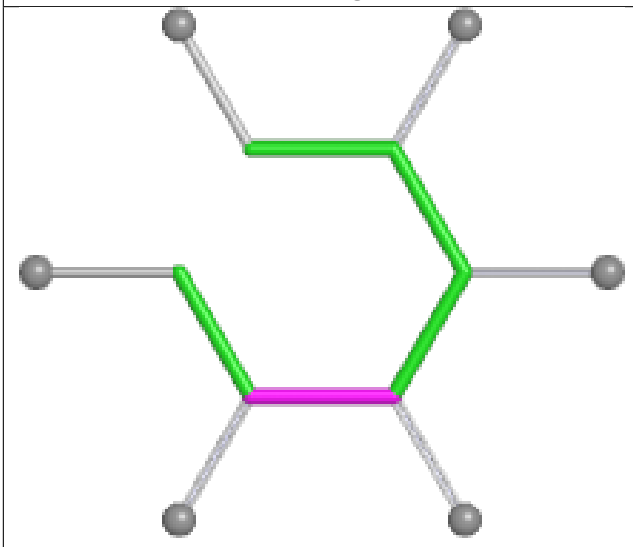


Bond angles



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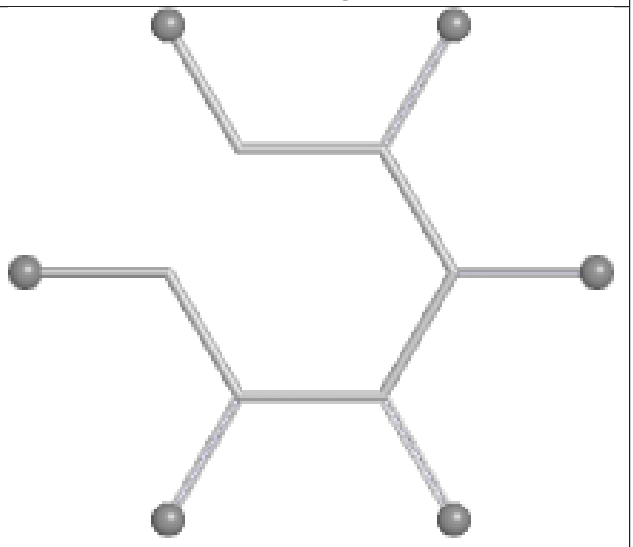
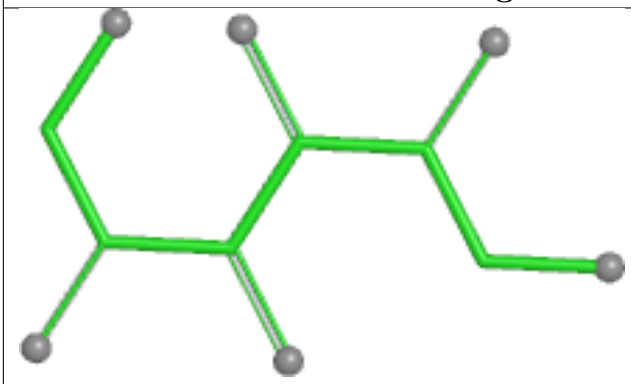


Rings

Ligand PSJ H 301 (A)



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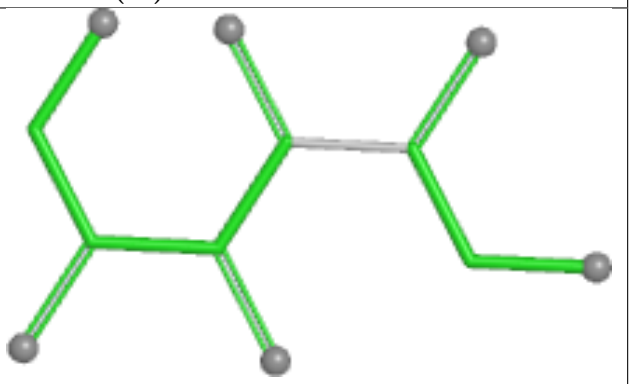
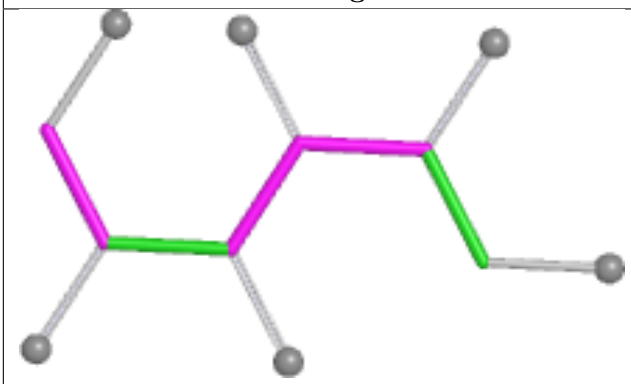


Bond angles



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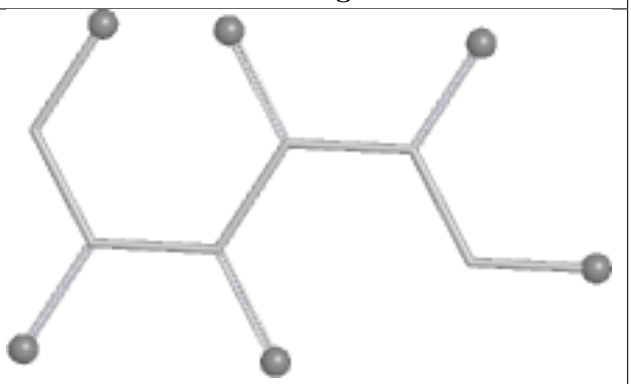
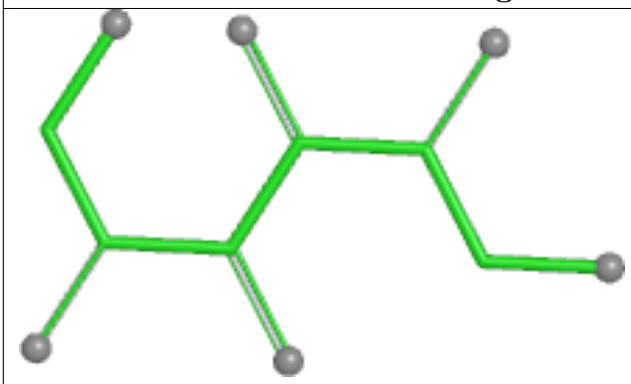


Rings

Ligand PSJ K 301 (A)



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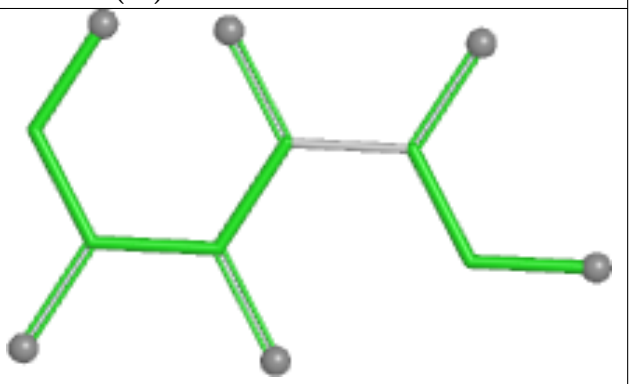
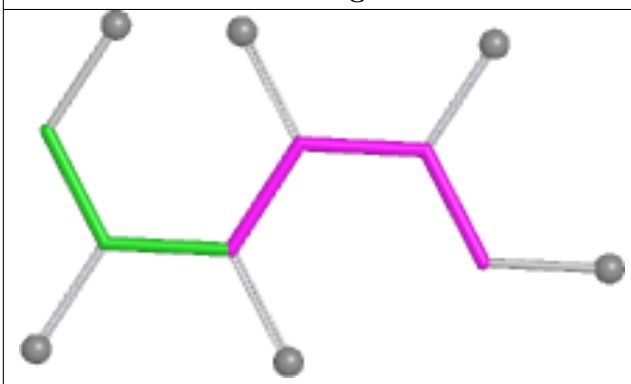


Bond angles



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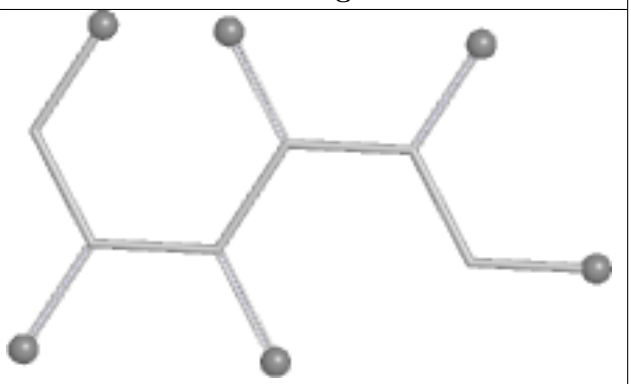
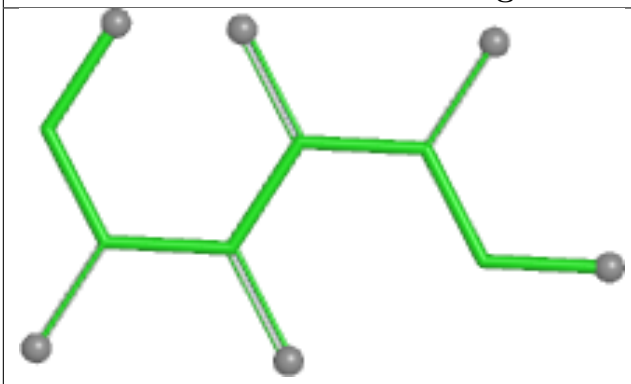
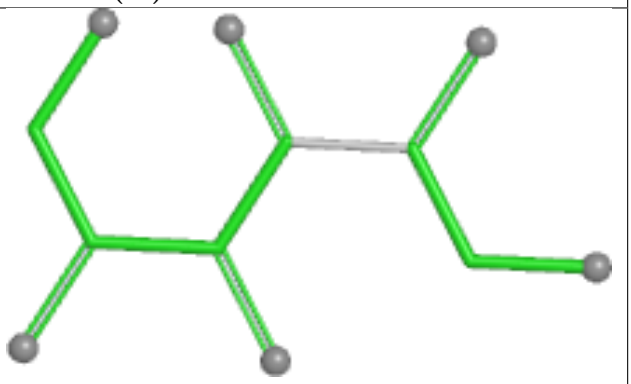


Rings

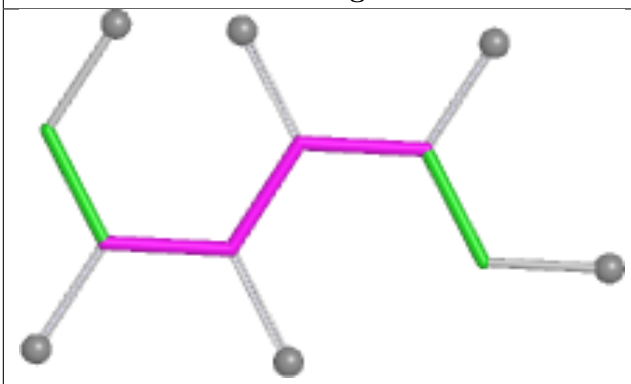
Ligand PSJ B 301 (A)



Bond lengths



Bond angles



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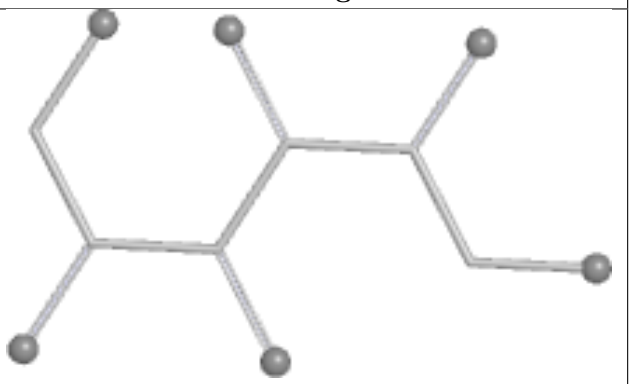
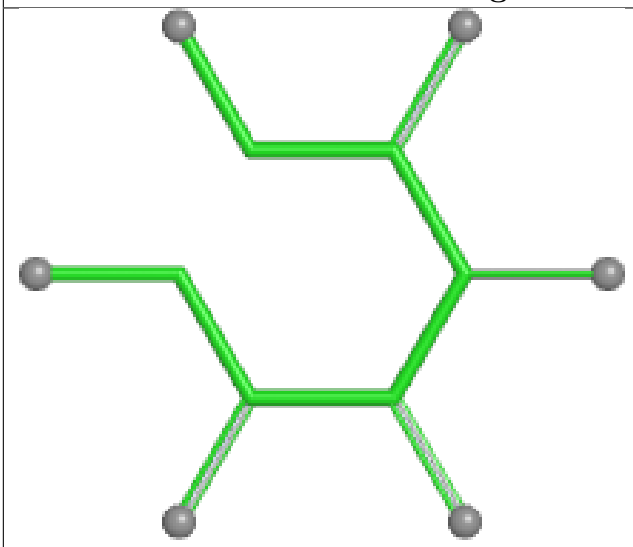
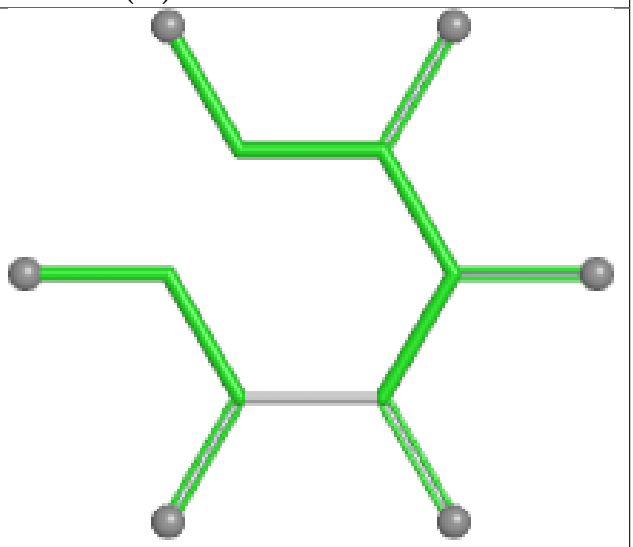


Rings

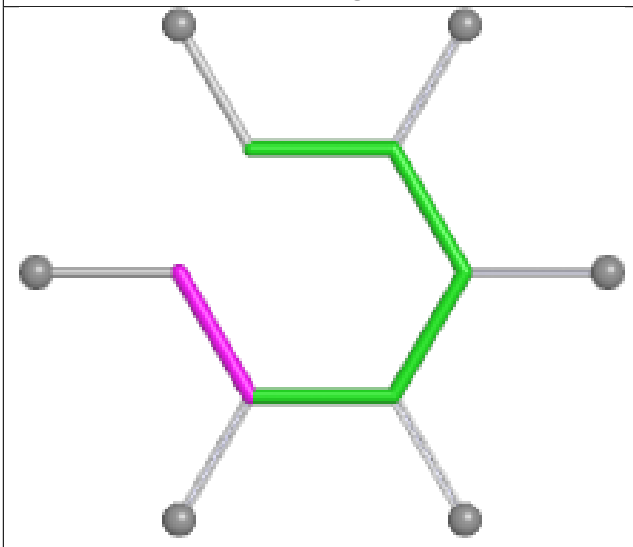
Ligand FUD O 302 (B)



Bond lengths



Bond angles



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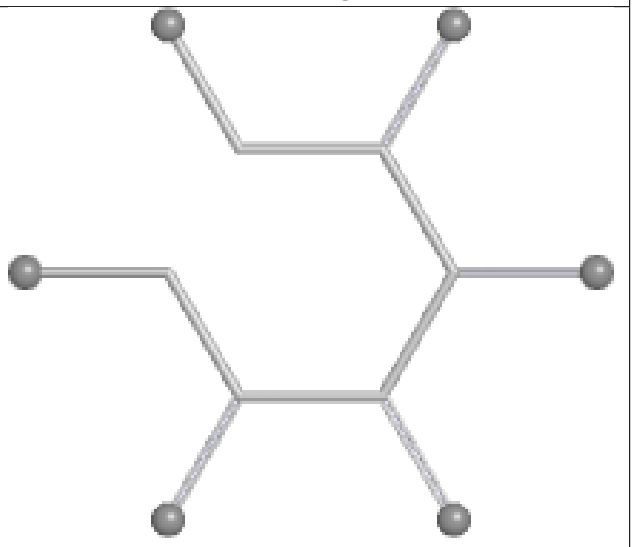
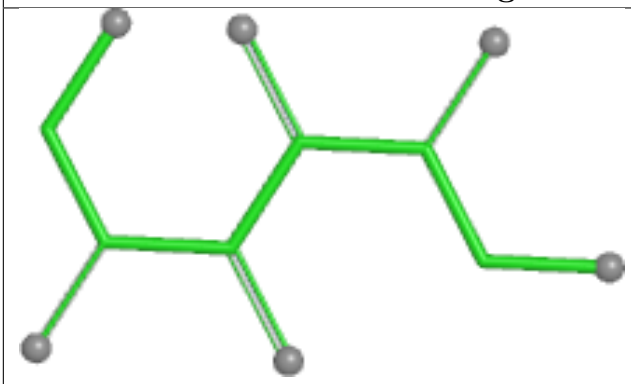
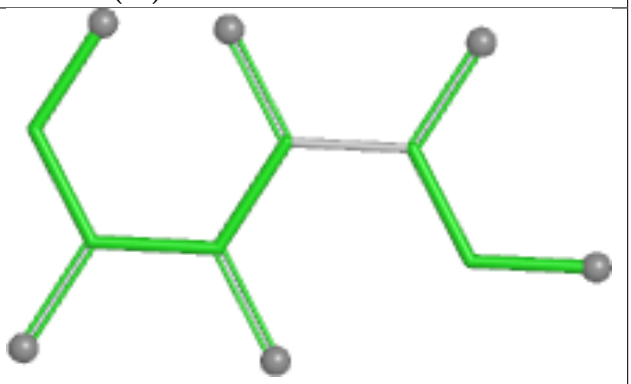


Rings

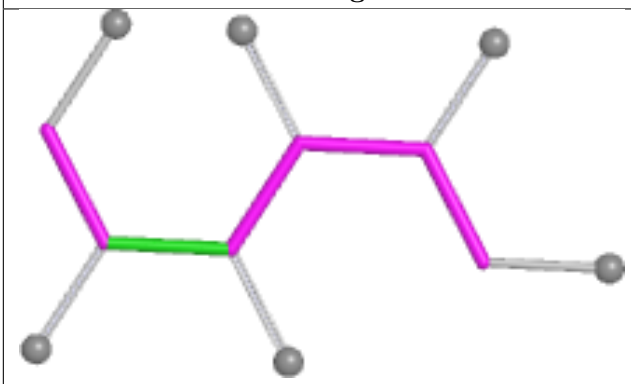
Ligand PSJ E 301 (A)



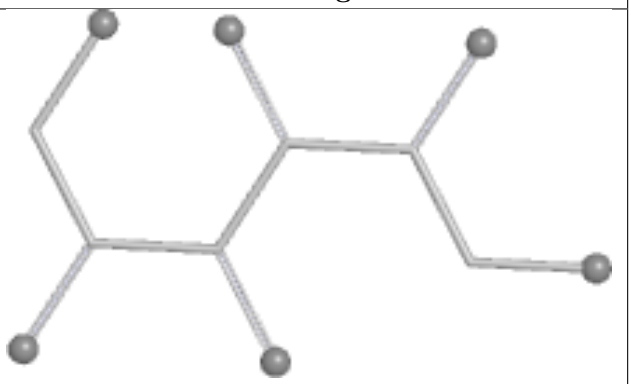
Bond lengths



Bond angles

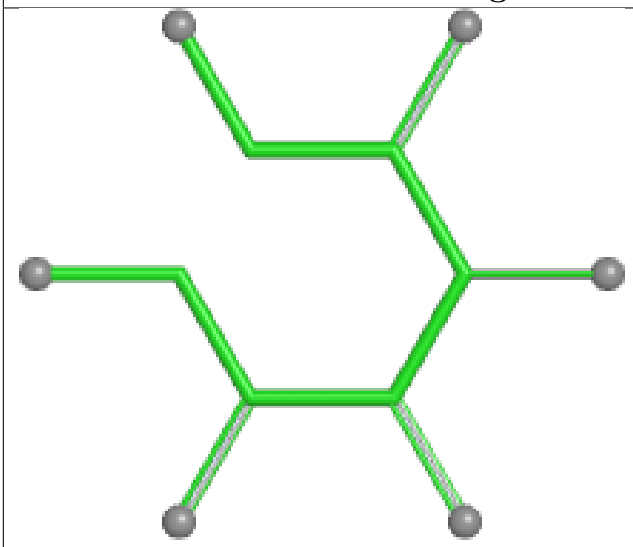


Torsions



Rings

Ligand FUD A 302 (B)



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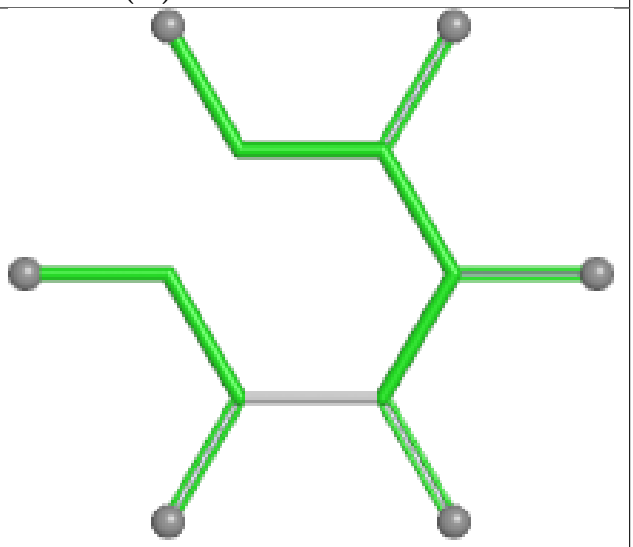

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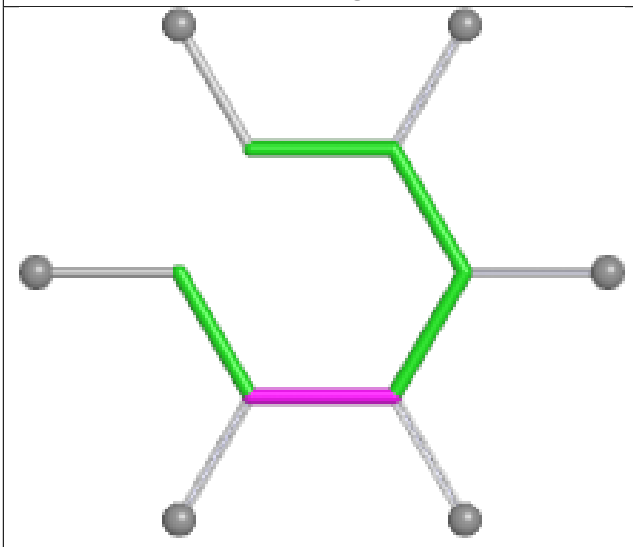

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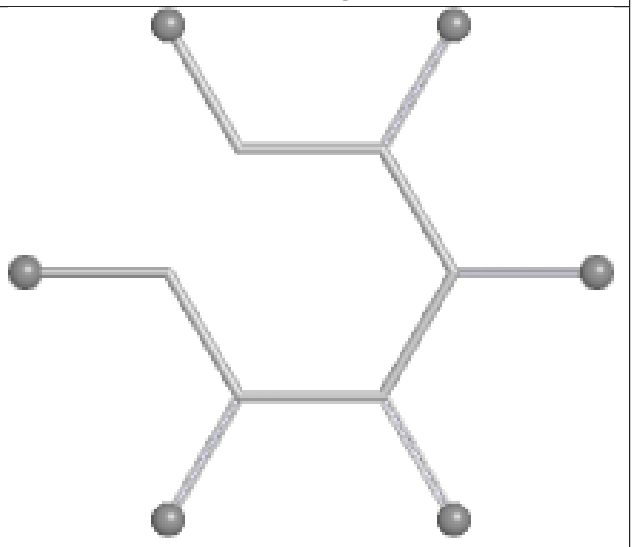
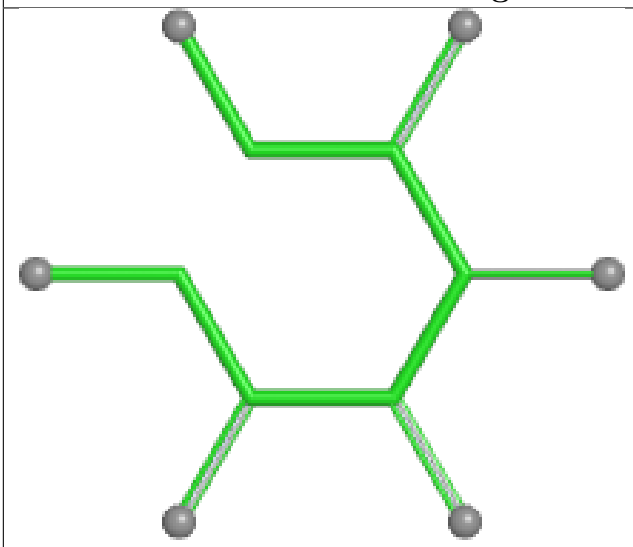


Rings

Ligand FUD F 302 (B)



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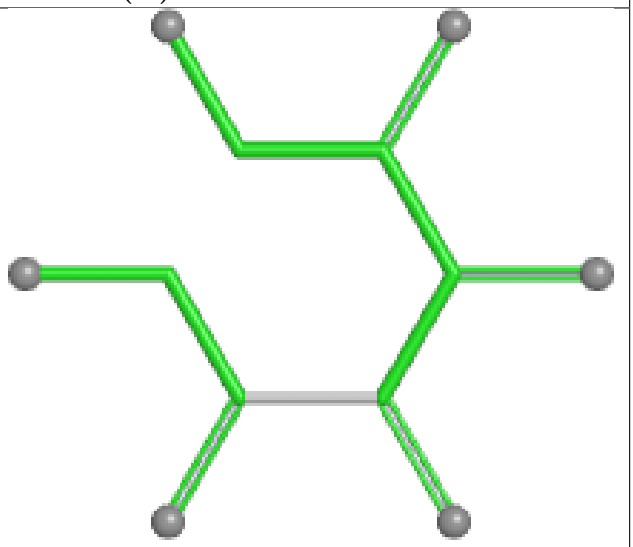
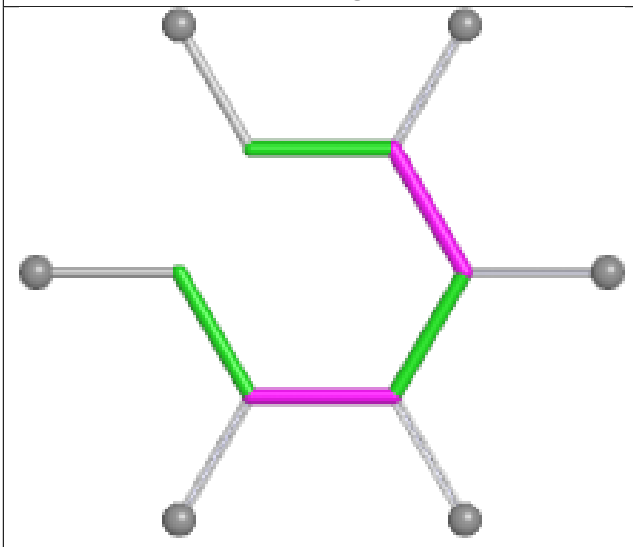


Bond angles



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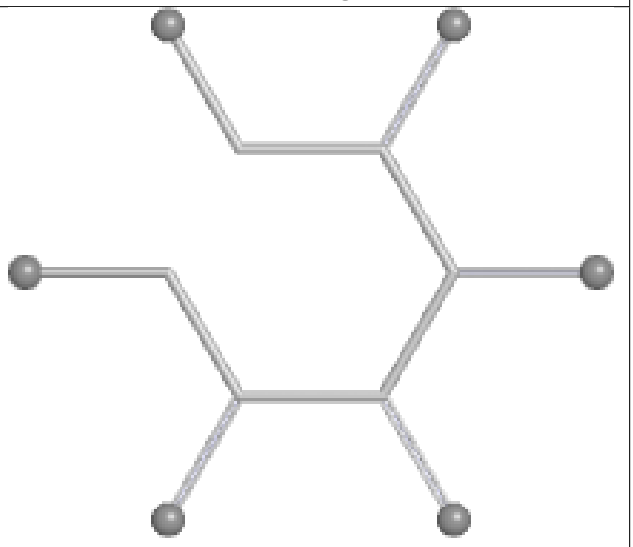
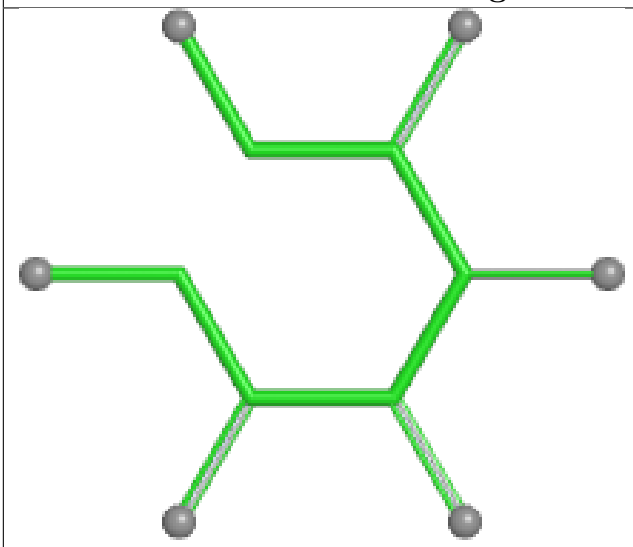


Rings

Ligand FUD K 302 (B)



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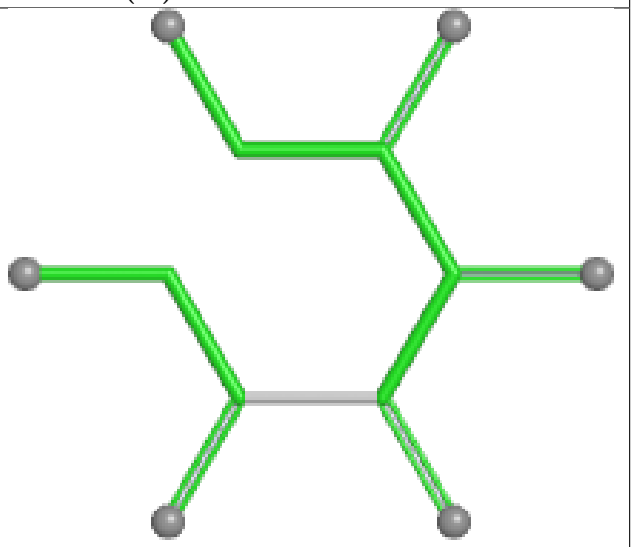
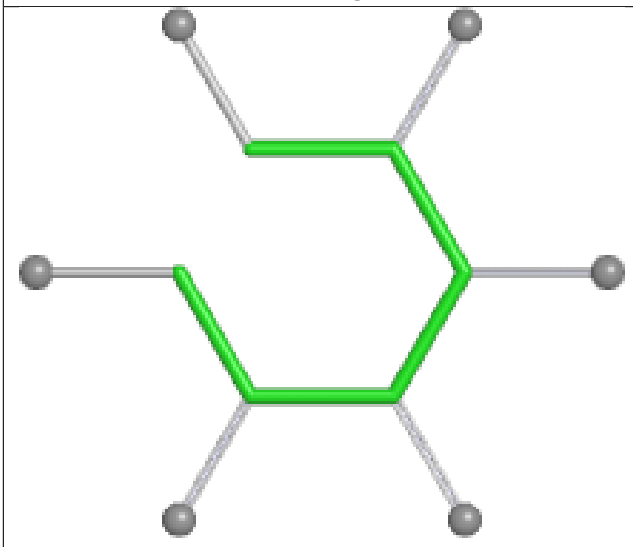


Bond angles



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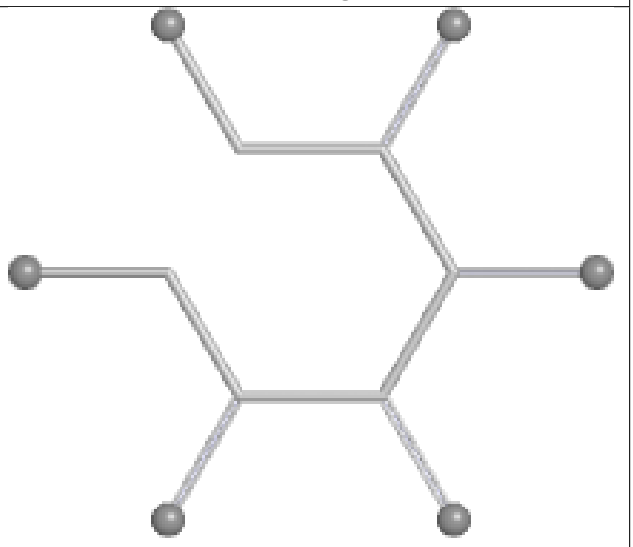
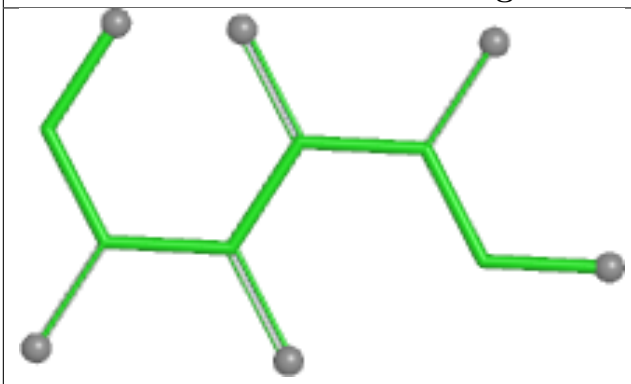


Rings

Ligand PSJ O 301 (A)



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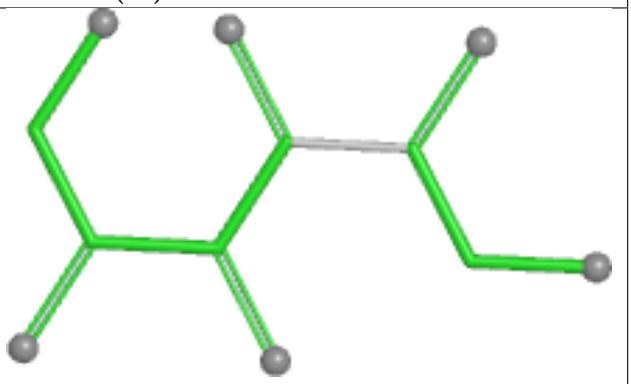

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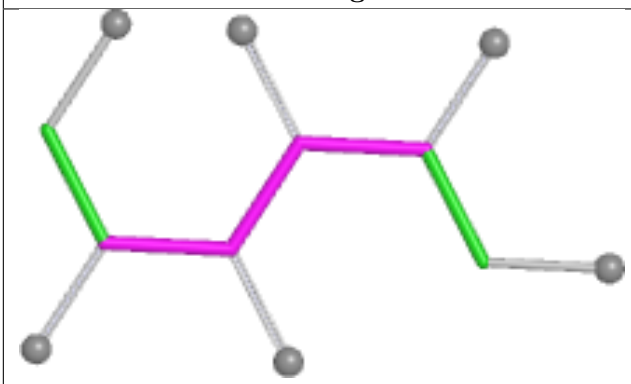

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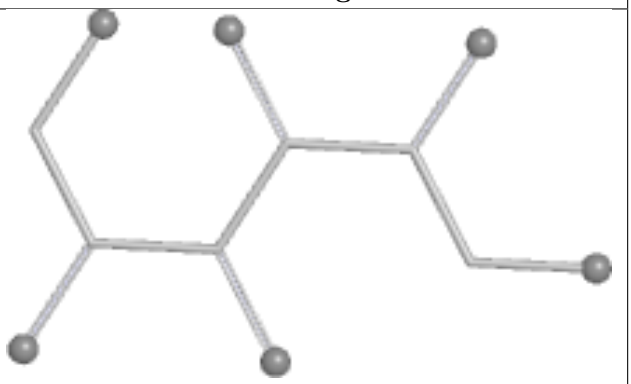
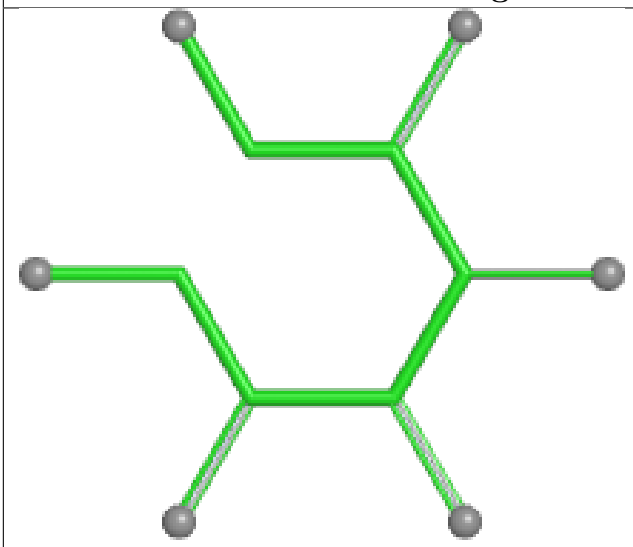


Rings

Ligand FUD E 302 (B)



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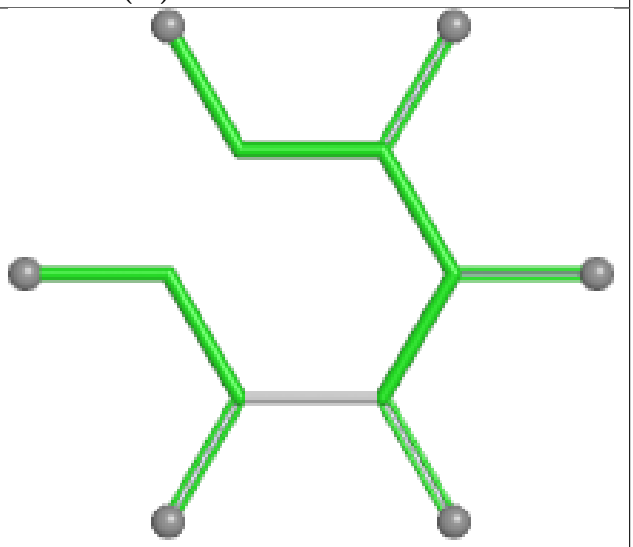

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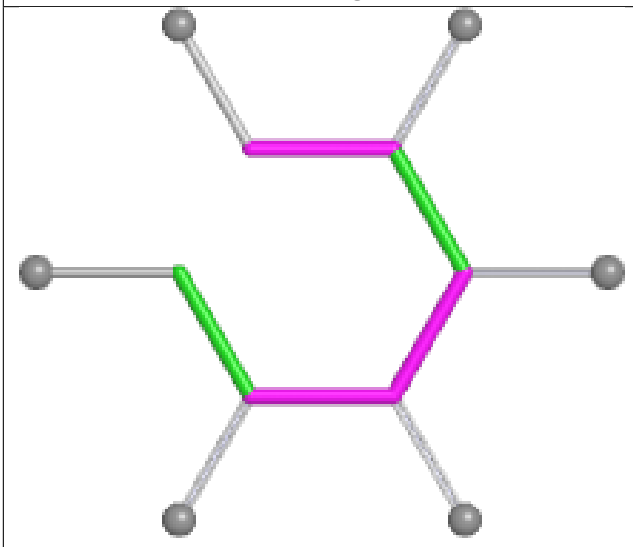

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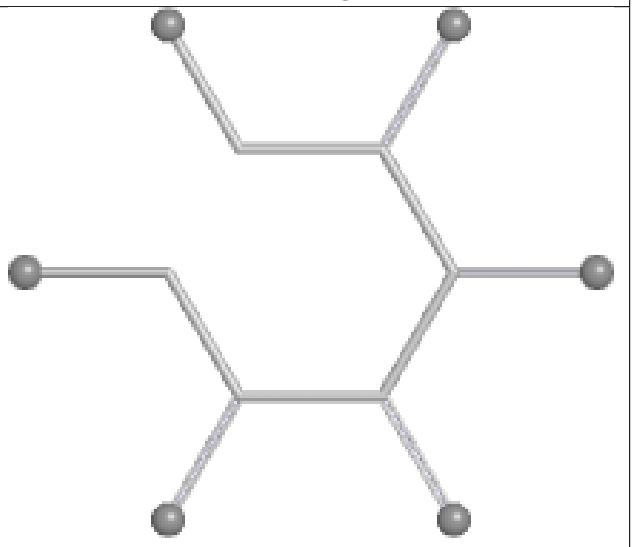
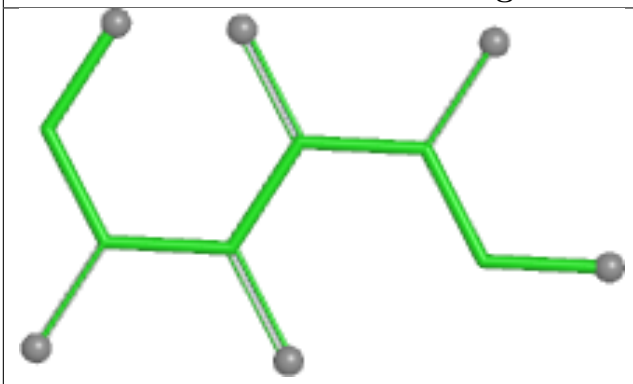


Rings

Ligand PSJ A 301 (A)



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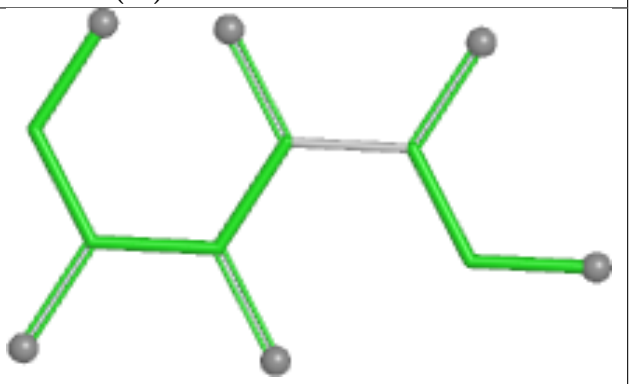

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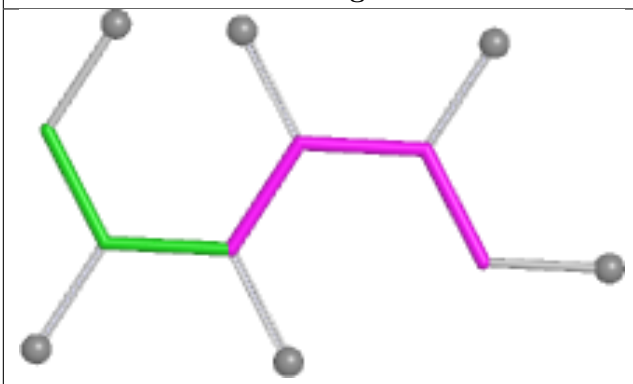

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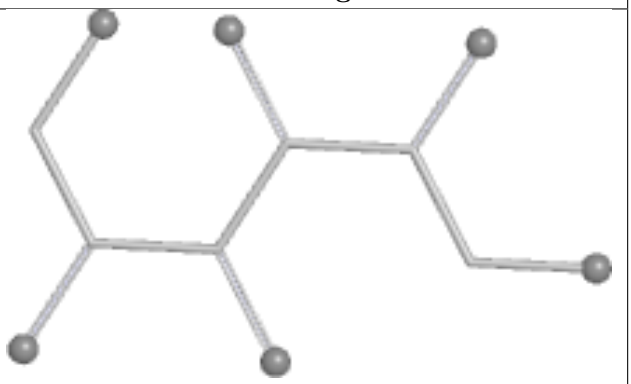
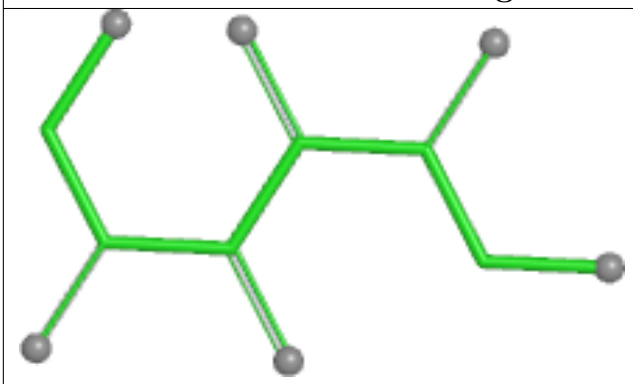


Rings

Ligand PSJ D 301 (A)



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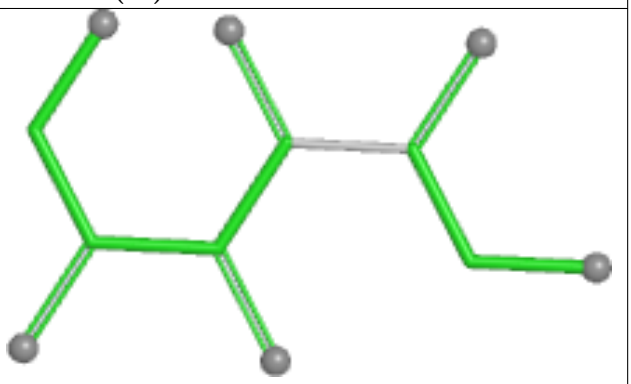
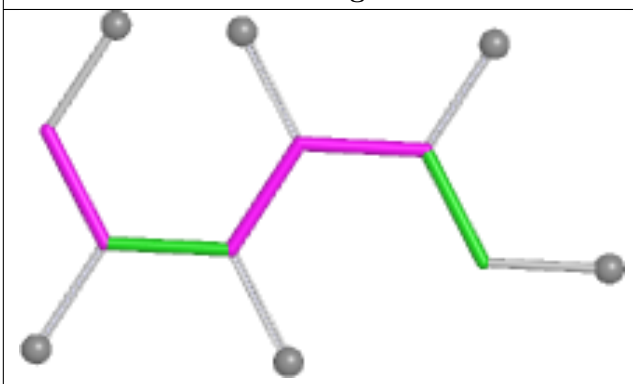


Bond angles



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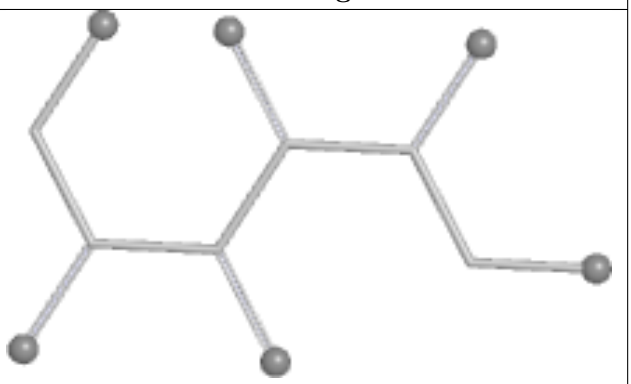
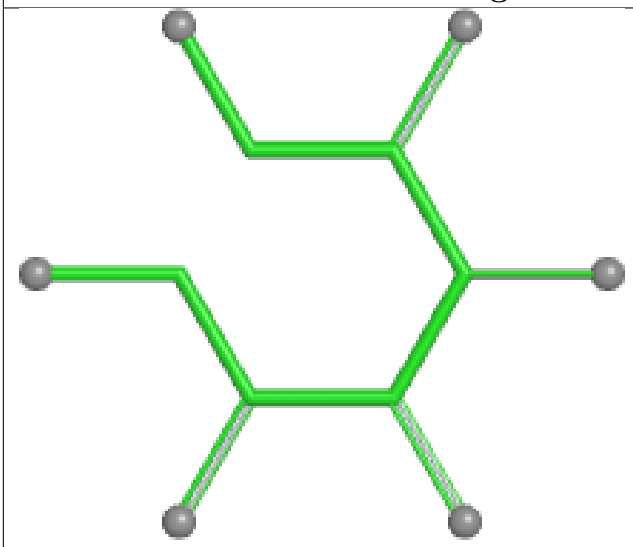


Rings

Ligand FUD B 302 (B)



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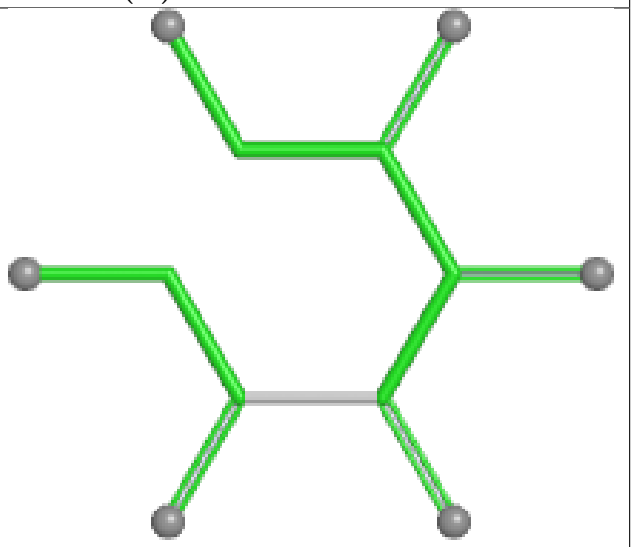
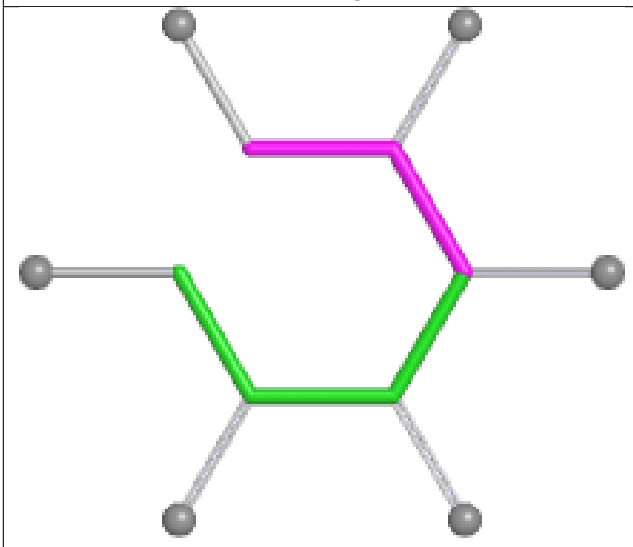


Bond angles



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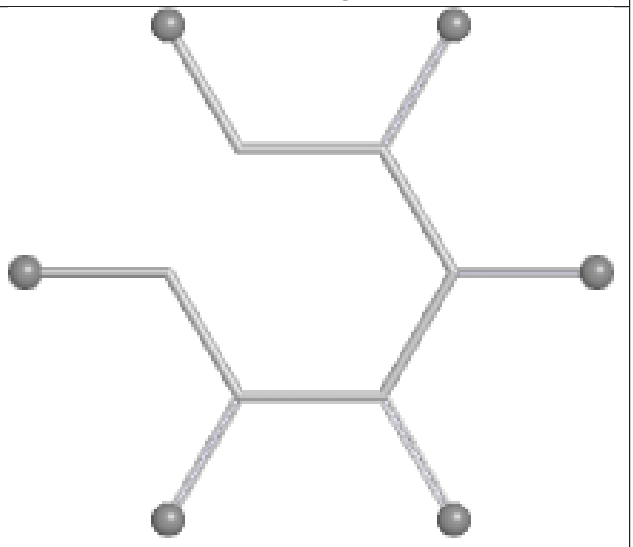
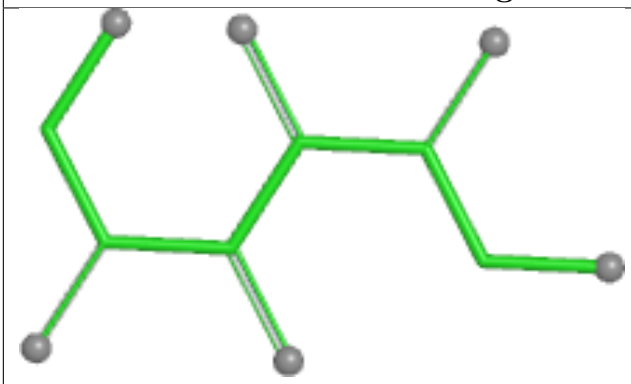


Rings

Ligand PSJ N 302 (A)



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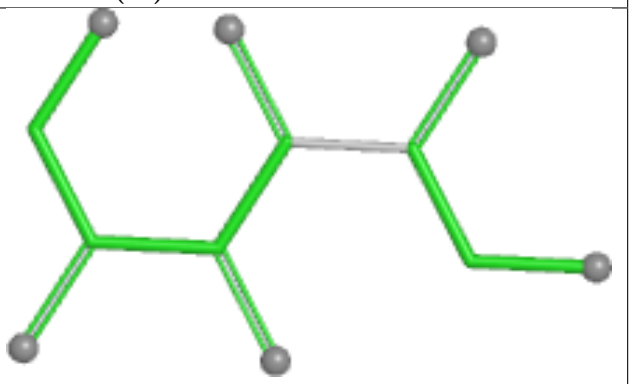

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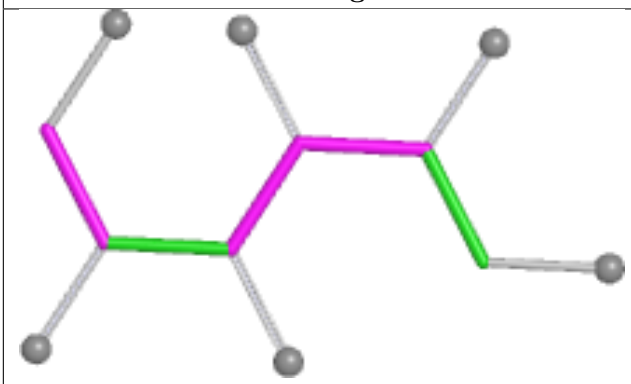

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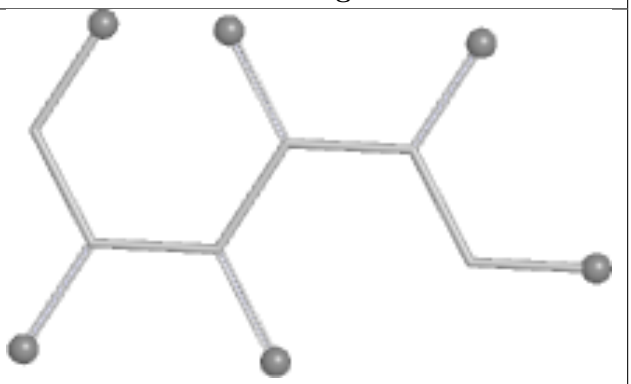
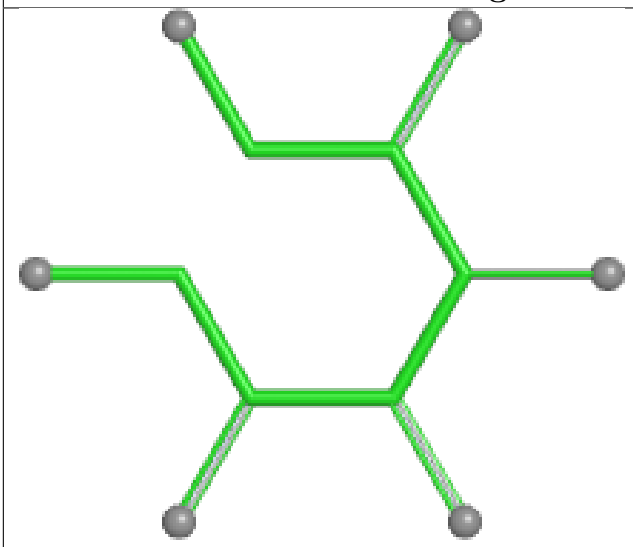


Rings

Ligand FUD D 302 (B)



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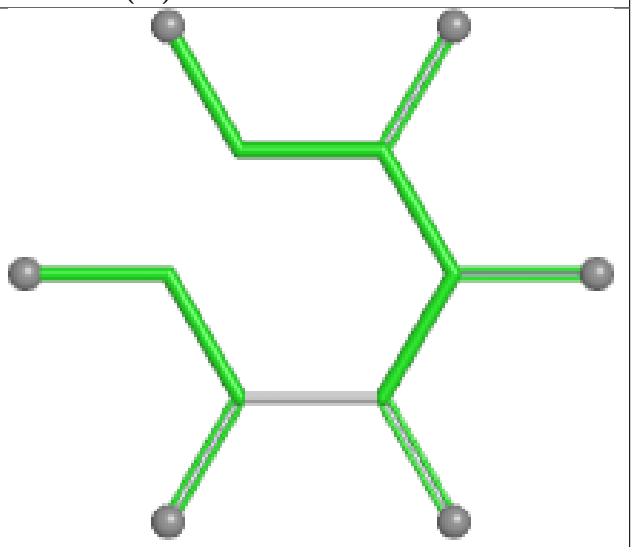

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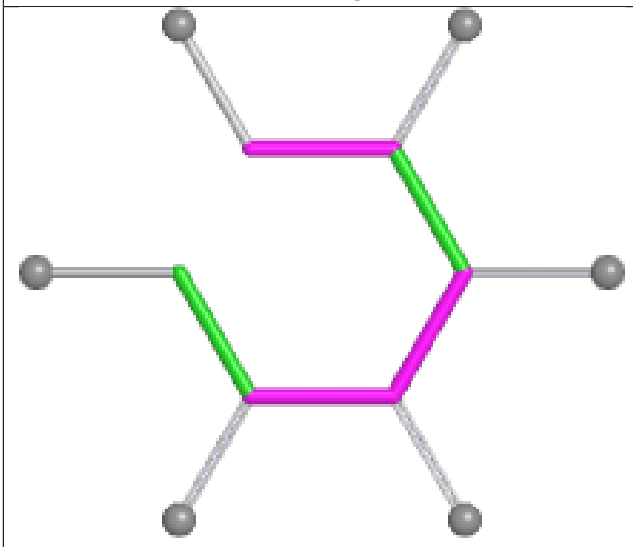

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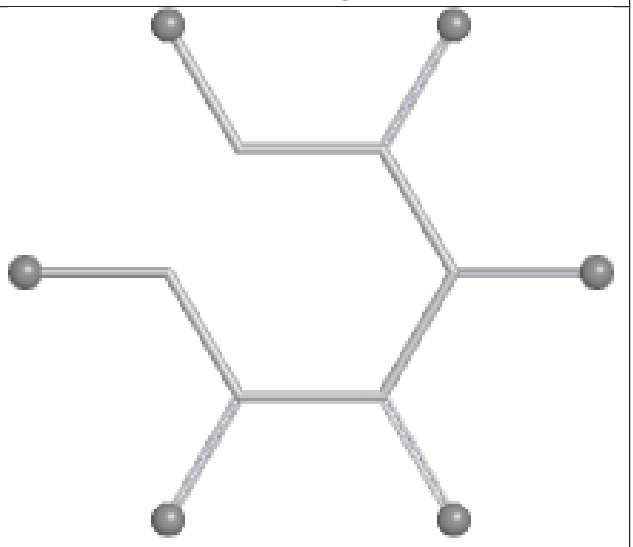
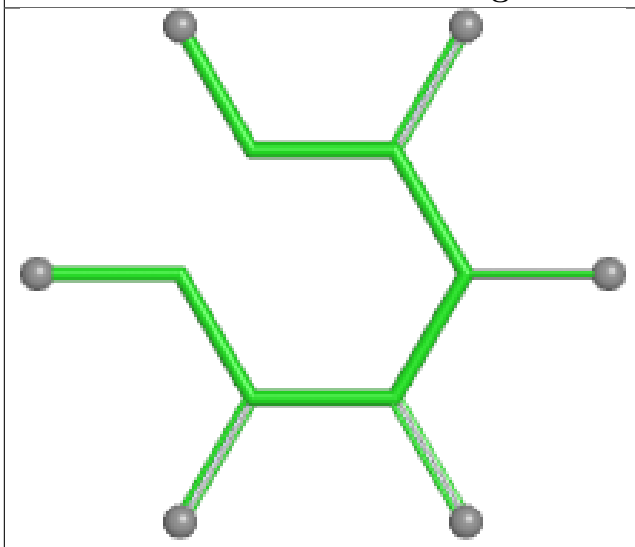


Rings

Ligand FUD P 302 (B)



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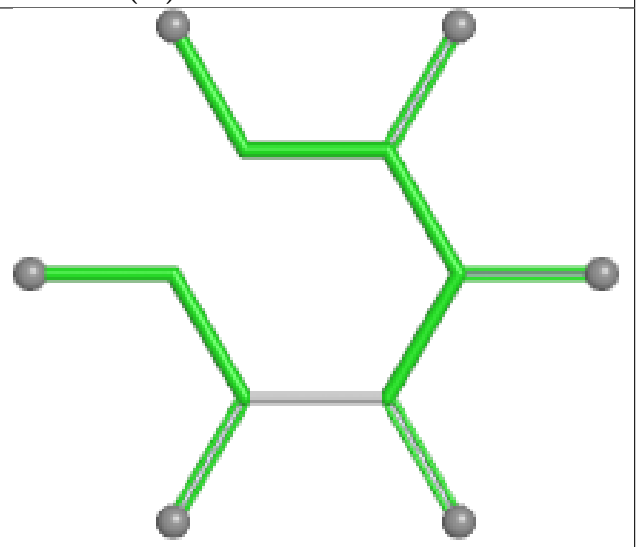
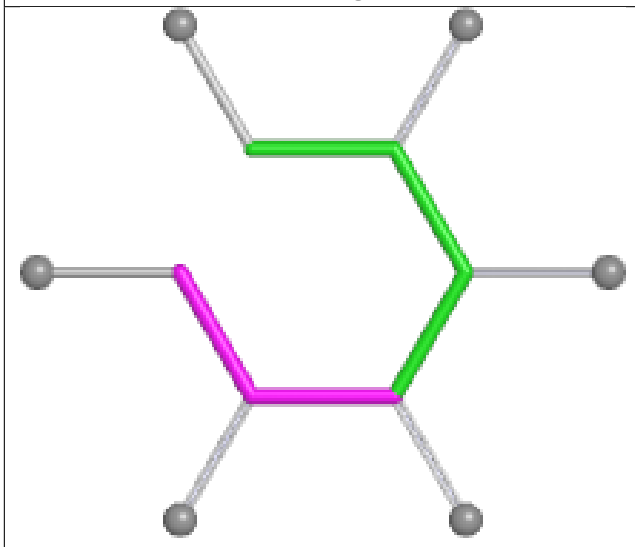


Bond angles



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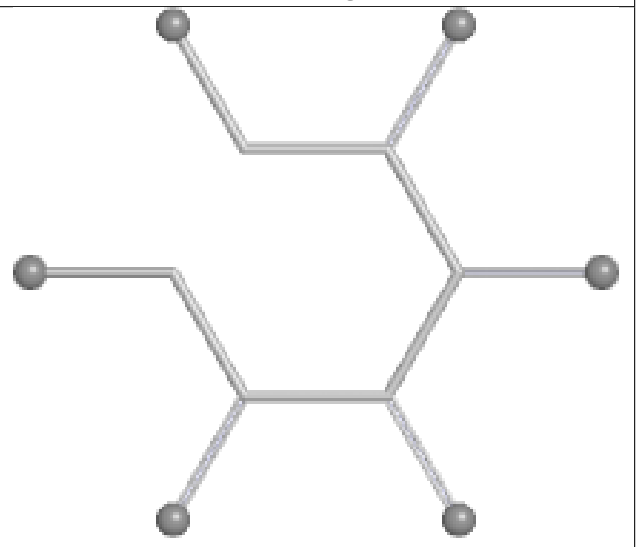
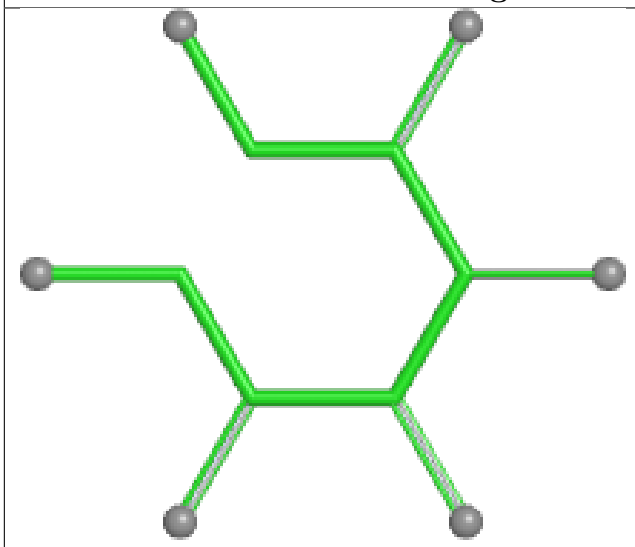


Rings

Ligand FUD N 303 (B)



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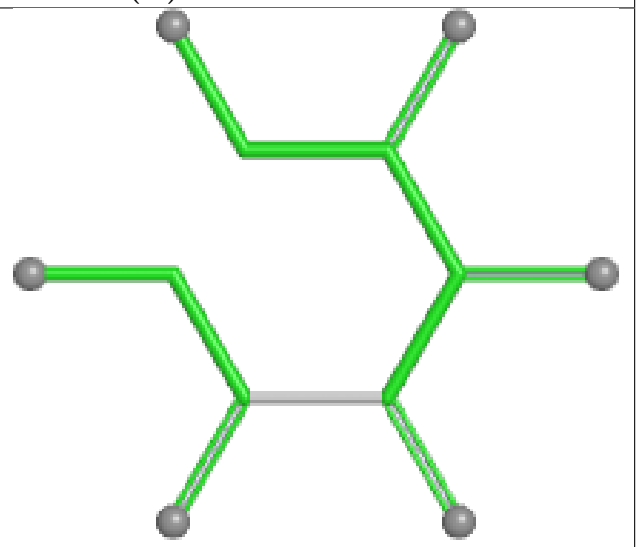
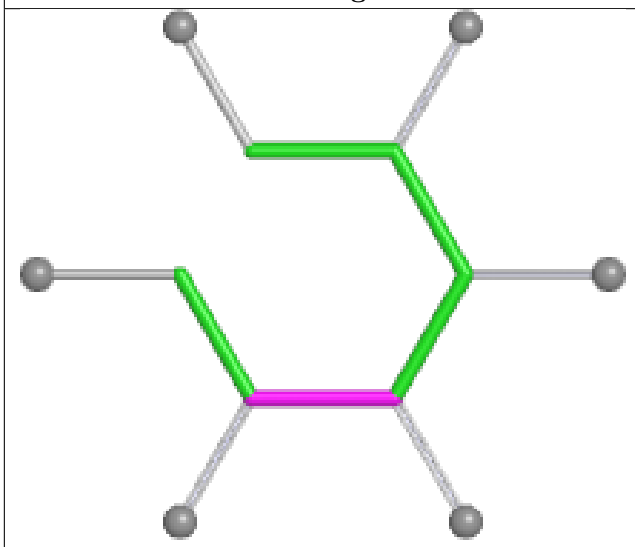


Bond angles



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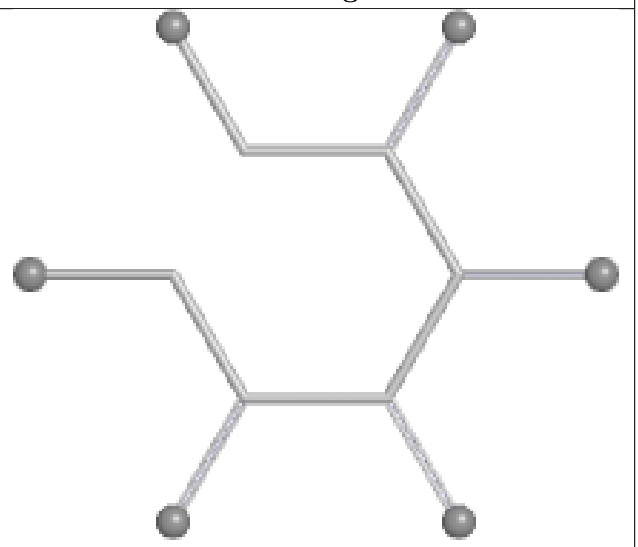
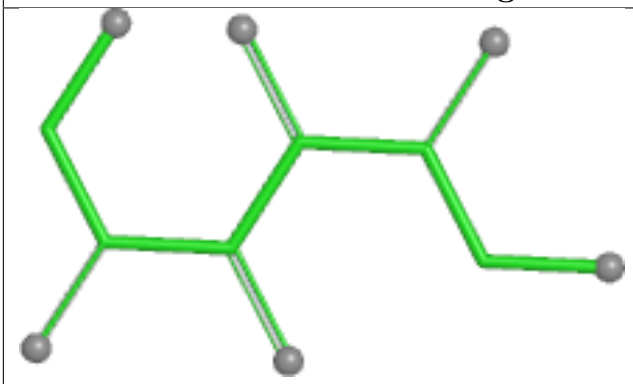


Rings

Ligand PSJ P 301 (A)



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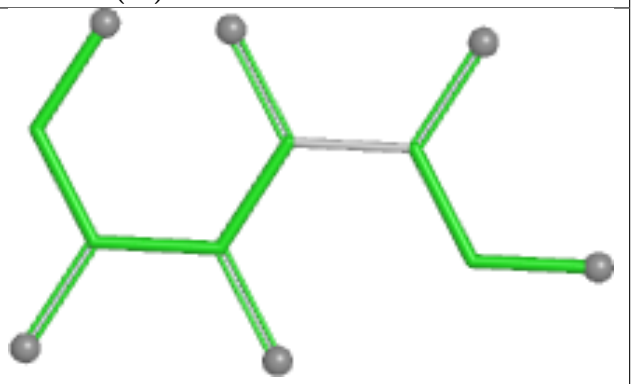
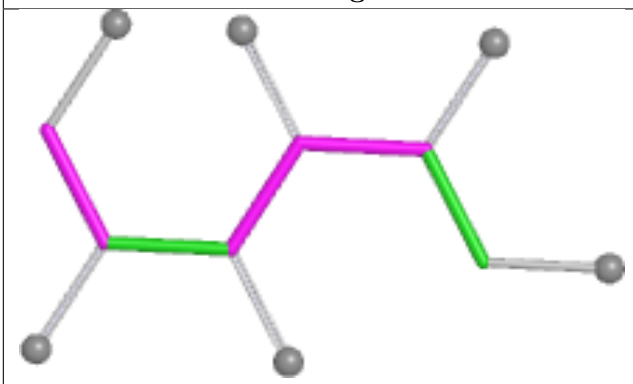


Bond angles



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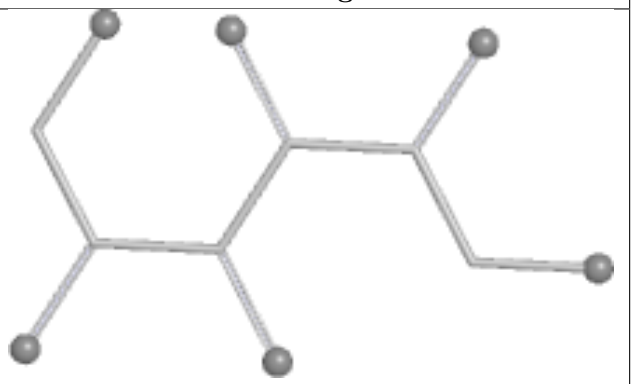
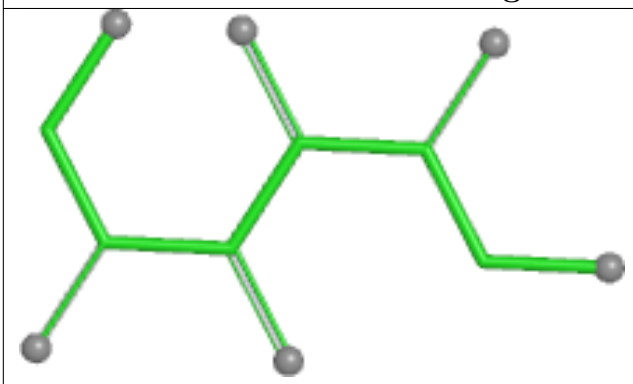
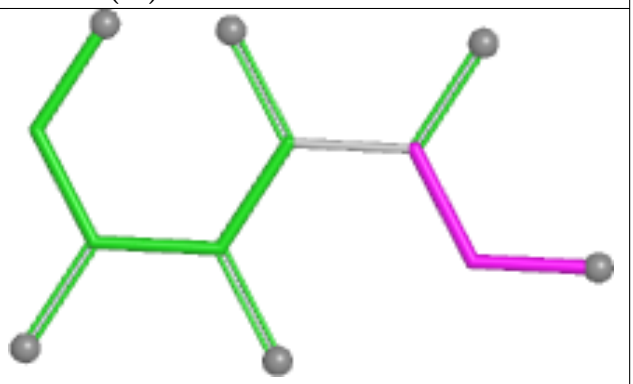


Rings

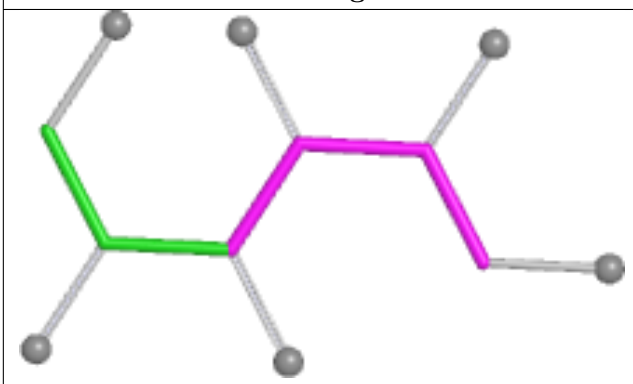
Ligand PSJ I 301 (A)



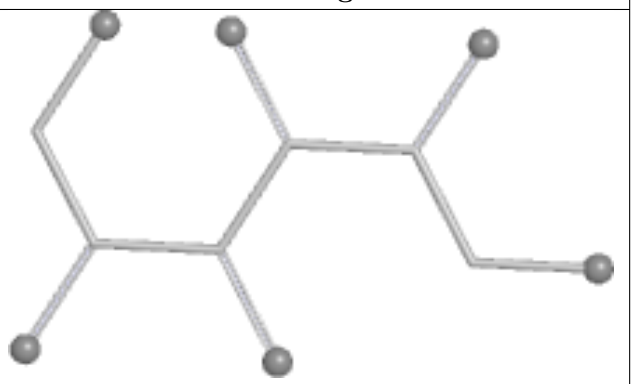
Bond lengths



Bond angles

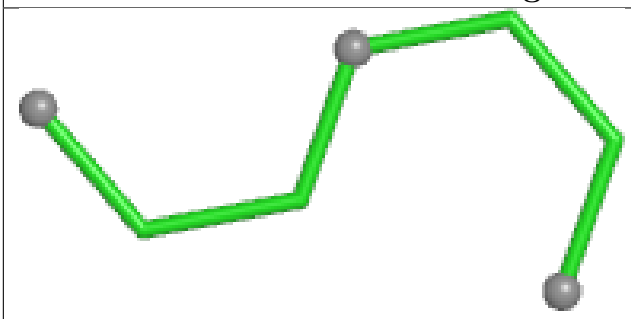


Torsions

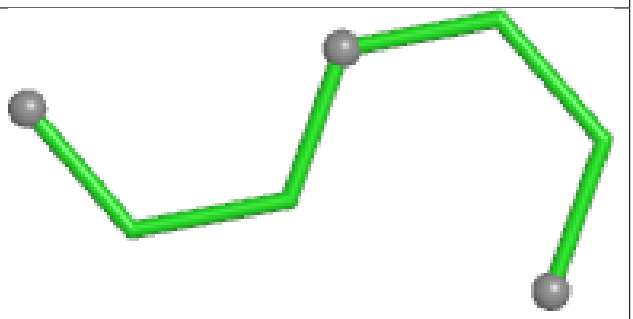


Rings

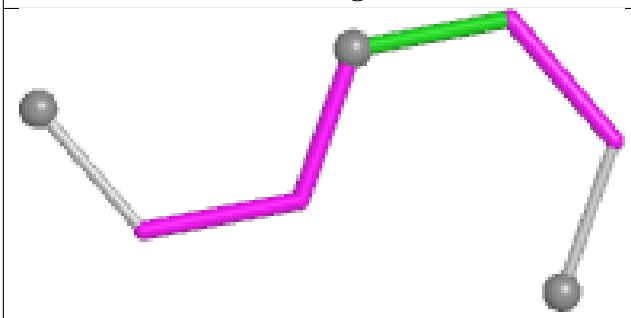
Ligand PEG C 305



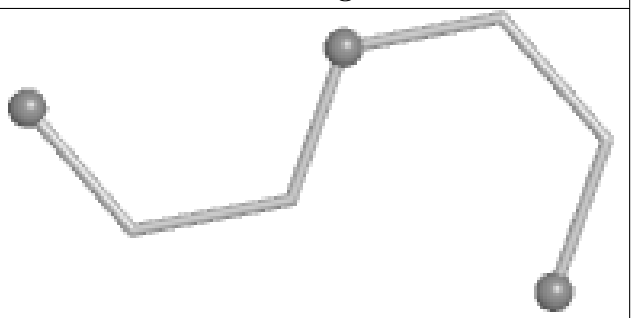
Bond lengths



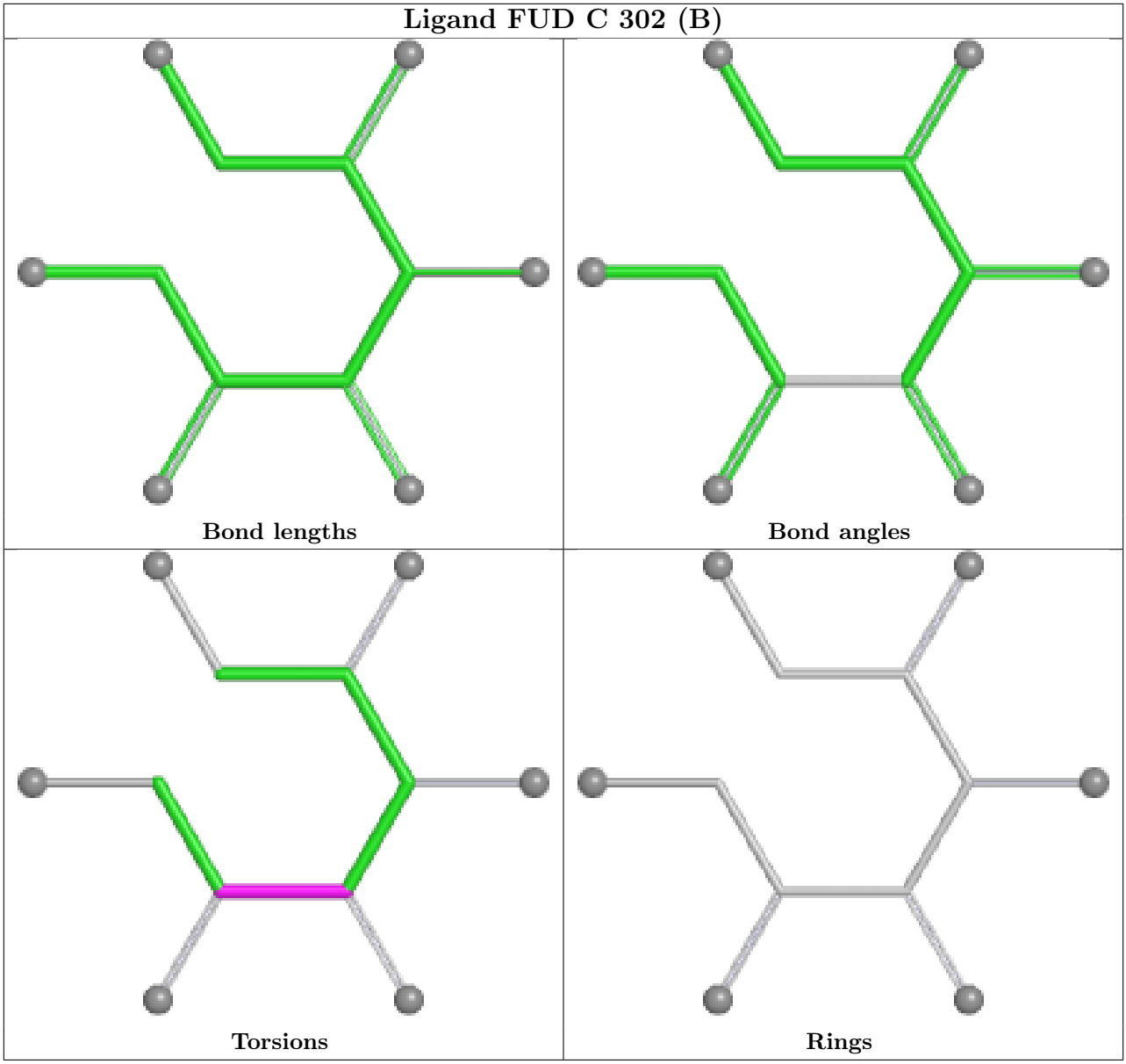
Bond angles



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/297 (99%)	-1.46	0	100	100	27, 44, 66, 83	0
1	B	288/297 (96%)	-1.45	0	100	100	28, 43, 66, 109	0
1	C	297/297 (100%)	-1.49	0	100	100	28, 45, 70, 93	0
1	D	289/297 (97%)	-1.46	0	100	100	25, 41, 62, 142	0
1	E	295/297 (99%)	-1.39	0	100	100	30, 52, 86, 109	0
1	F	289/297 (97%)	-1.39	0	100	100	30, 49, 76, 143	0
1	G	296/297 (99%)	-1.38	0	100	100	30, 47, 71, 94	0
1	H	289/297 (97%)	-1.43	0	100	100	29, 46, 69, 133	0
1	I	296/297 (99%)	-1.41	0	100	100	28, 53, 86, 111	0
1	J	289/297 (97%)	-1.37	0	100	100	31, 49, 75, 132	0
1	K	297/297 (100%)	-1.49	0	100	100	28, 44, 70, 113	0
1	L	288/297 (96%)	-1.46	0	100	100	27, 43, 65, 126	0
1	M	296/297 (99%)	-1.40	0	100	100	29, 46, 72, 91	0
1	N	288/297 (96%)	-1.47	0	100	100	30, 46, 69, 111	0
1	O	296/297 (99%)	-1.46	0	100	100	29, 45, 69, 79	0
1	P	289/297 (97%)	-1.47	0	100	100	26, 41, 62, 140	0
All	All	4678/4752 (98%)	-1.44	0	100	100	25, 46, 74, 143	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	G	304	1/1	0.97	0.04	47,47,47,47	0
5	NA	J	301	1/1	0.97	0.03	42,42,42,42	0
5	NA	A	304	1/1	0.98	0.06	36,36,36,36	0
5	NA	C	304	1/1	0.98	0.04	42,42,42,42	0
5	NA	K	304	1/1	0.98	0.06	39,39,39,39	0
5	NA	O	304	1/1	0.98	0.03	43,43,43,43	0
6	PEG	C	305	7/7	0.98	0.05	52,58,59,62	0
2	PSJ	I	301[A]	12/12	0.99	0.03	46,57,73,75	12
2	PSJ	L	301[A]	12/12	0.99	0.04	49,58,64,67	12
2	PSJ	M	301[A]	12/12	0.99	0.04	48,65,77,83	12
2	PSJ	N	302[A]	12/12	0.99	0.03	42,55,61,61	12
2	PSJ	P	301[A]	12/12	0.99	0.04	41,52,58,60	12
3	FUD	F	302[B]	12/12	0.99	0.04	50,60,65,68	12
3	FUD	B	302[B]	12/12	0.99	0.04	49,58,62,66	12
3	FUD	G	302[B]	12/12	0.99	0.04	55,69,79,81	12
3	FUD	H	302[B]	12/12	0.99	0.04	47,57,65,67	12
3	FUD	I	302[B]	12/12	0.99	0.05	50,54,58,59	12
3	FUD	J	303[B]	12/12	0.99	0.05	49,58,62,62	12
3	FUD	L	302[B]	12/12	0.99	0.04	51,59,63,65	12
3	FUD	M	302[B]	12/12	0.99	0.05	54,64,68,68	12
3	FUD	P	302[B]	12/12	0.99	0.04	43,51,56,56	12
5	NA	E	304	1/1	0.99	0.03	34,34,34,34	0
2	PSJ	E	301[A]	12/12	0.99	0.03	50,60,72,75	12
2	PSJ	F	301[A]	12/12	0.99	0.03	44,60,65,68	12
2	PSJ	A	301[A]	12/12	0.99	0.03	42,54,64,68	12
2	PSJ	B	301[A]	12/12	0.99	0.03	45,58,63,65	12
2	PSJ	C	301[A]	12/12	0.99	0.04	51,59,70,74	12
5	NA	N	301	1/1	0.99	0.03	43,43,43,43	0
2	PSJ	D	301[A]	12/12	0.99	0.03	44,52,57,58	12
2	PSJ	H	301[A]	12/12	0.99	0.03	45,55,61,61	12
3	FUD	O	302[B]	12/12	1.00	0.04	52,59,63,66	12
3	FUD	C	302[B]	12/12	1.00	0.03	52,56,63,66	12

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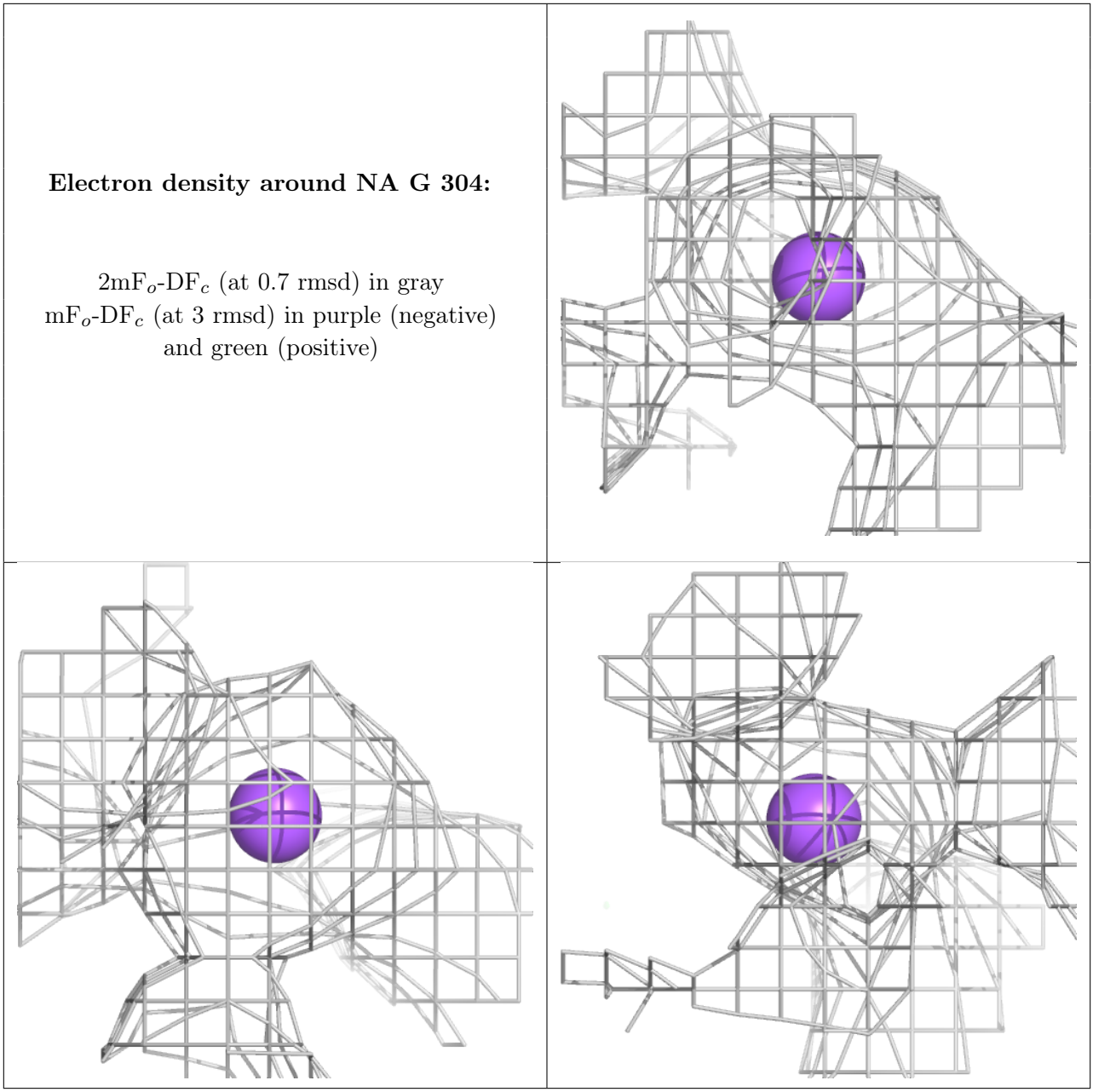
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	303	1/1	1.00	0.01	25,25,25,25	0
4	MG	F	303	1/1	1.00	0.01	28,28,28,28	0
4	MG	A	303	1/1	1.00	0.01	17,17,17,17	0
4	MG	B	303	1/1	1.00	0.01	21,21,21,21	0
4	MG	C	303	1/1	1.00	0.01	18,18,18,18	0
4	MG	D	303	1/1	1.00	0.01	17,17,17,17	0
4	MG	G	303	1/1	1.00	0.01	21,21,21,21	0
4	MG	H	303	1/1	1.00	0.01	20,20,20,20	0
4	MG	I	303	1/1	1.00	0.03	27,27,27,27	0
4	MG	J	304	1/1	1.00	0.01	27,27,27,27	0
4	MG	K	303	1/1	1.00	0.02	19,19,19,19	0
4	MG	L	303	1/1	1.00	0.01	20,20,20,20	0
4	MG	M	303	1/1	1.00	0.01	21,21,21,21	0
4	MG	N	304	1/1	1.00	0.01	18,18,18,18	0
4	MG	O	303	1/1	1.00	0.00	21,21,21,21	0
4	MG	P	303	1/1	1.00	0.00	16,16,16,16	0
3	FUD	D	302[B]	12/12	1.00	0.05	45,48,49,49	12
2	PSJ	O	301[A]	12/12	1.00	0.03	54,65,72,73	12
2	PSJ	G	301[A]	12/12	1.00	0.03	49,56,62,65	12
3	FUD	E	302[B]	12/12	1.00	0.04	54,65,80,83	12
2	PSJ	J	302[A]	12/12	1.00	0.03	47,61,70,74	12
3	FUD	K	302[B]	12/12	1.00	0.05	42,45,48,49	12
3	FUD	A	302[B]	12/12	1.00	0.03	43,48,58,58	12
2	PSJ	K	301[A]	12/12	1.00	0.02	40,55,64,67	0
3	FUD	N	303[B]	12/12	1.00	0.04	49,54,60,60	12

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.

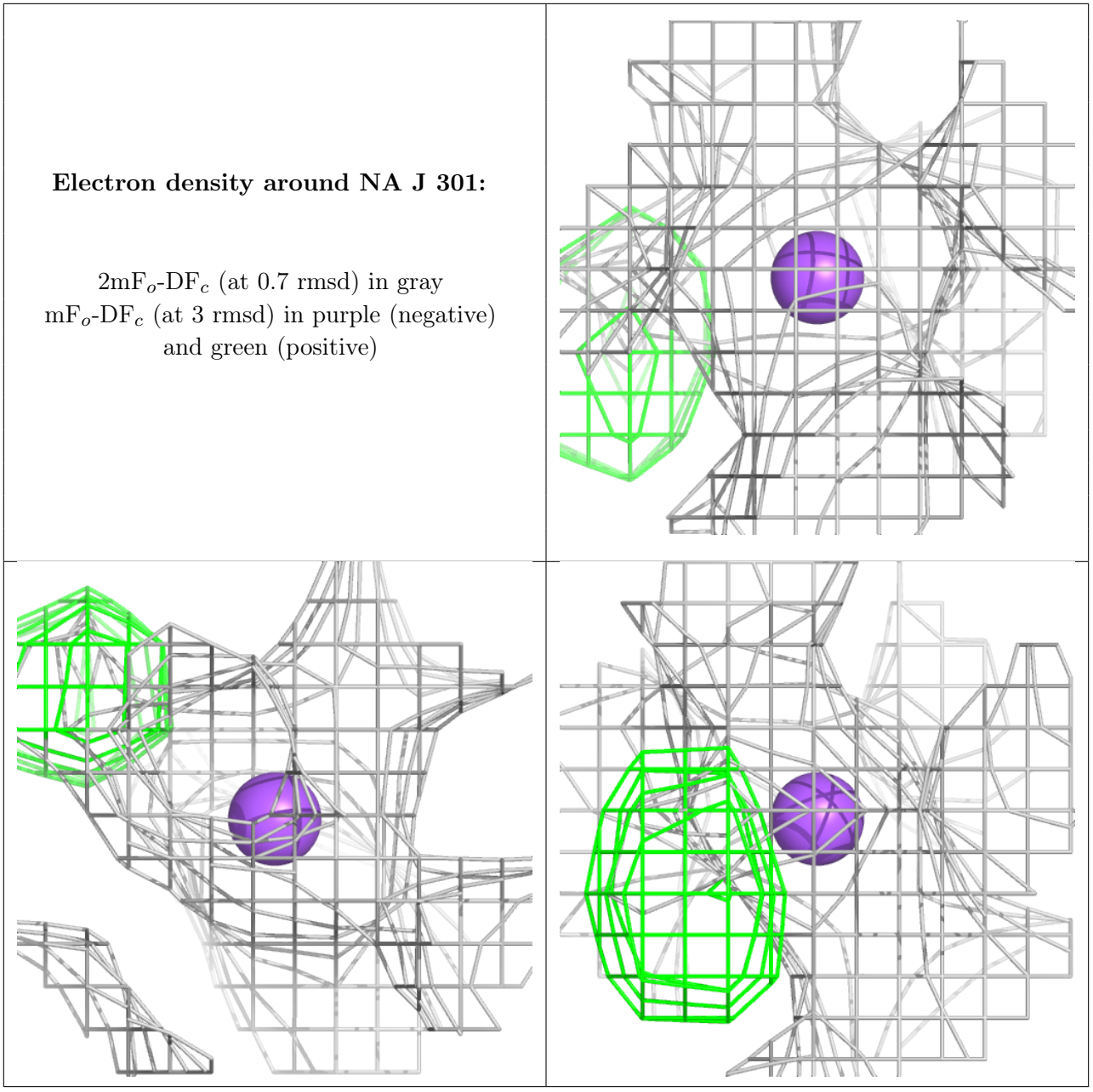
Electron density around NA G 304:

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



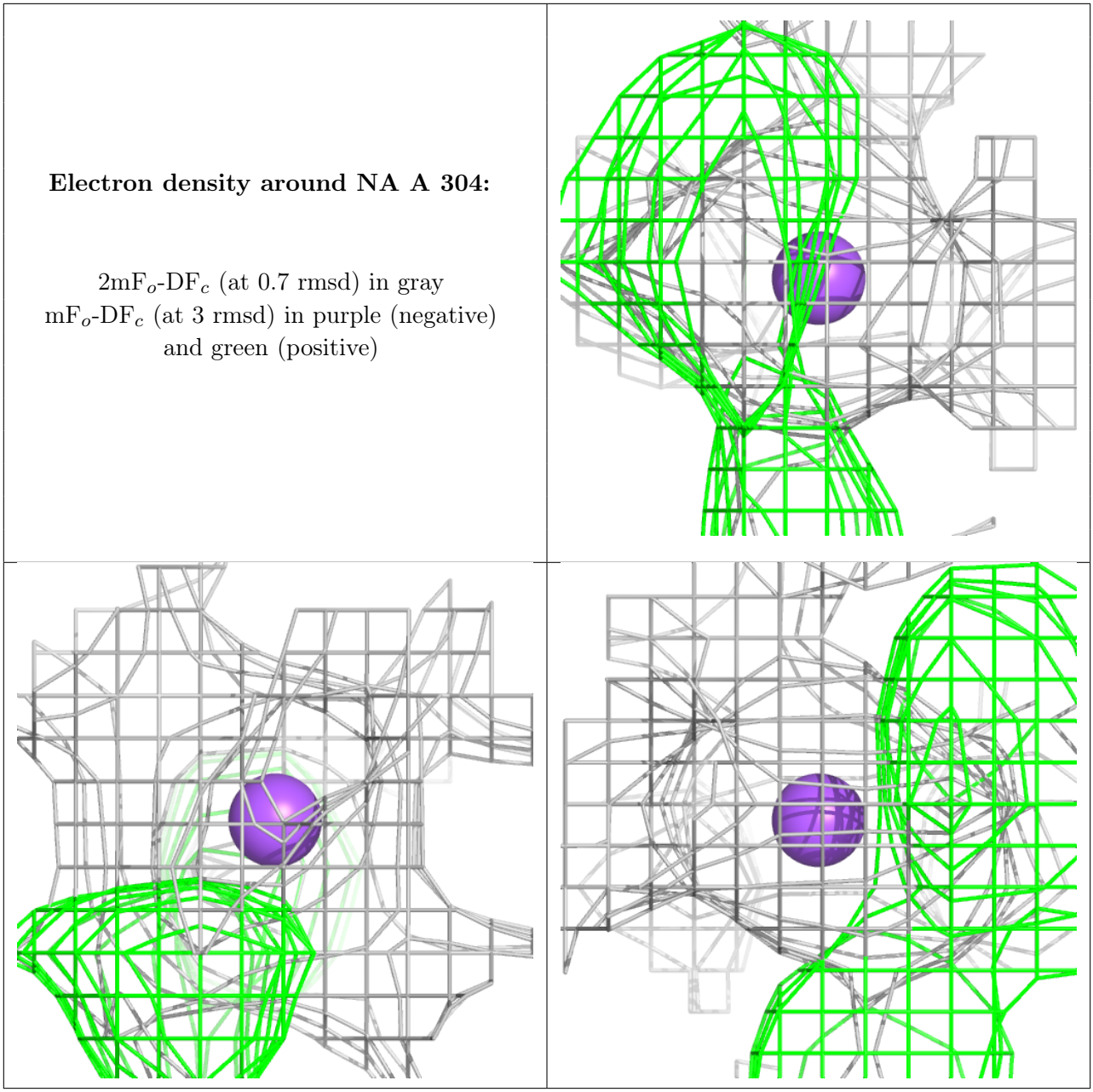
Electron density around NA J 301:

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



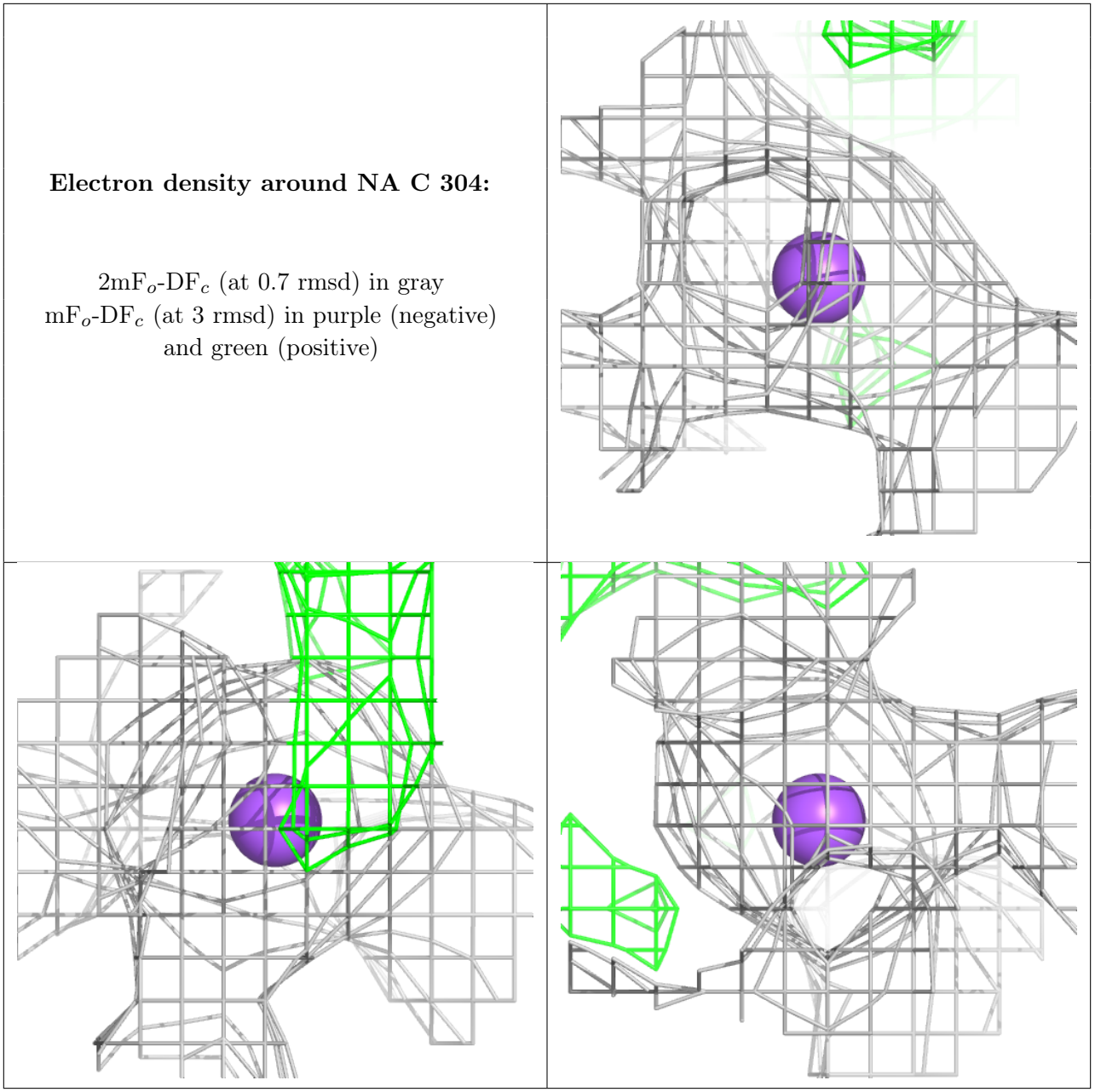
Electron density around NA A 304:

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



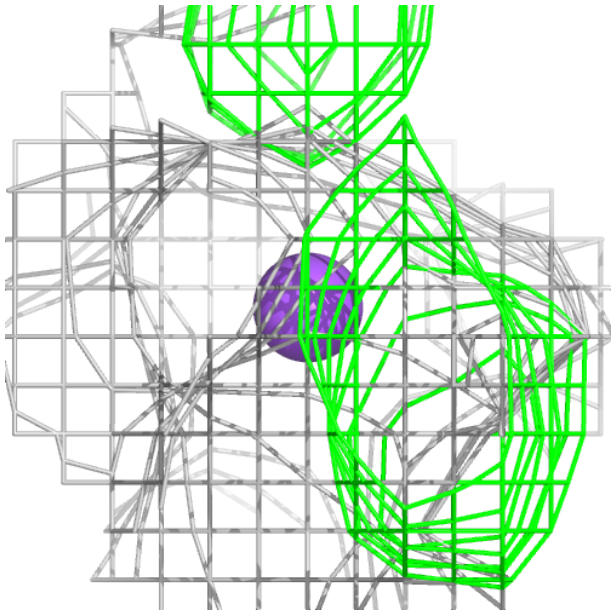
Electron density around NA C 304:

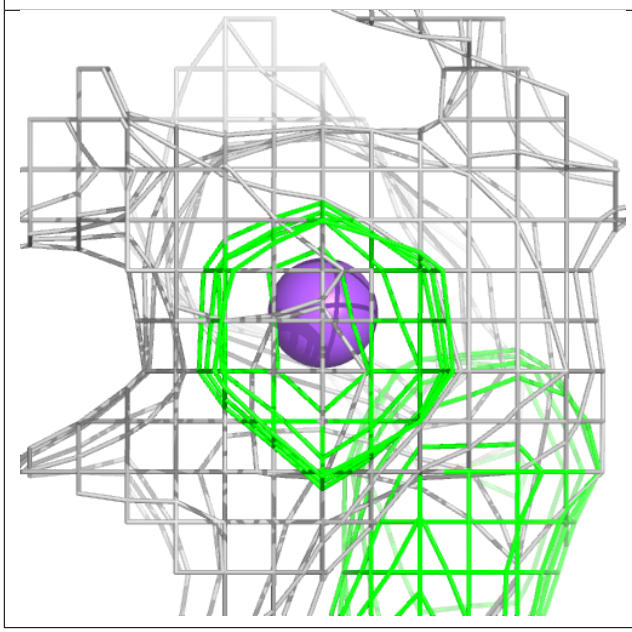
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

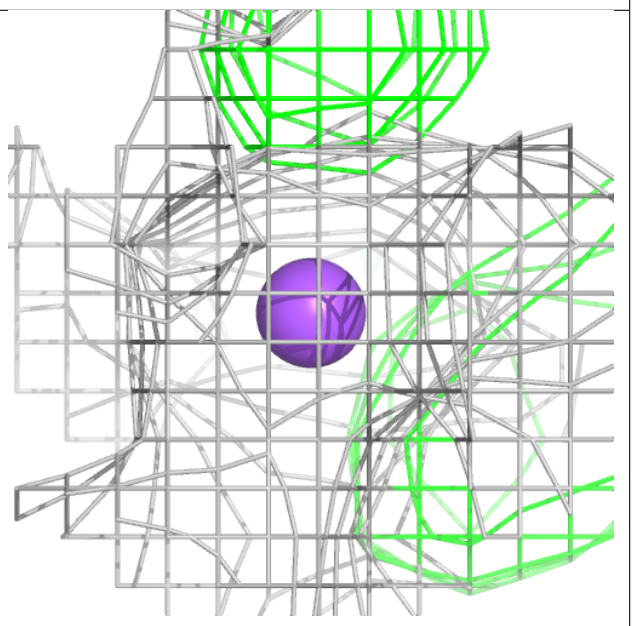


Electron density around NA K 304:

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

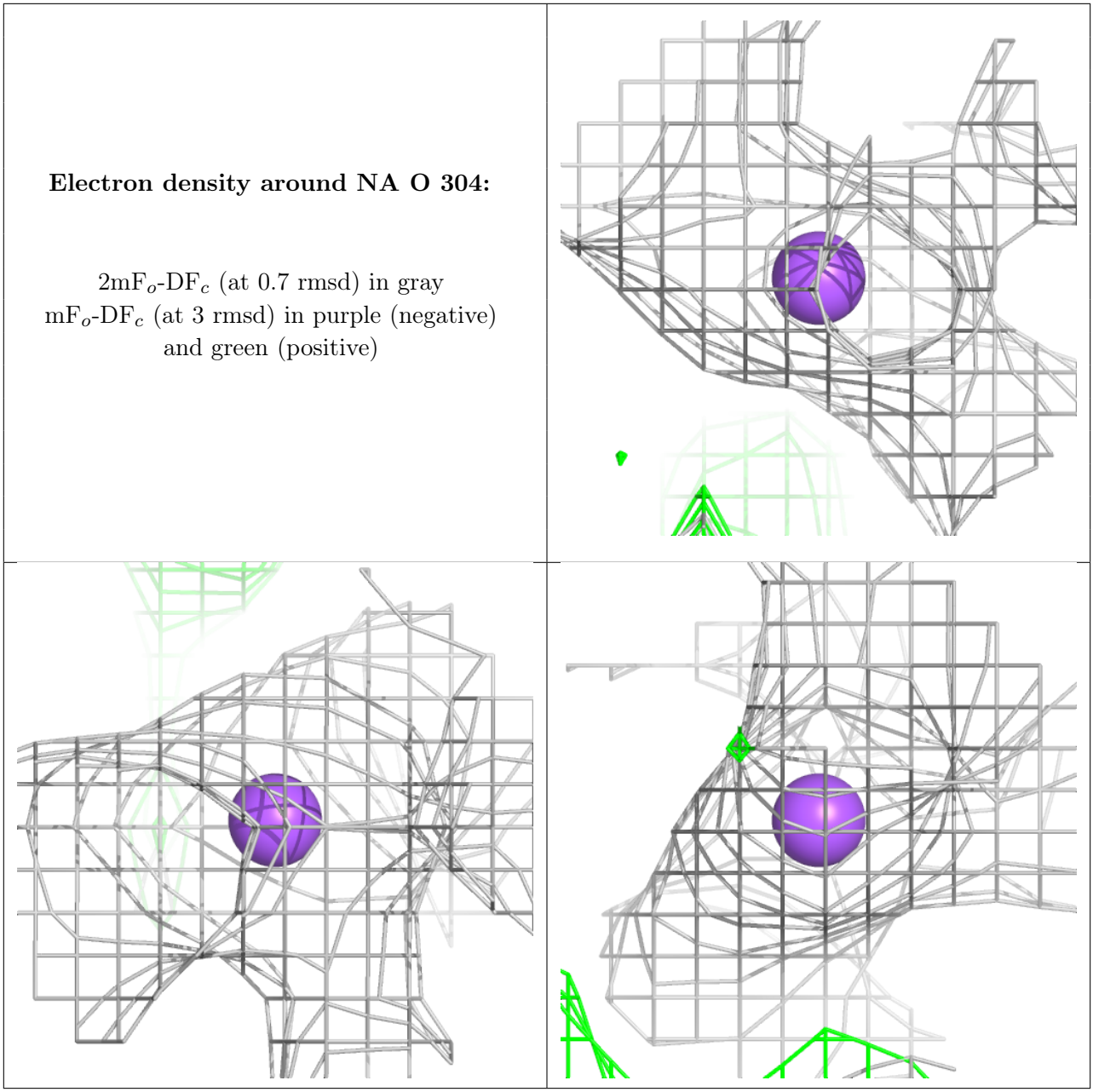






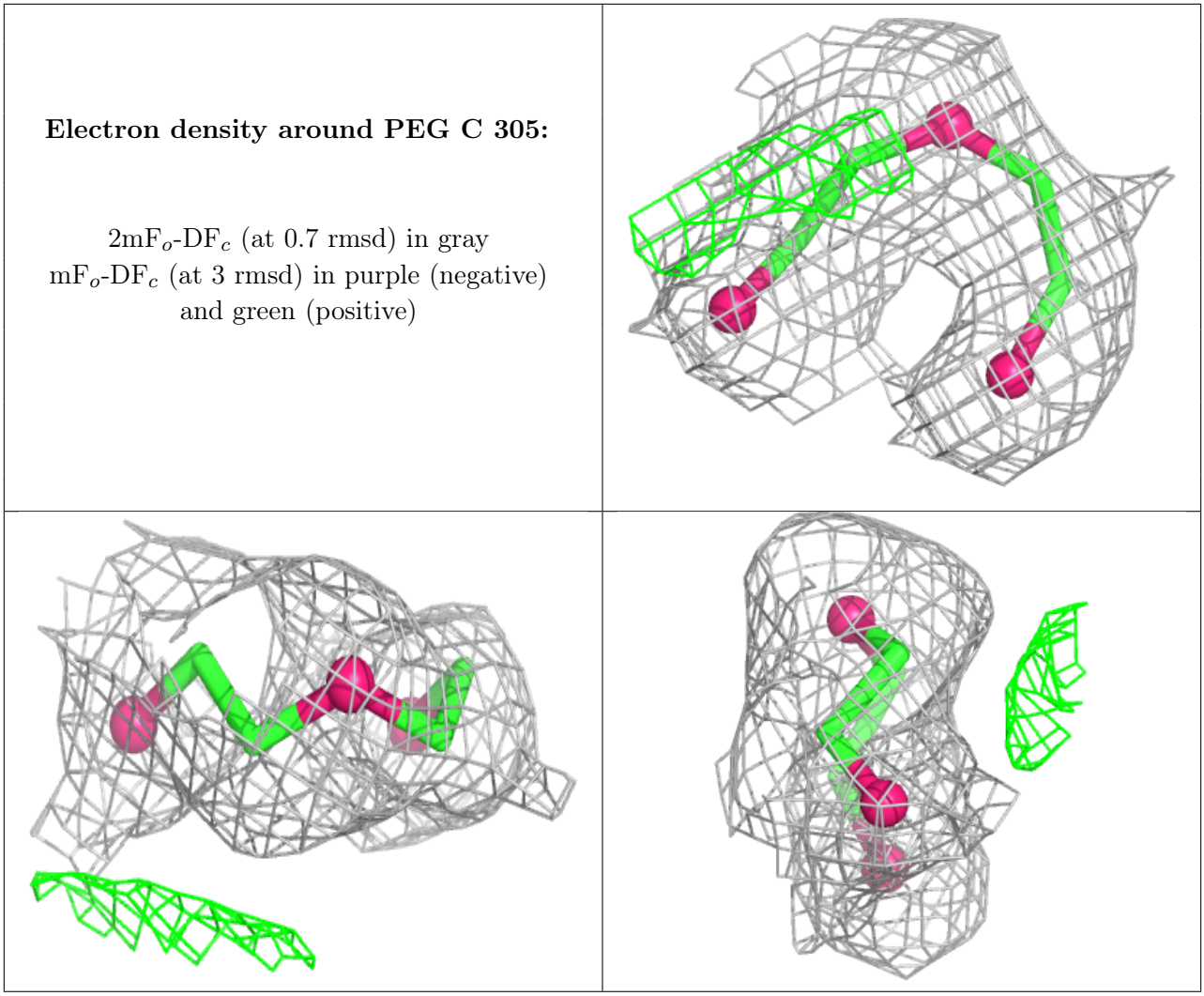
Electron density around NA O 304:

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



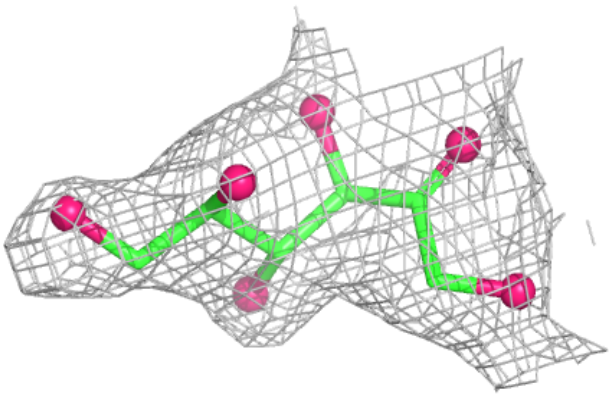
Electron density around PEG C 305:

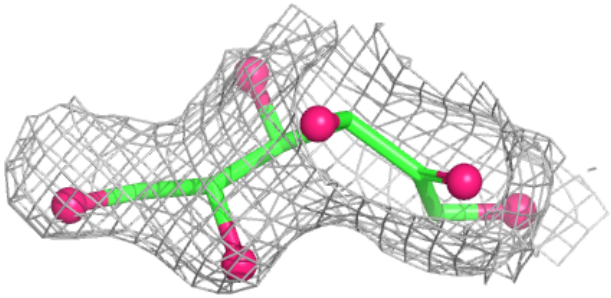
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

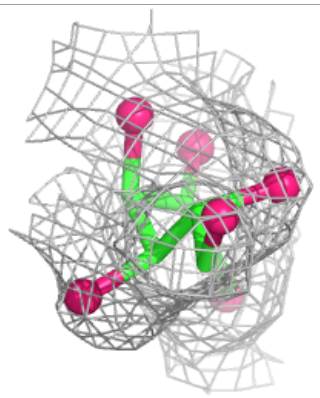


Electron density around PSJ I 301 (A):

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

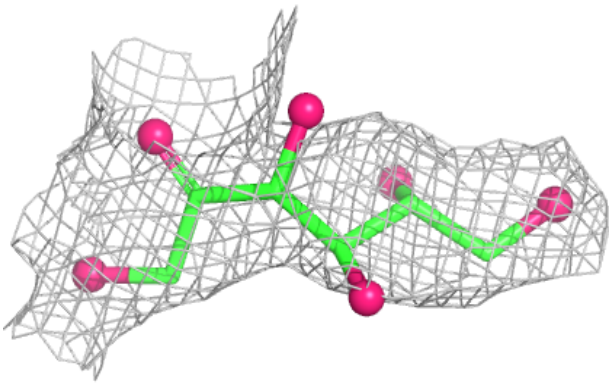


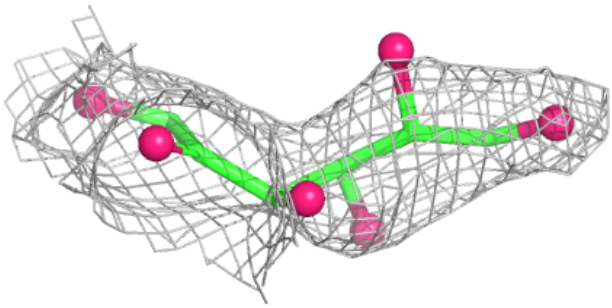


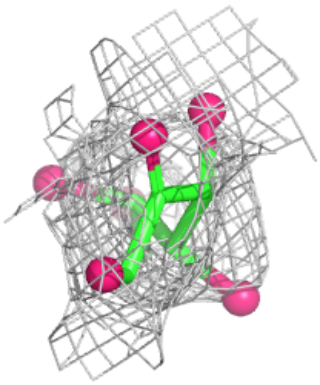


Electron density around PSJ L 301 (A):

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

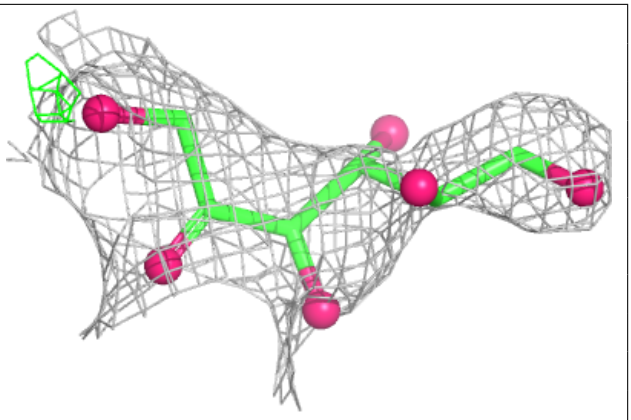


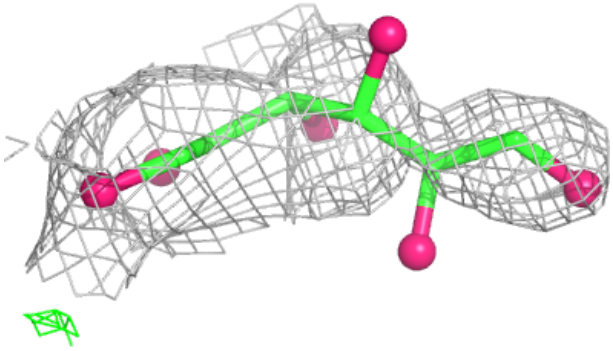


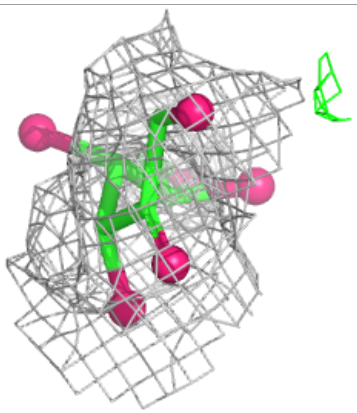


Electron density around PSJ M 301 (A):

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

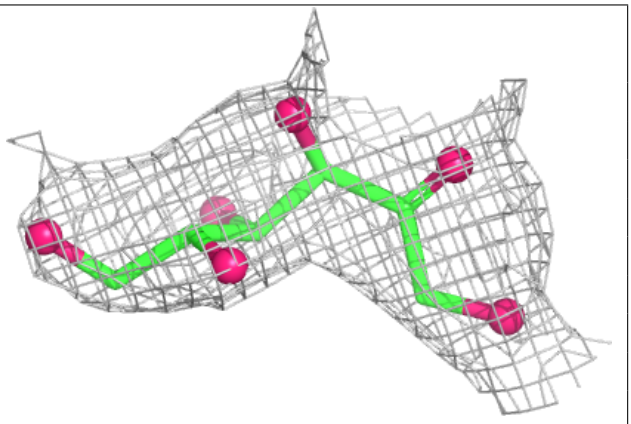


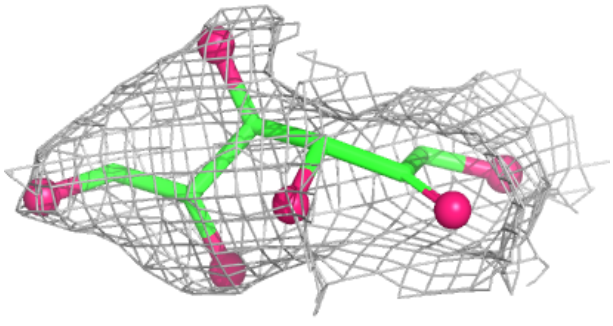


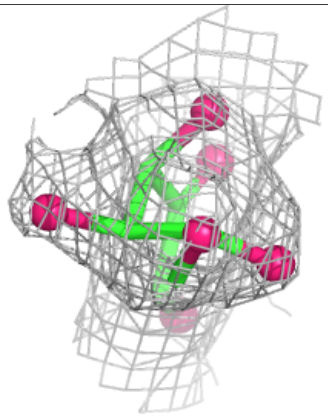


Electron density around PSJ N 302 (A):

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

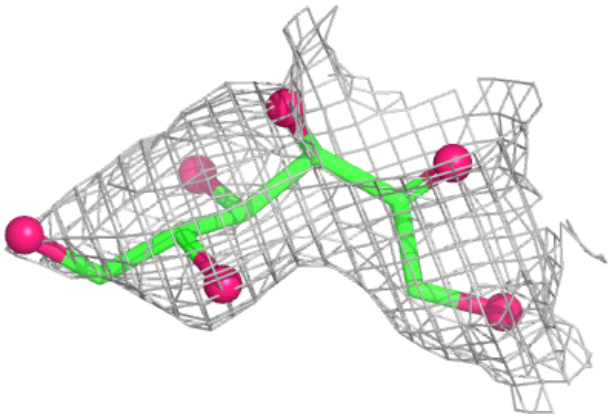


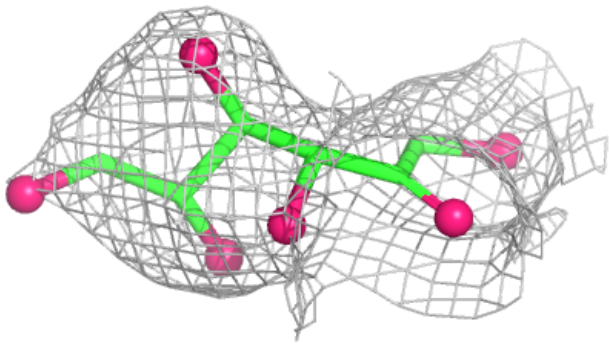


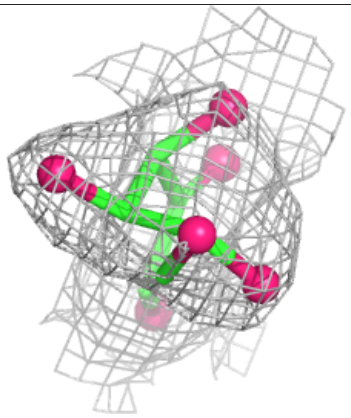


Electron density around PSJ P 301 (A):

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

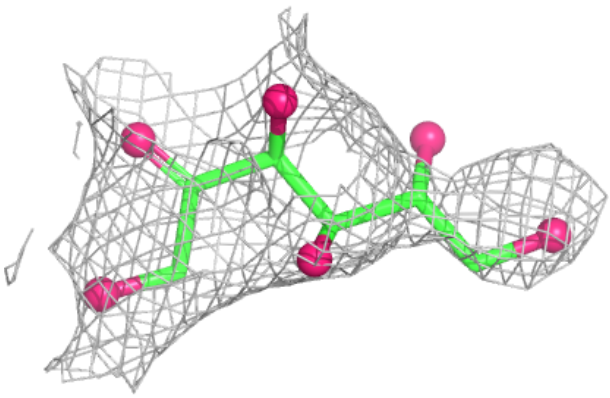


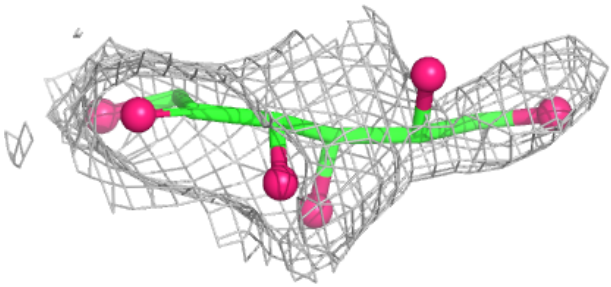


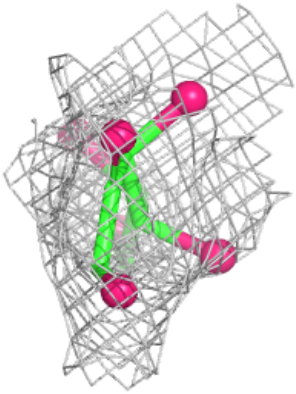


Electron density around FUD F 302 (B):

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

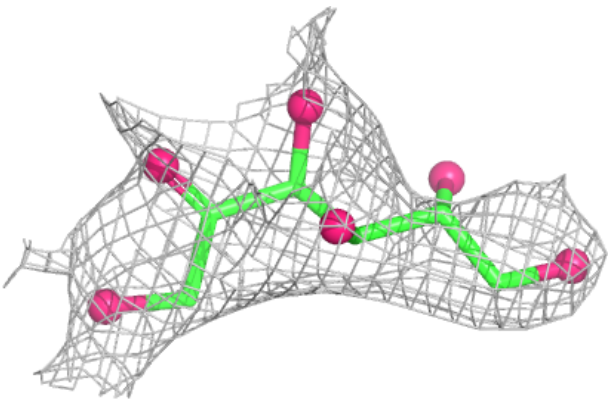


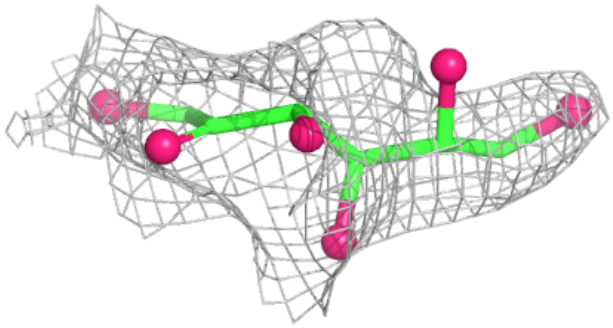




Electron density around FUD B 302 (B):

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

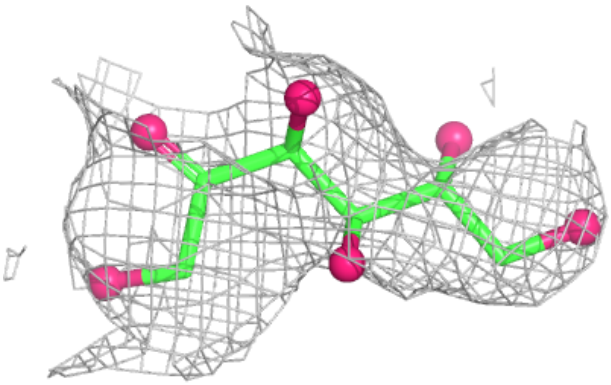


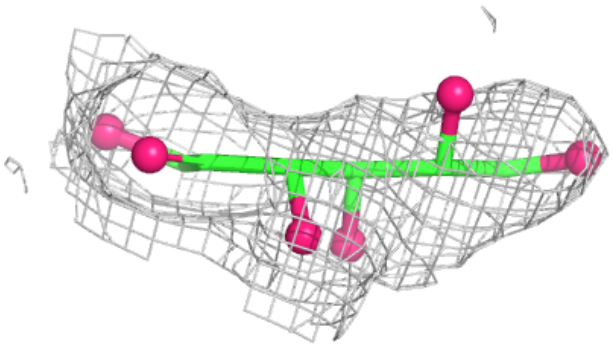


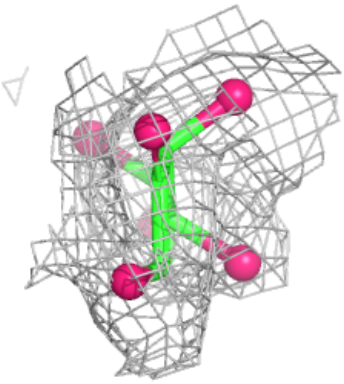


Electron density around FUD G 302 (B):

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

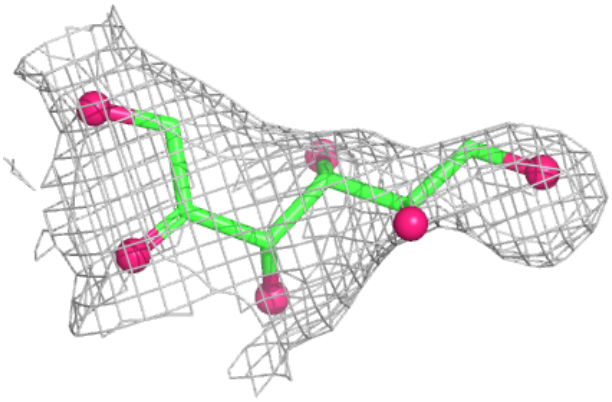


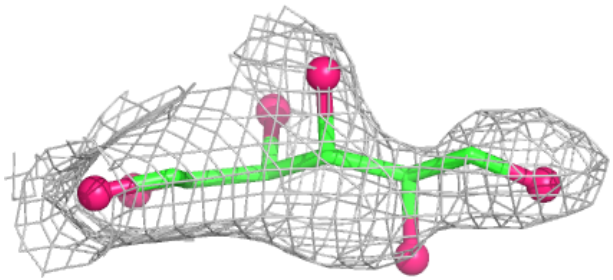


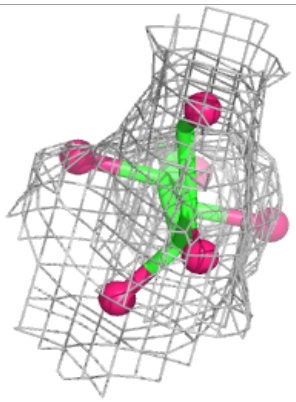


Electron density around FUD H 302 (B):

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

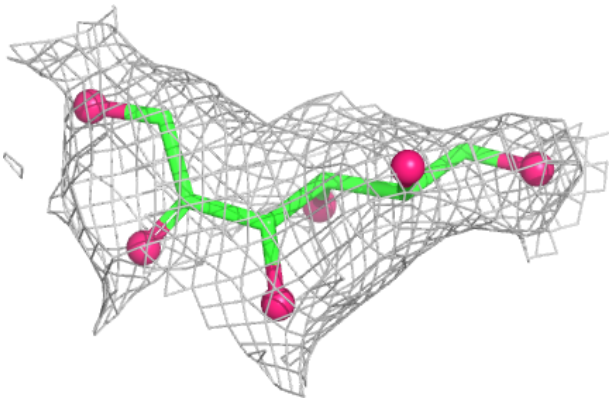


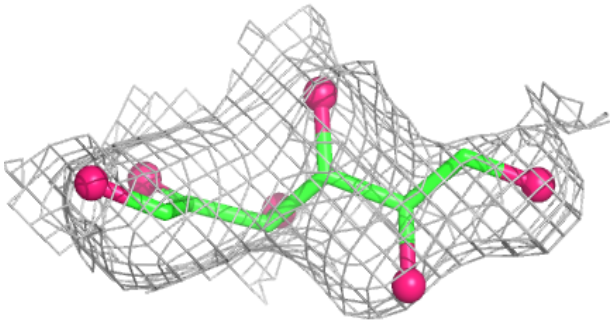


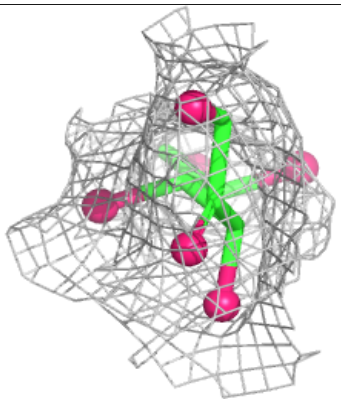


Electron density around FUD I 302 (B):

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

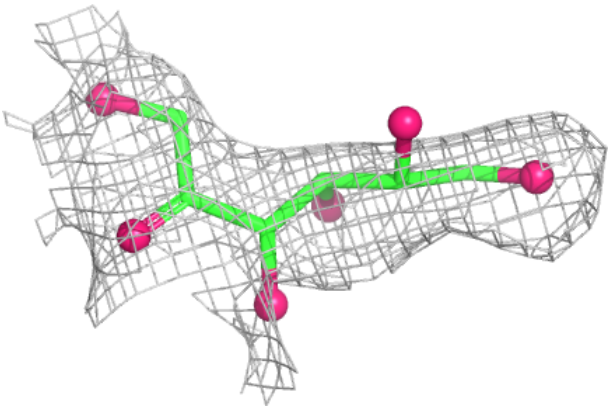


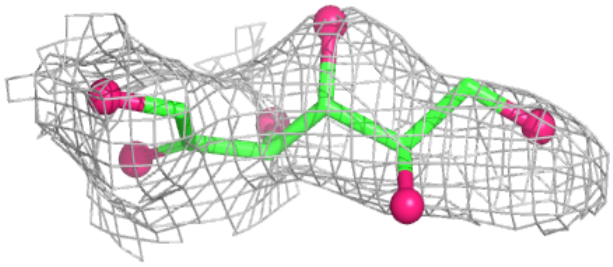


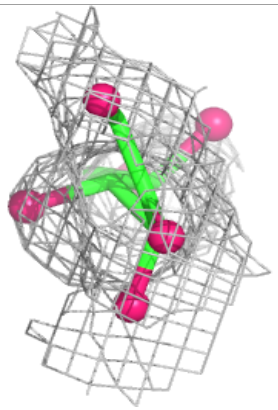


Electron density around FUD J 303 (B):

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



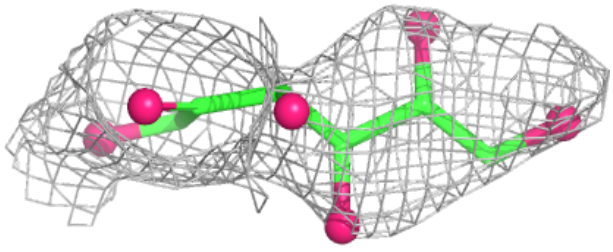


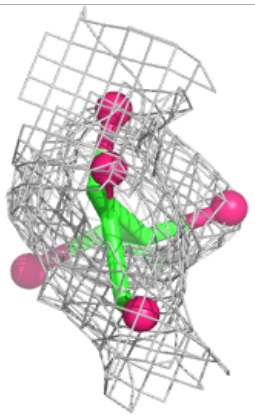


Electron density around FUD L 302 (B):

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

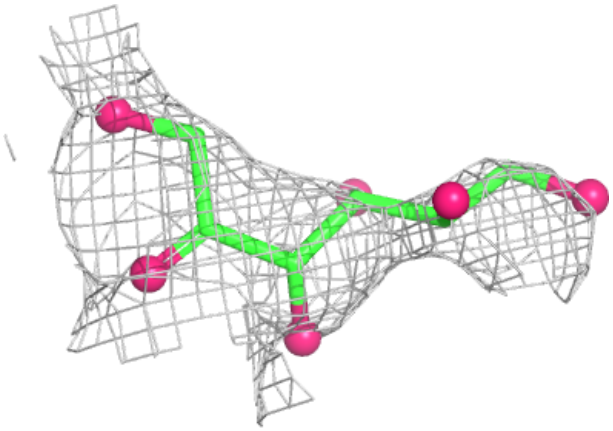


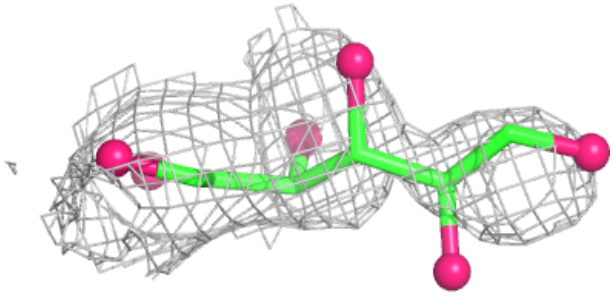


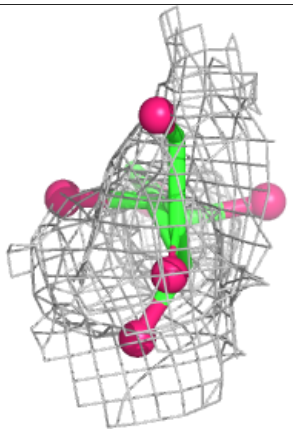


Electron density around FUD M 302 (B):

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

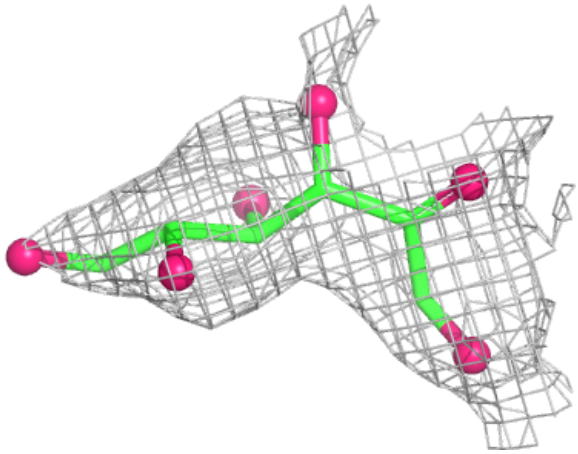


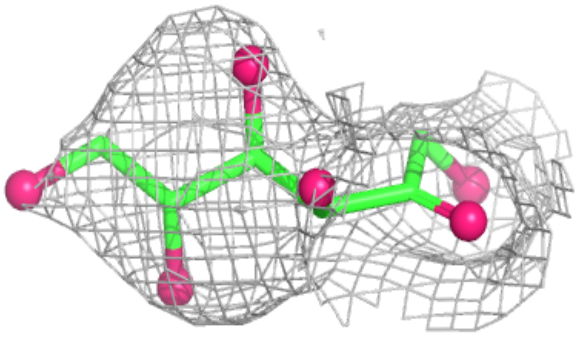


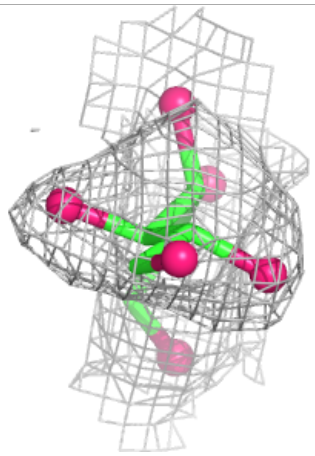


Electron density around FUD P 302 (B):

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

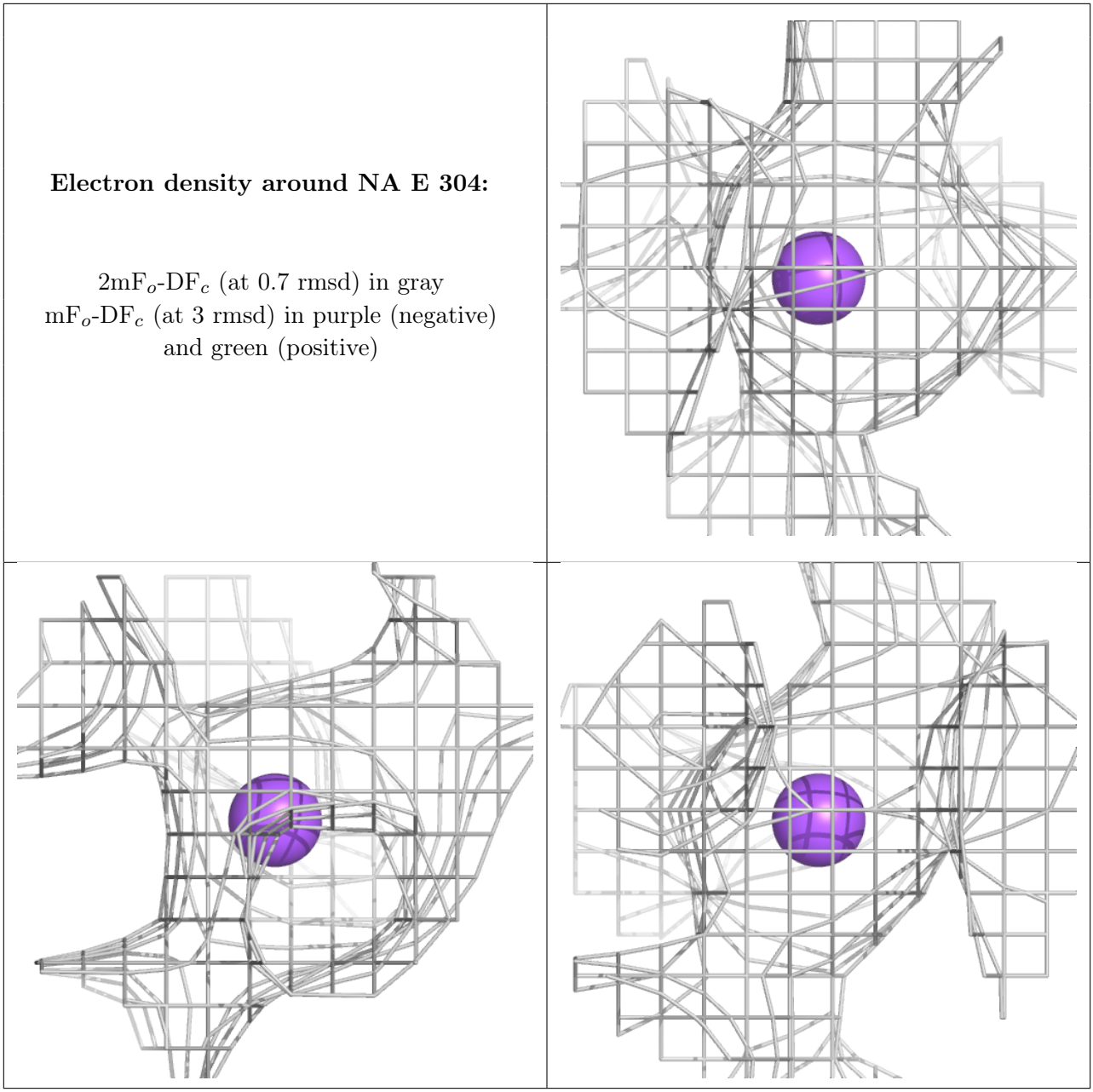






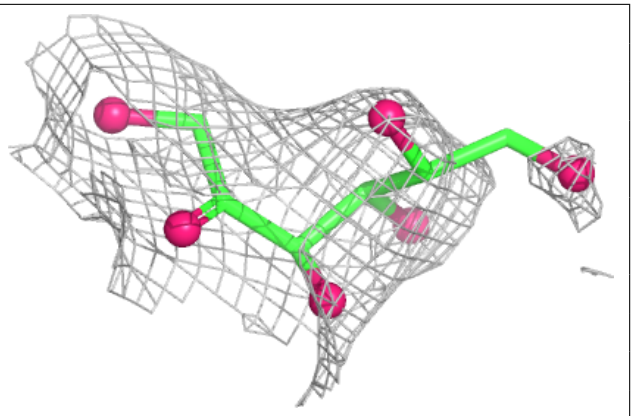
Electron density around NA E 304:

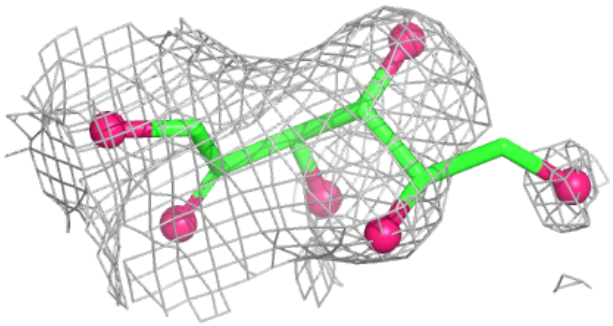
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

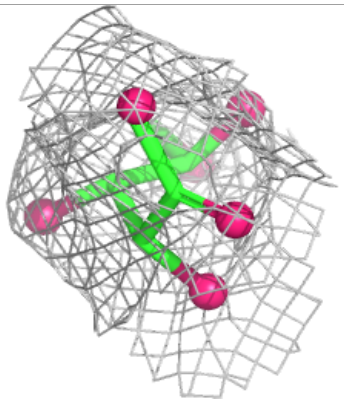


Electron density around PSJ E 301 (A):

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

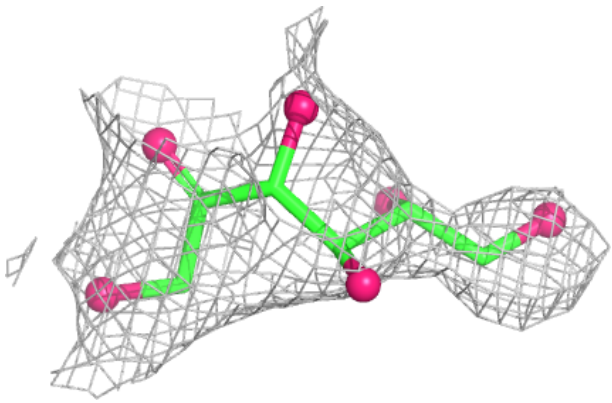


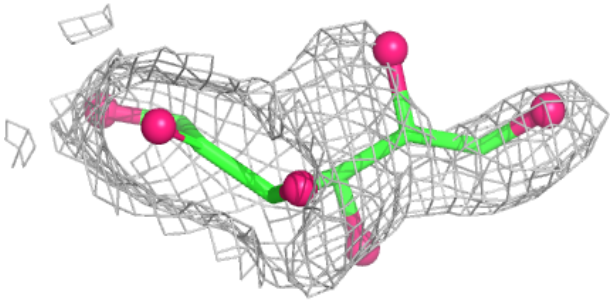


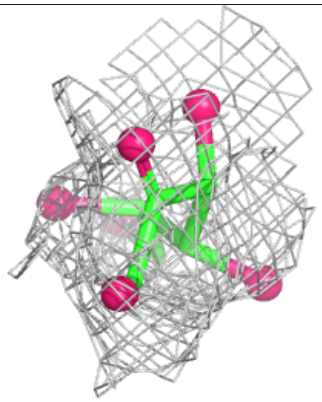


Electron density around PSJ F 301 (A):

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

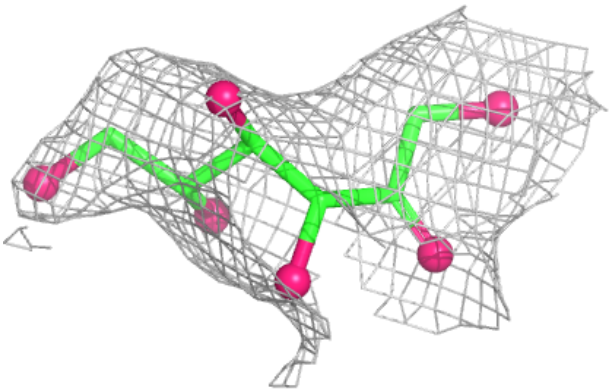


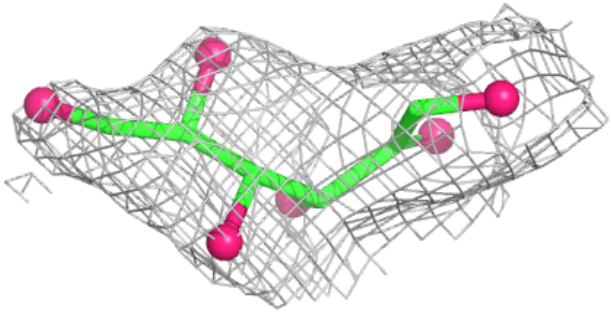


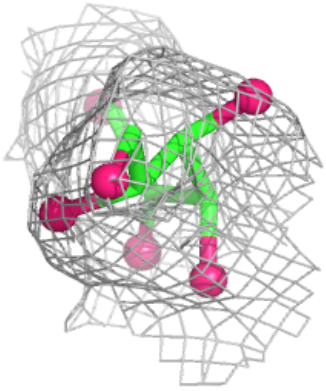


Electron density around PSJ A 301 (A):

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

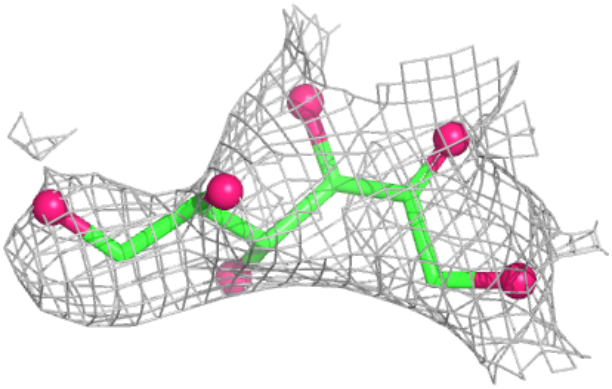


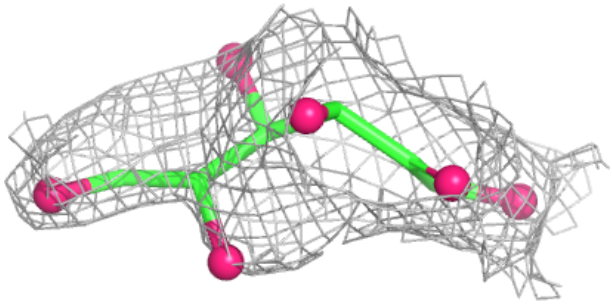


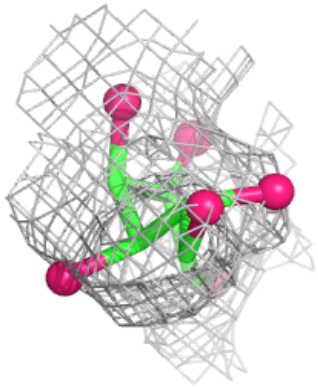


Electron density around PSJ B 301 (A):

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

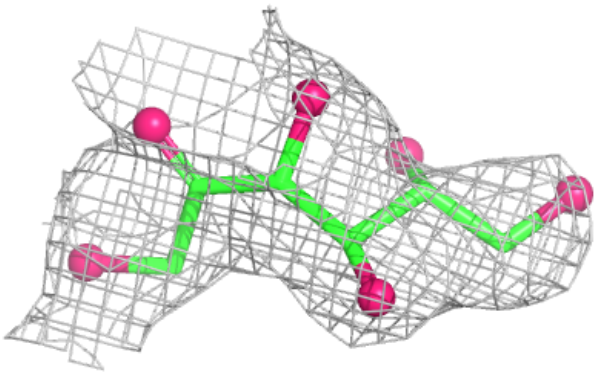


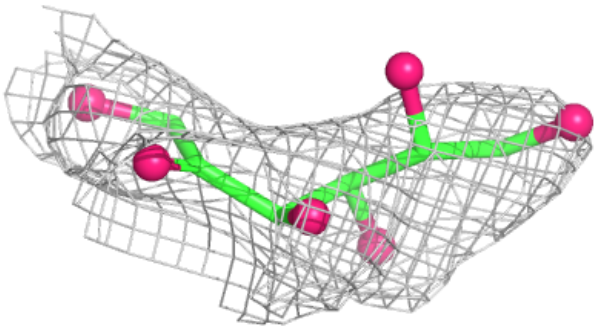


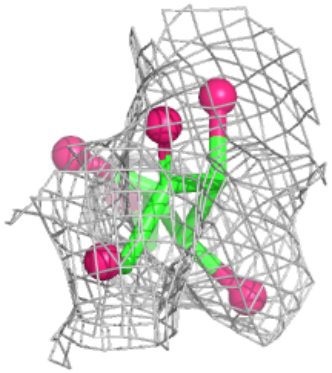


Electron density around PSJ C 301 (A):

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

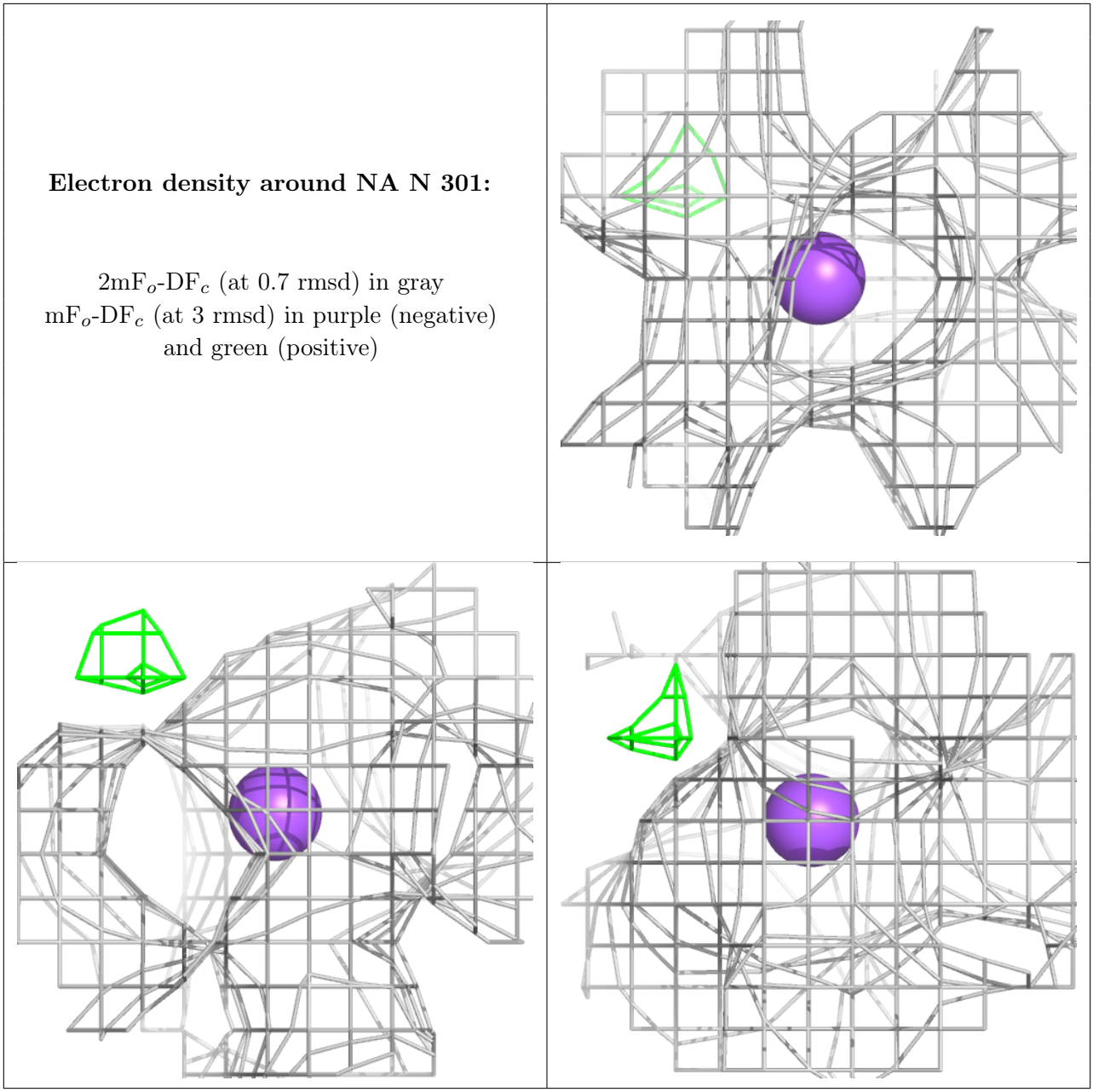






Electron density around NA N 301:

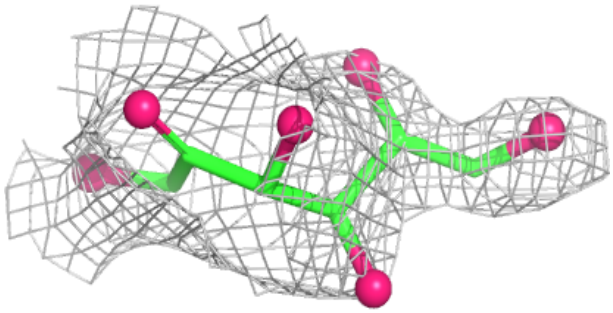
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

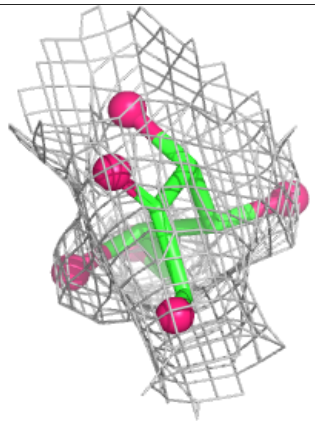


Electron density around PSJ D 301 (A):

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

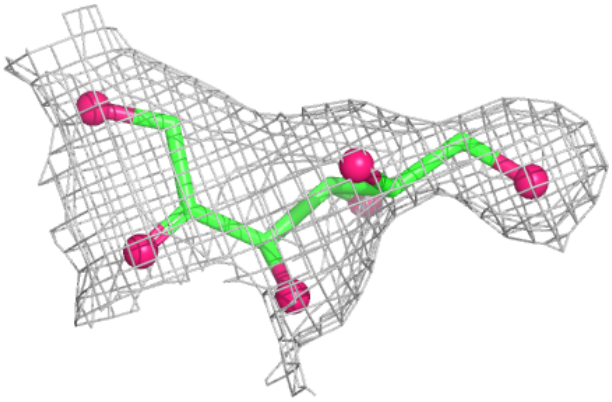


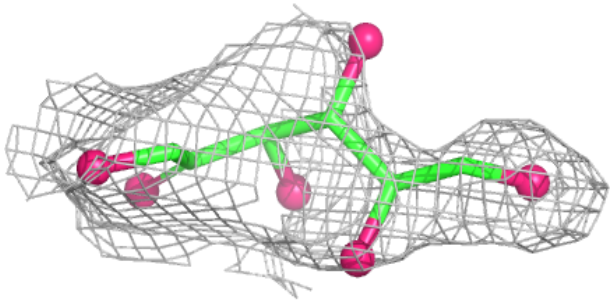


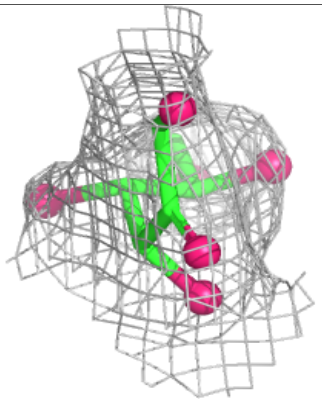


Electron density around PSJ H 301 (A):

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

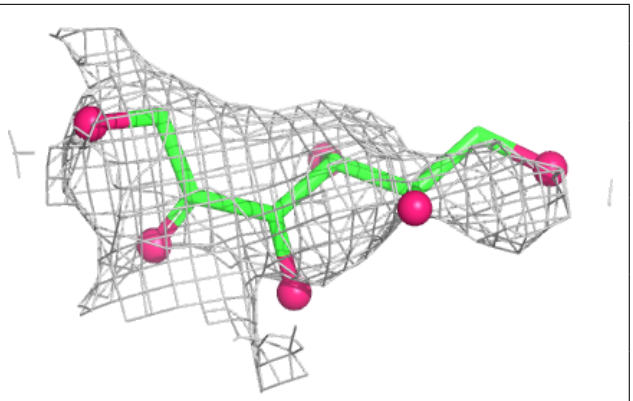


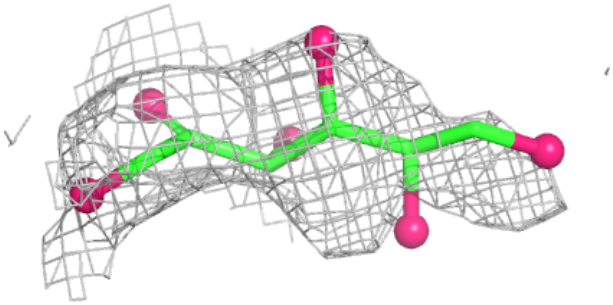


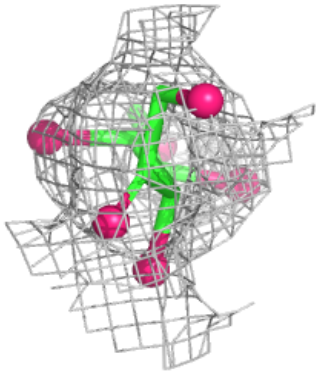


Electron density around FUD O 302 (B):

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

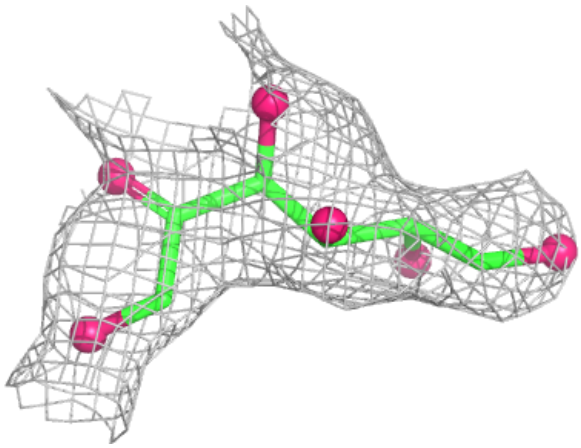


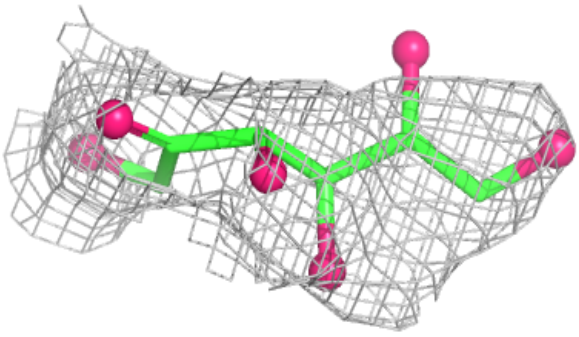


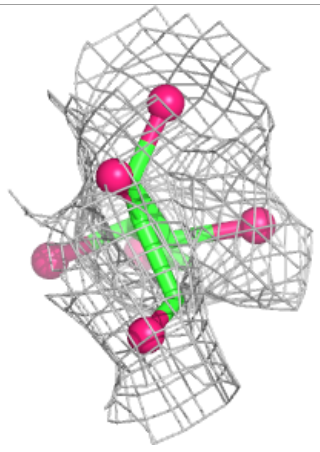


Electron density around FUD C 302 (B):

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

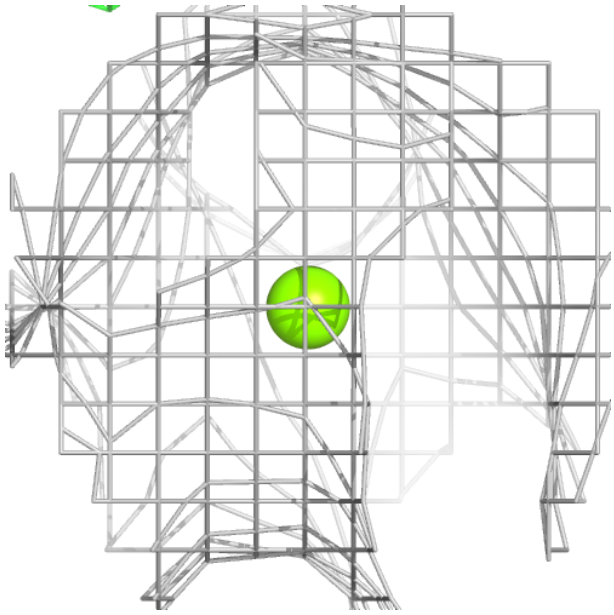


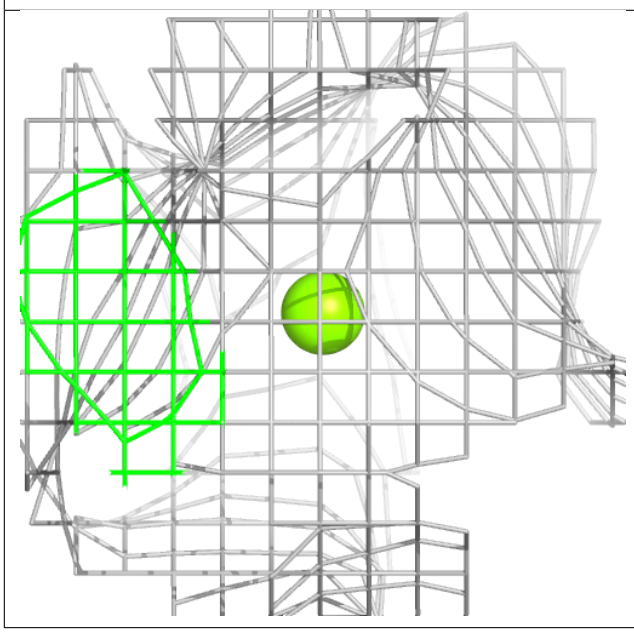


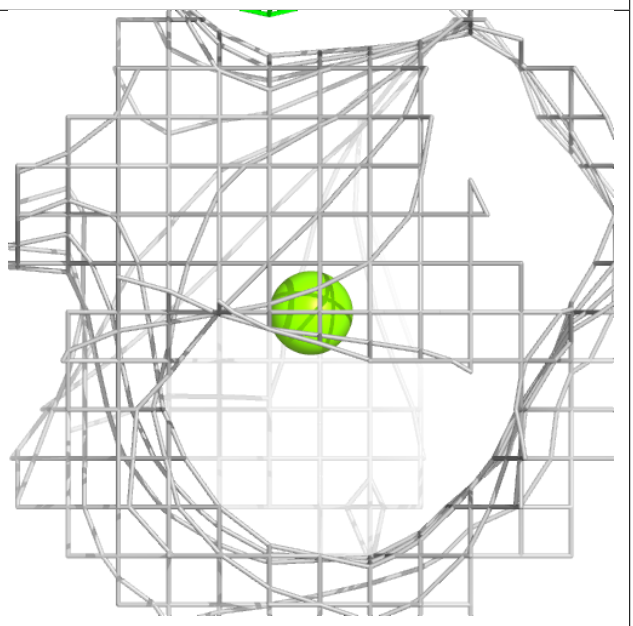


Electron density around MG E 303:

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

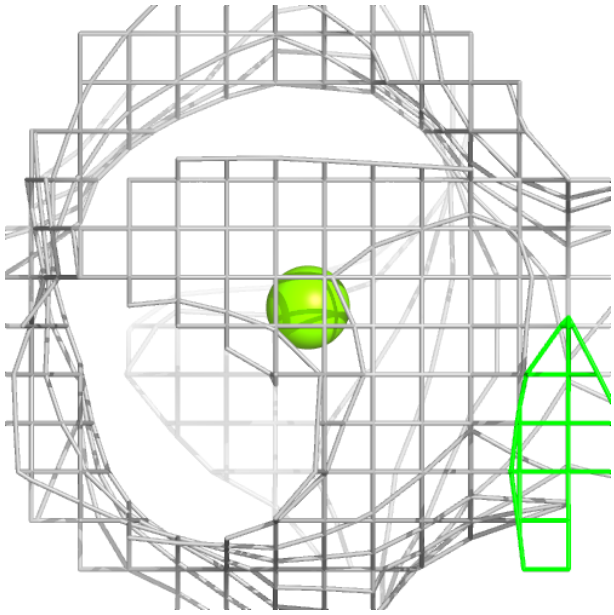


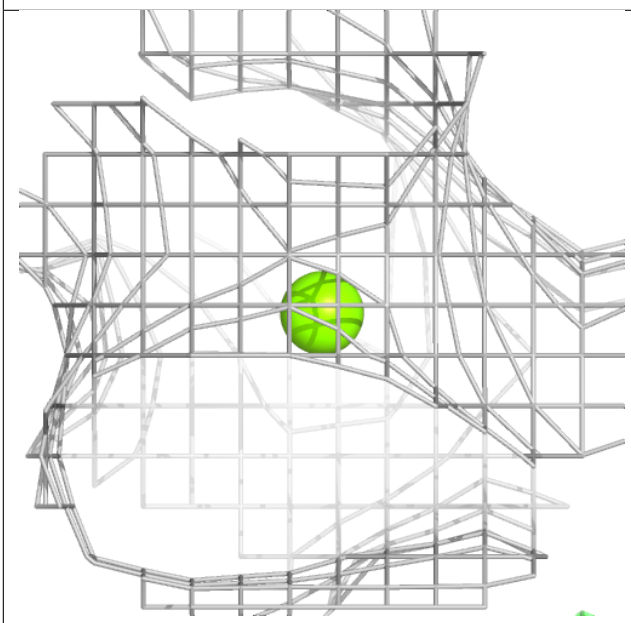


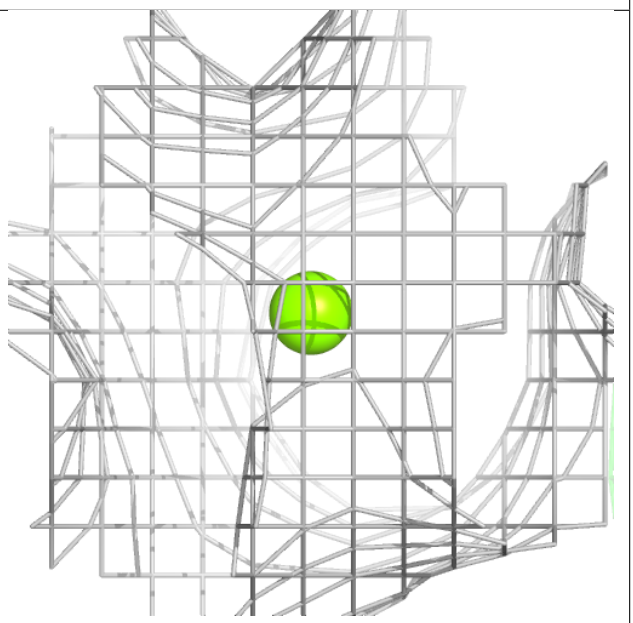


Electron density around MG F 303:

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

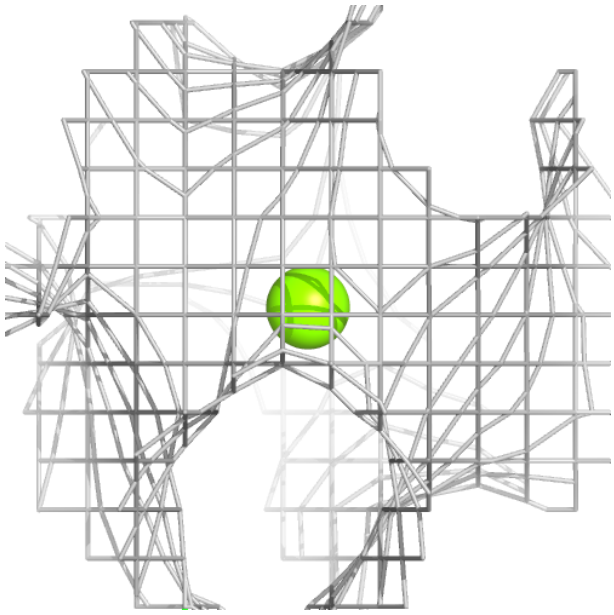


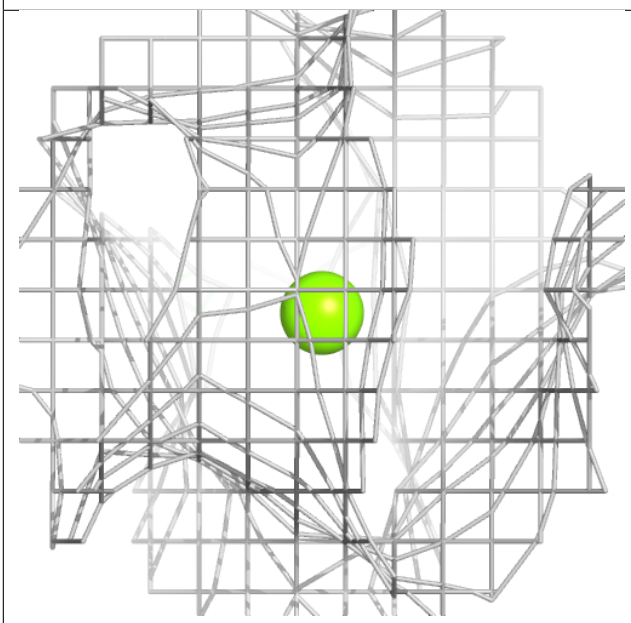


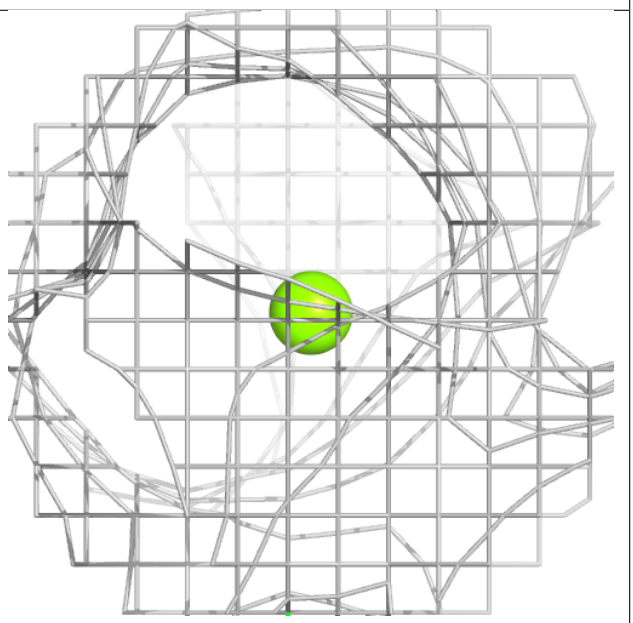


Electron density around MG A 303:

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

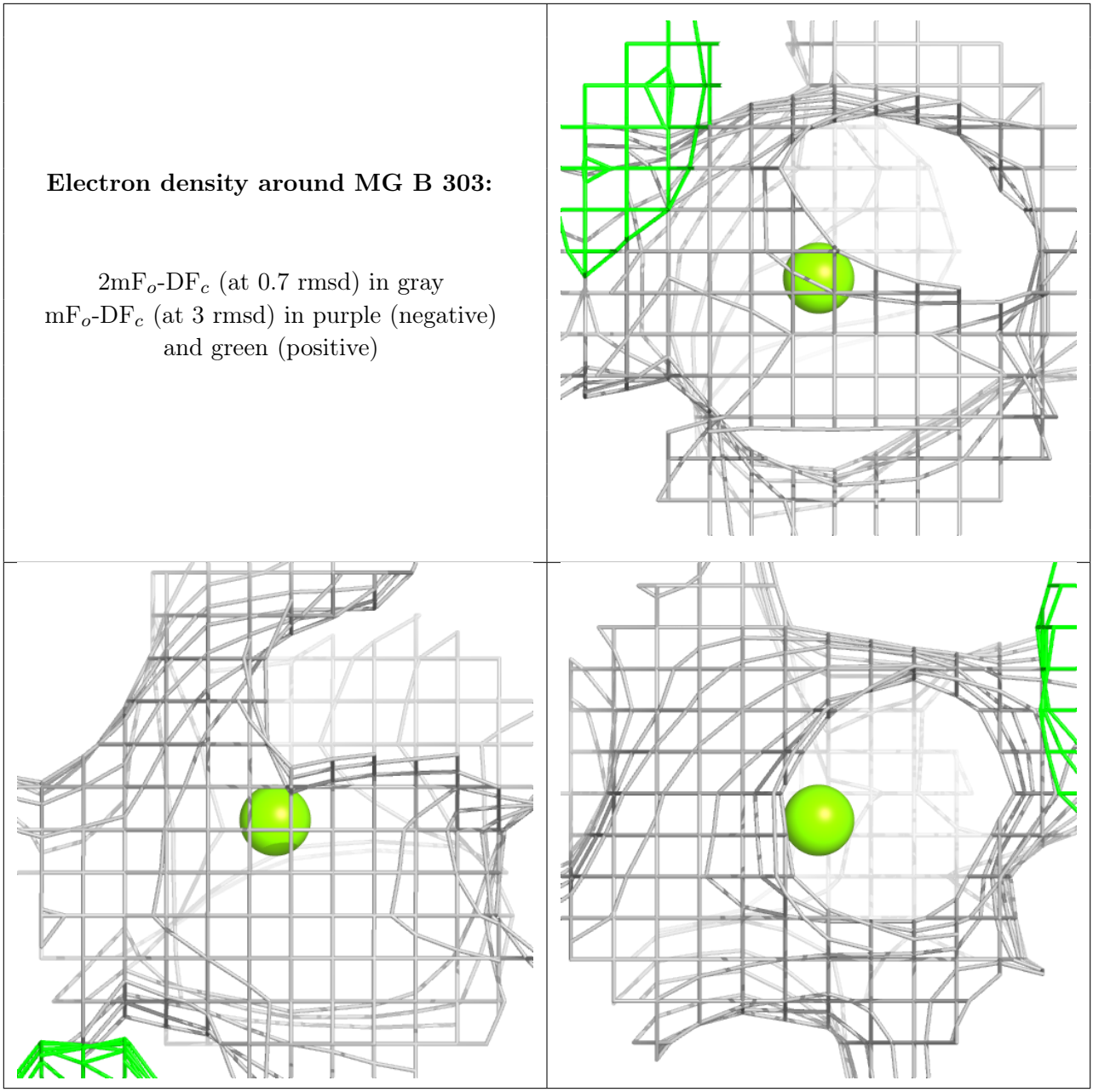






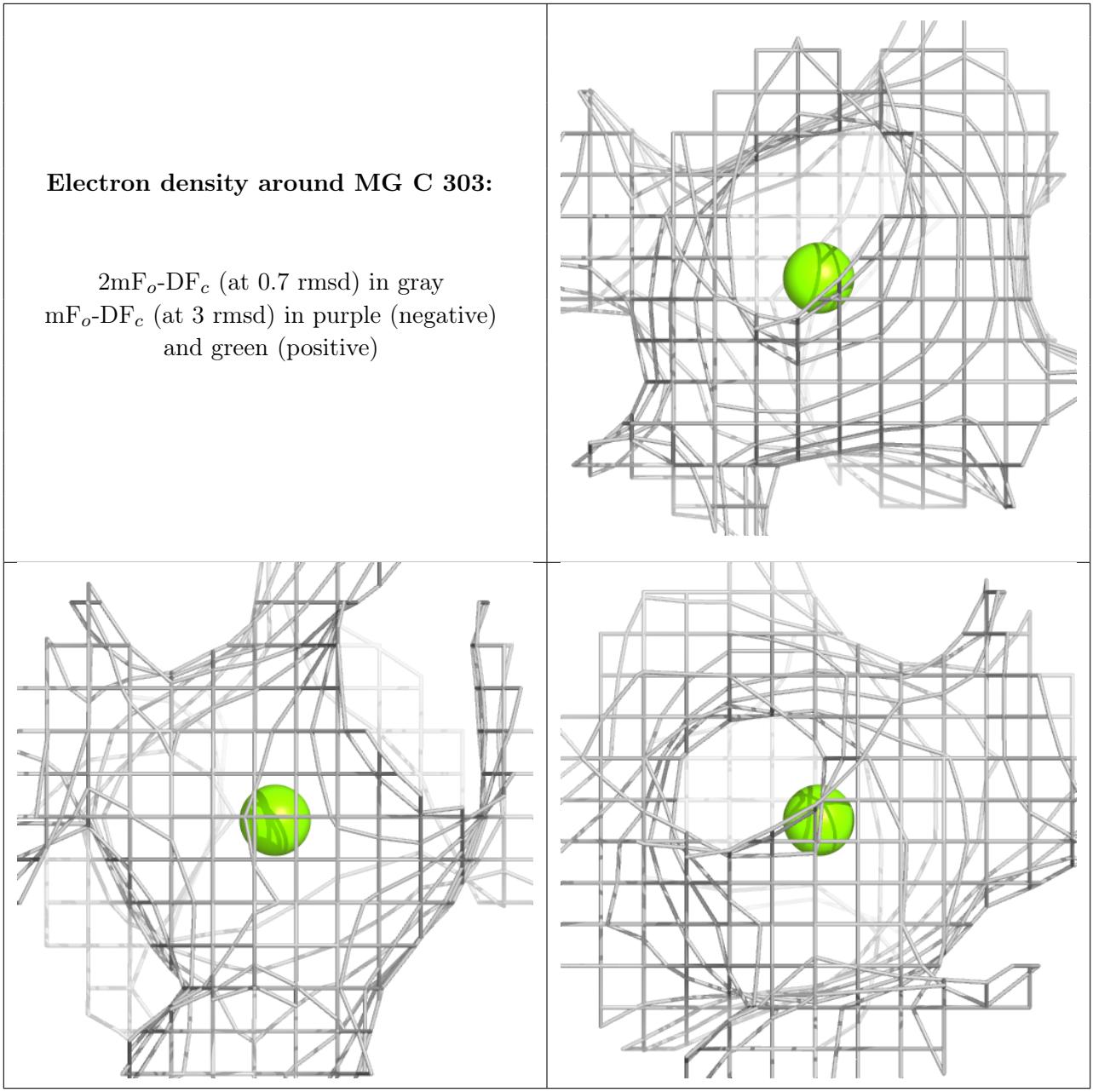
Electron density around MG B 303:

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



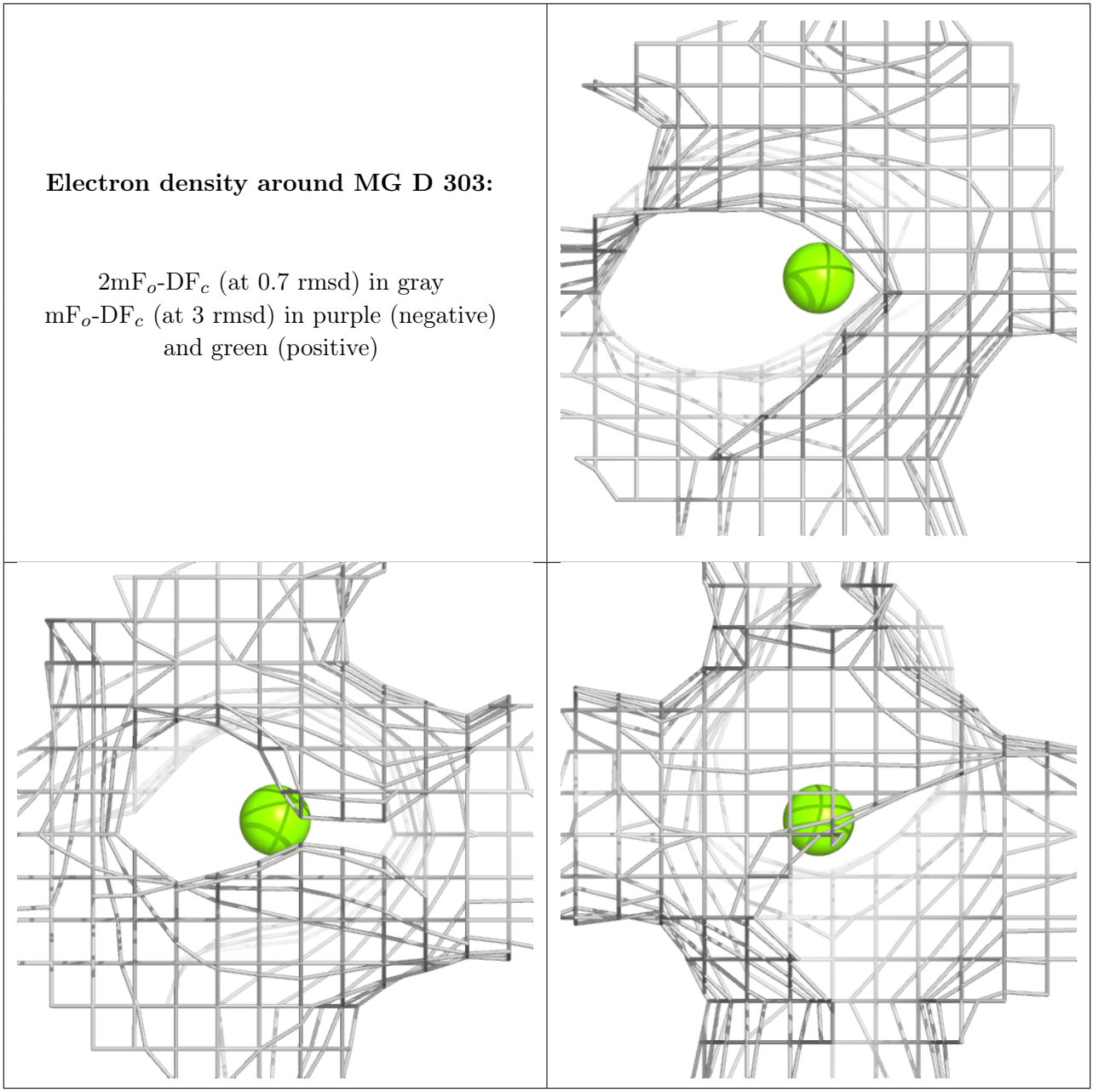
Electron density around MG C 303:

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



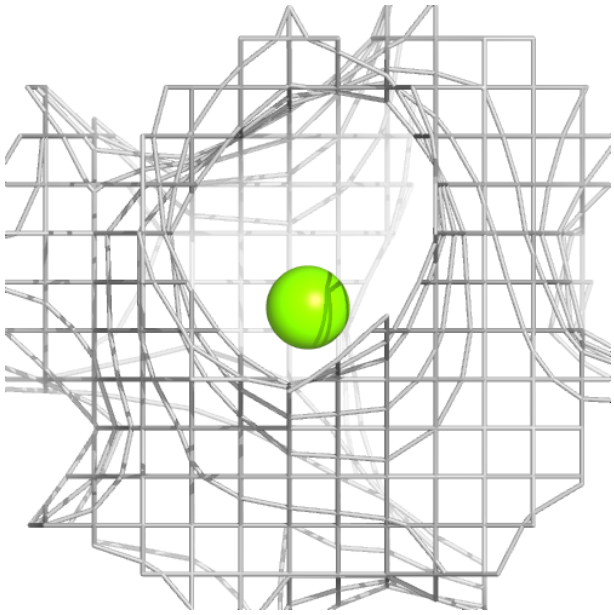
Electron density around MG D 303:

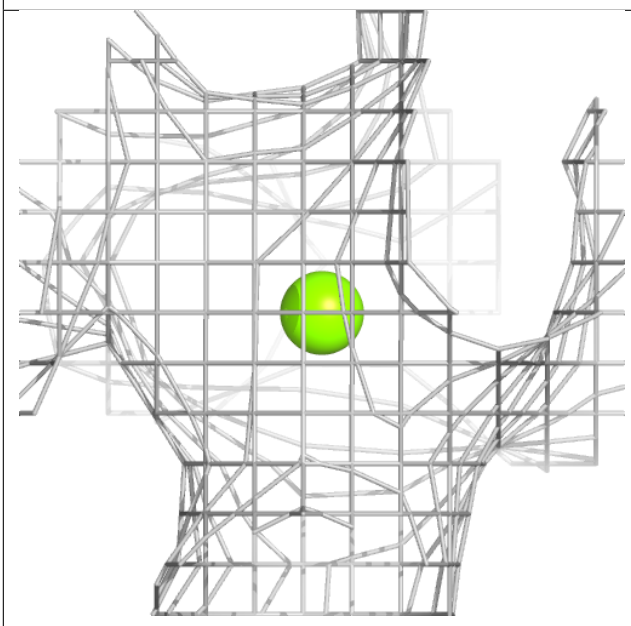
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

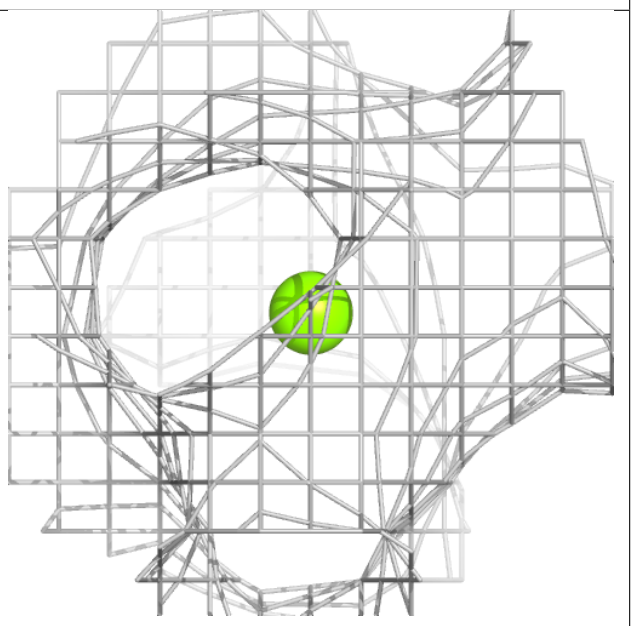


Electron density around MG G 303:

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

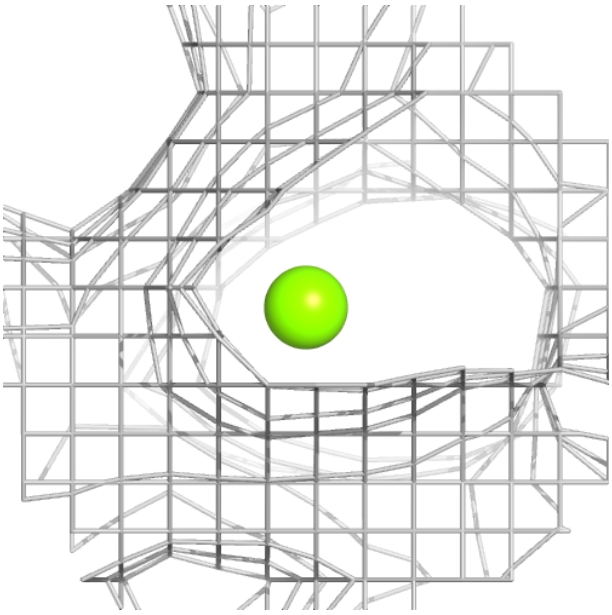


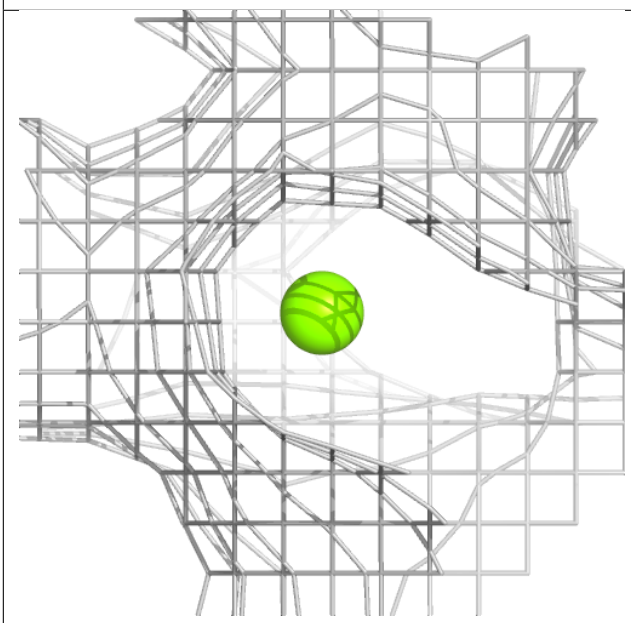


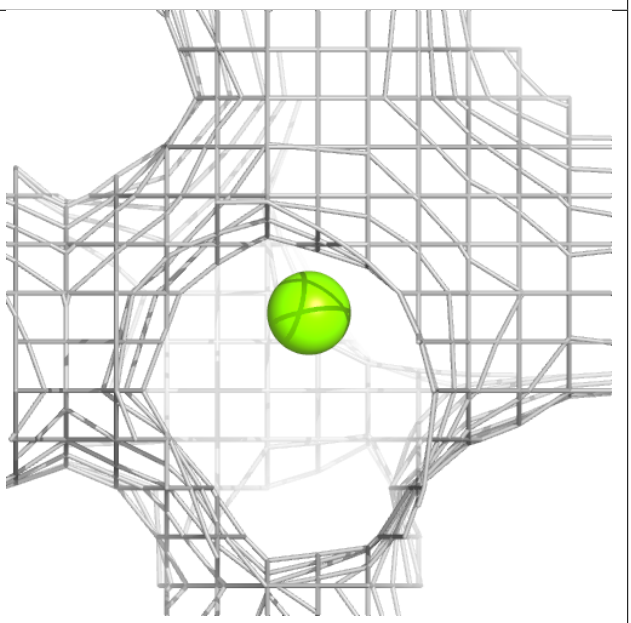


Electron density around MG H 303:

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

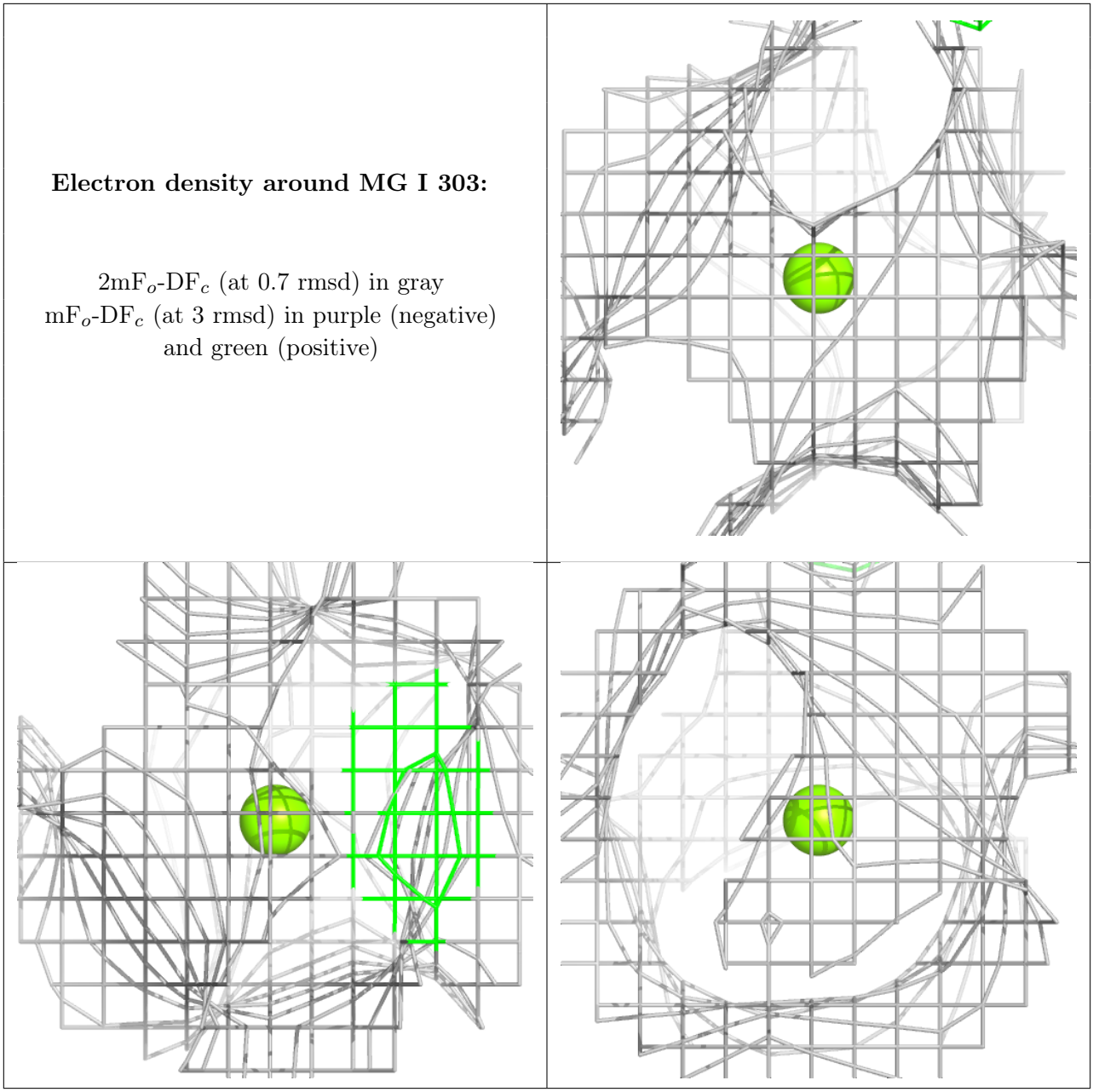






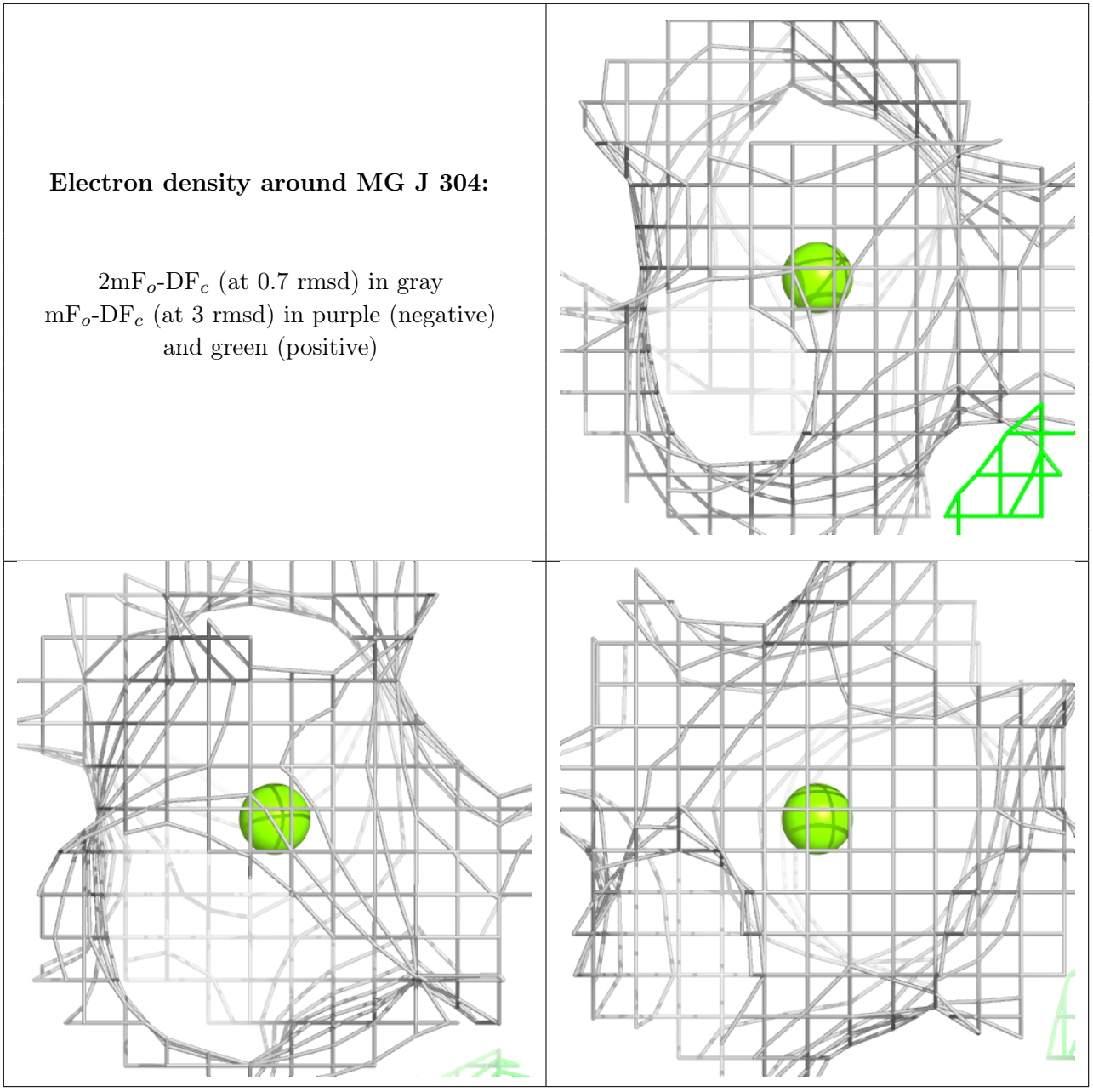
Electron density around MG I 303:

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



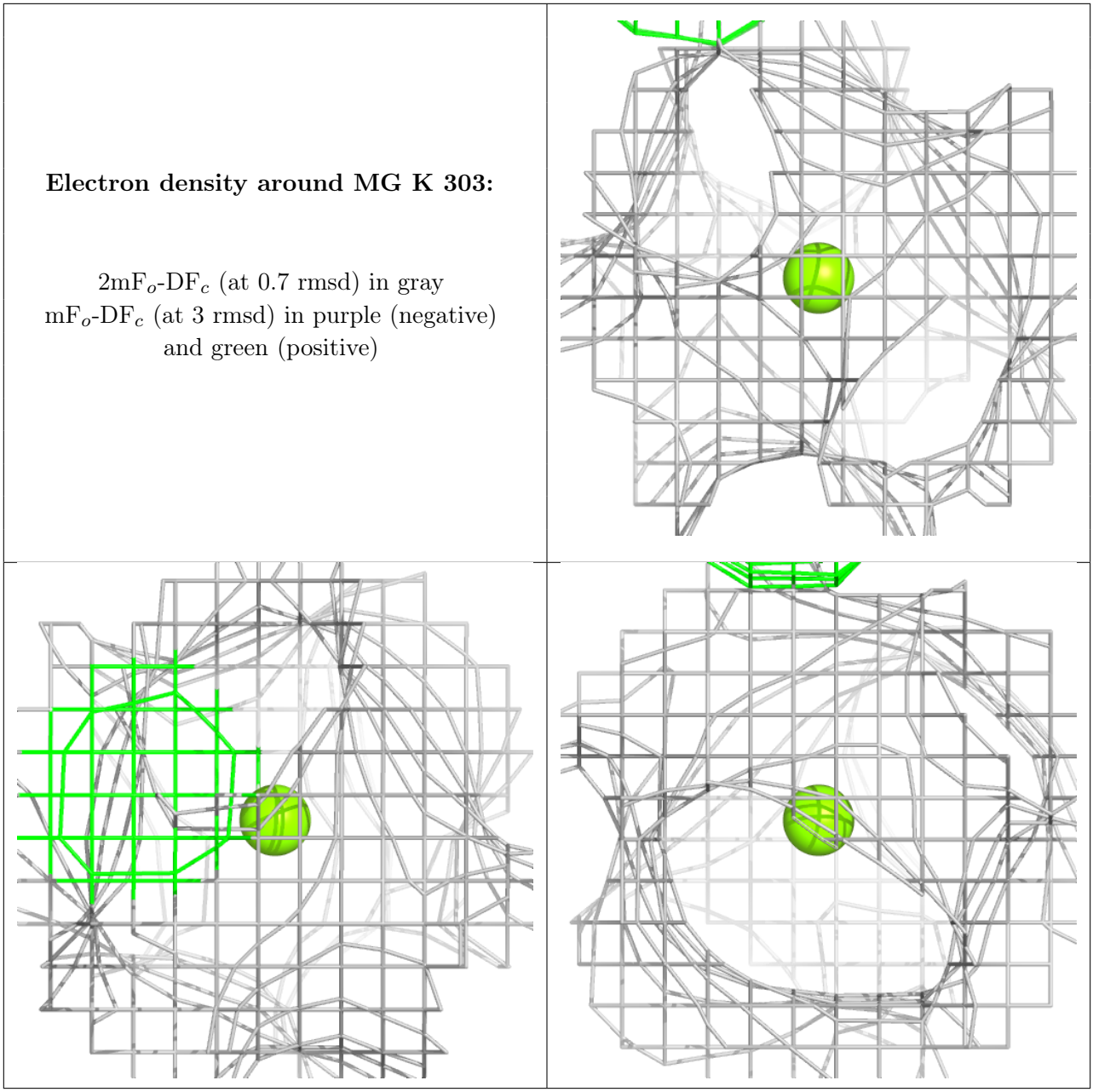
Electron density around MG J 304:

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



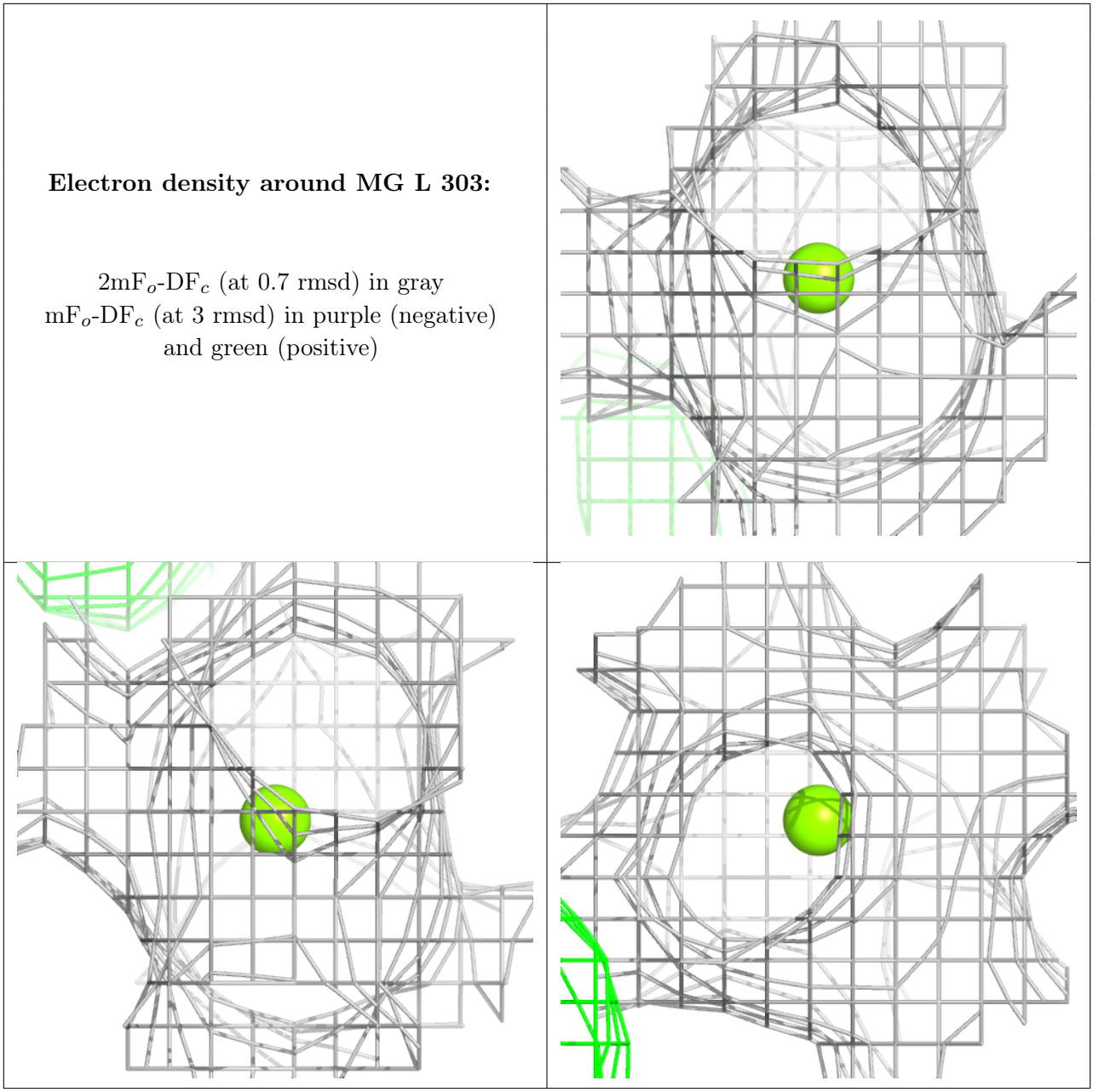
Electron density around MG K 303:

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



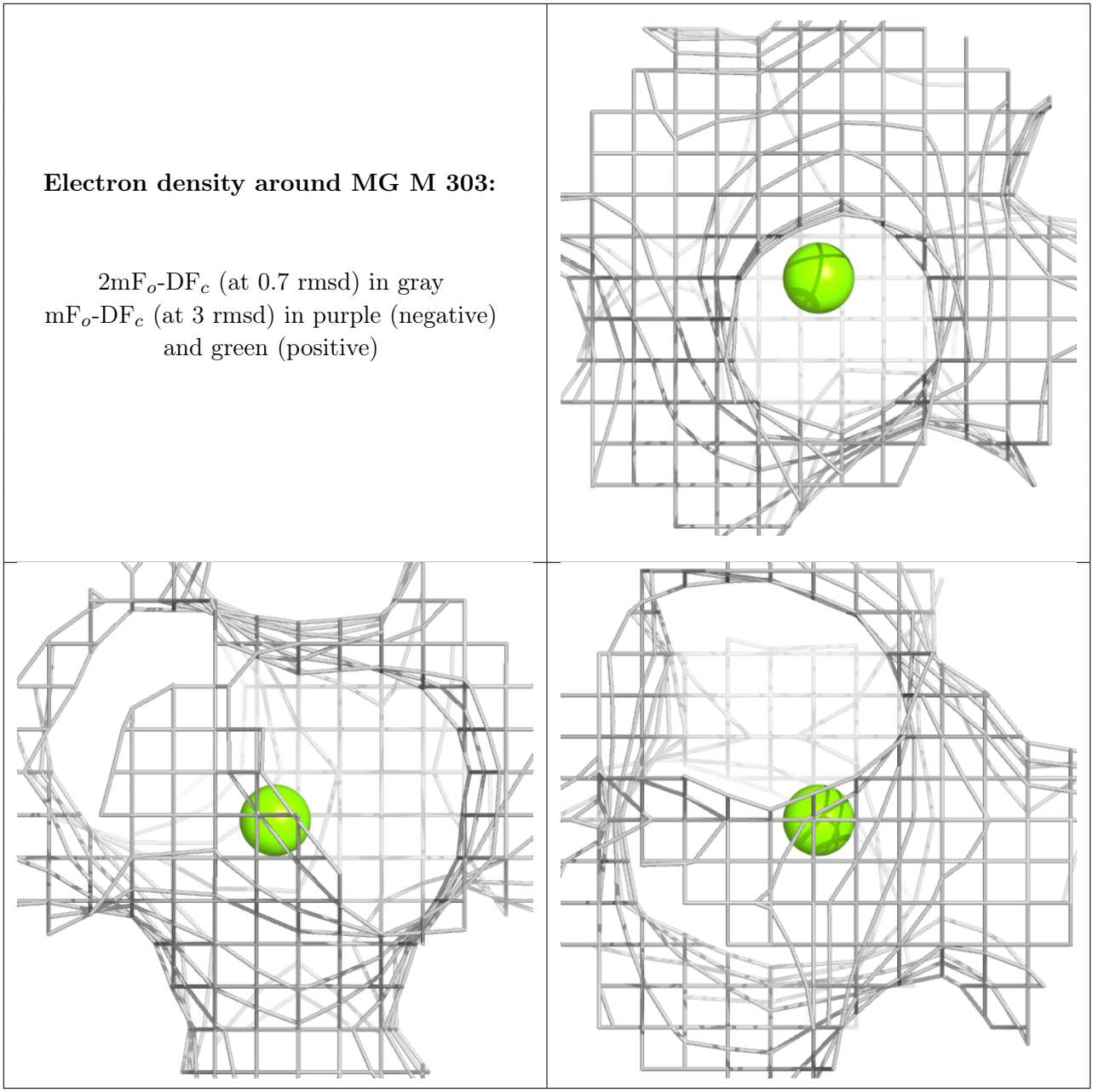
Electron density around MG L 303:

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



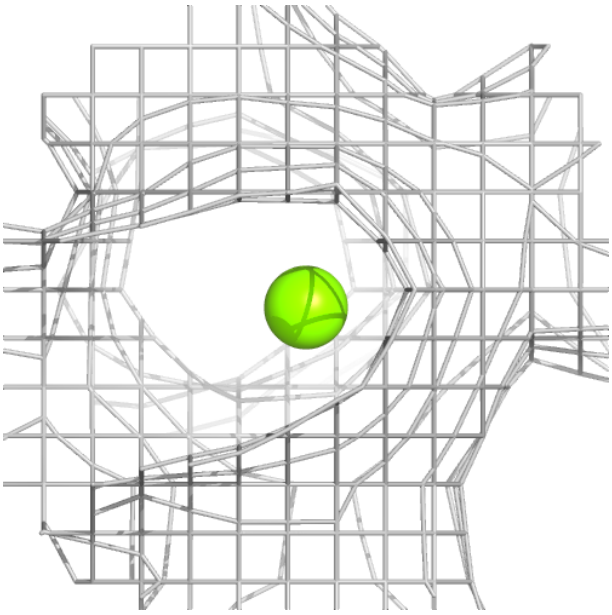
Electron density around MG M 303:

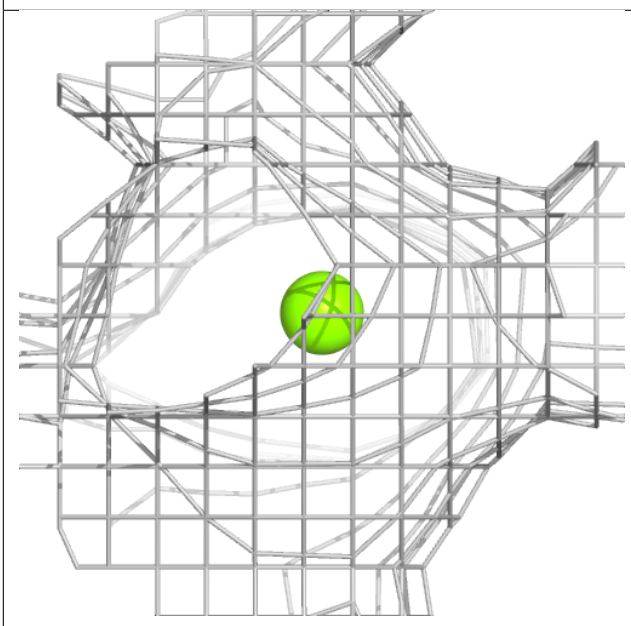
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

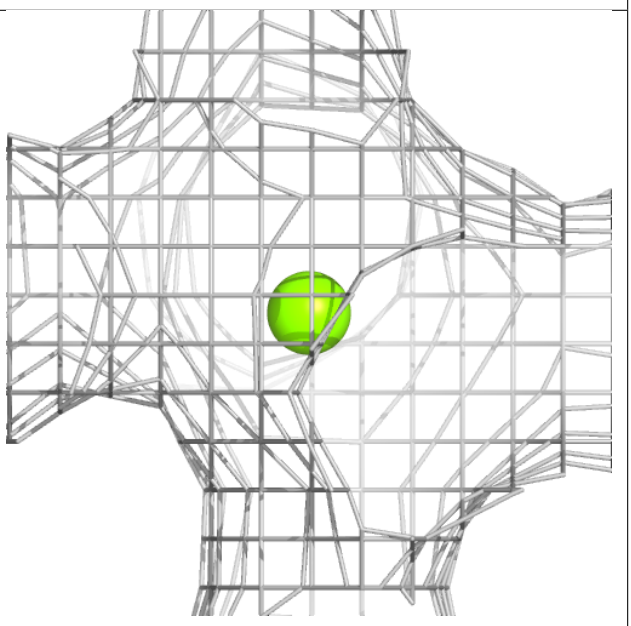


Electron density around MG N 304:

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

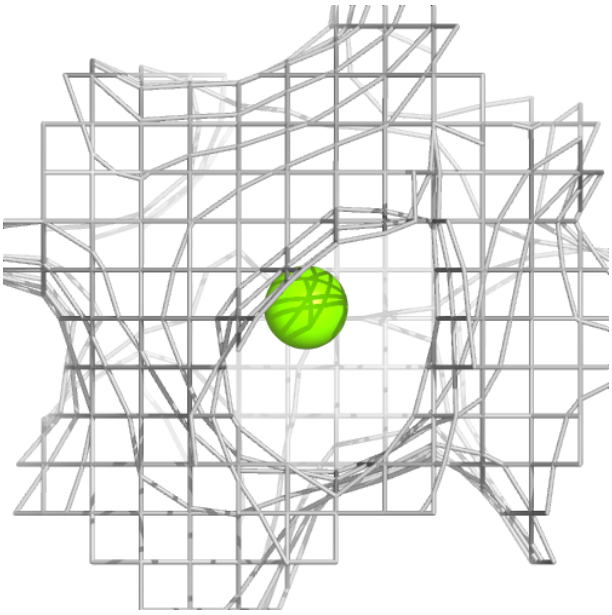


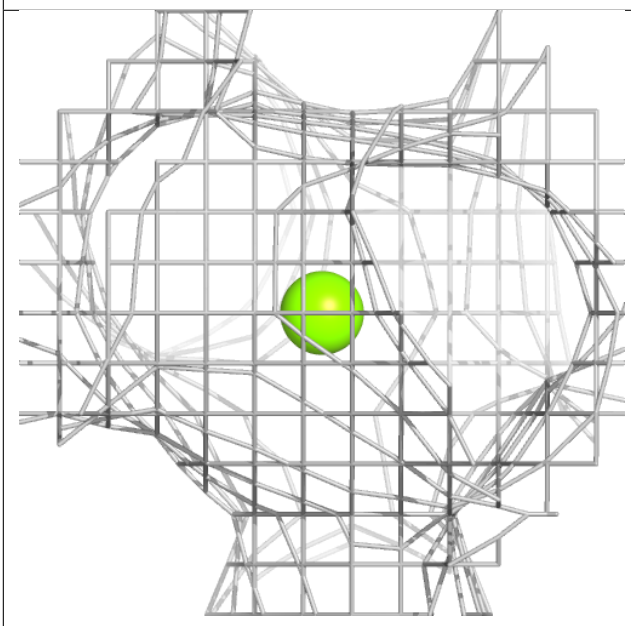


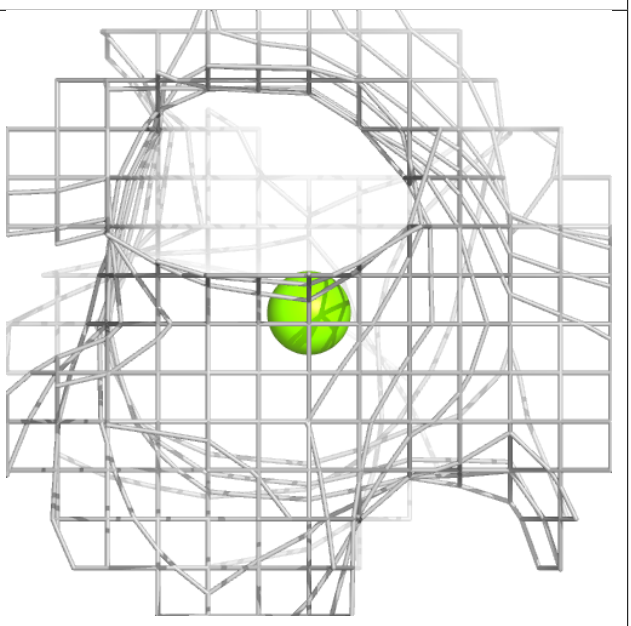


Electron density around MG O 303:

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

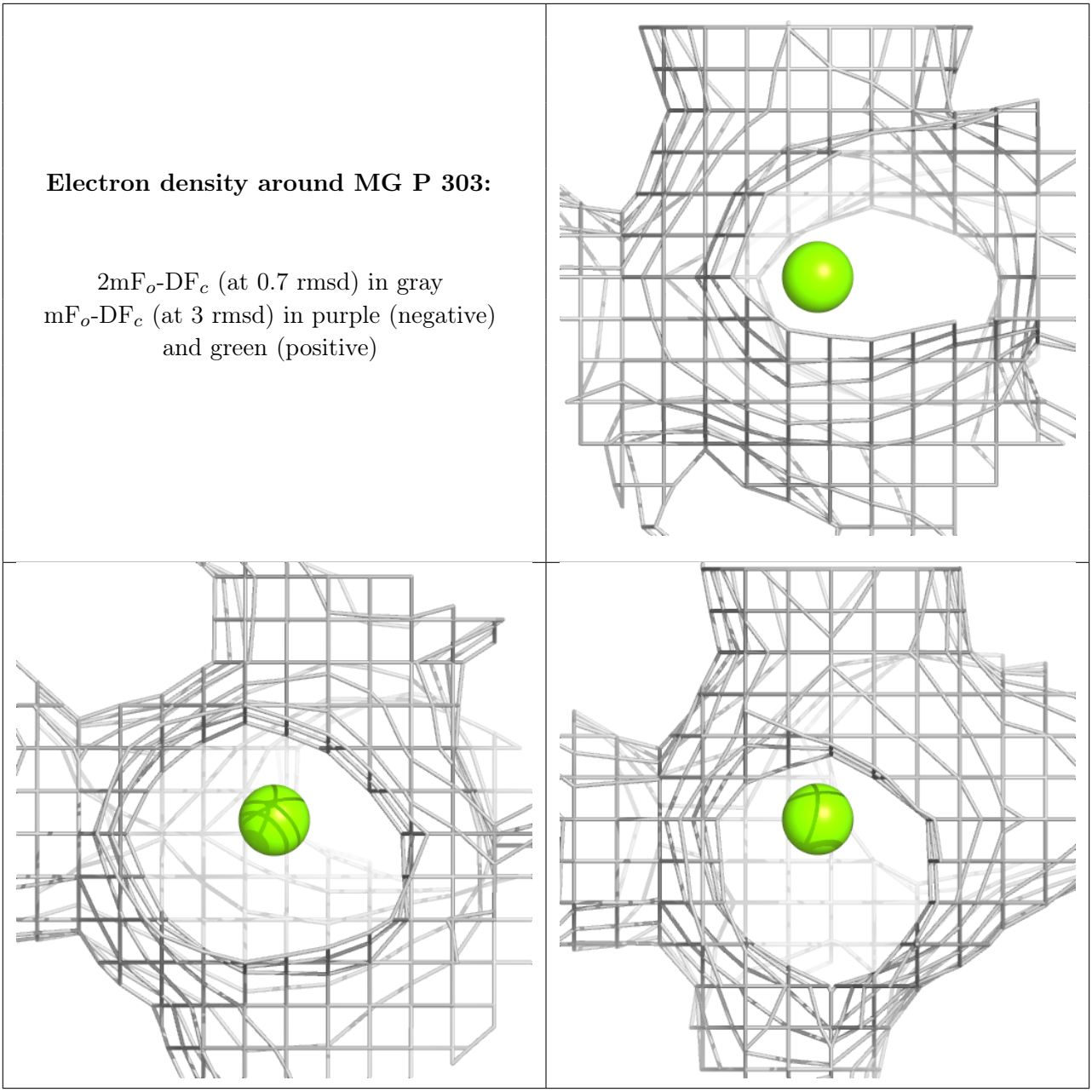






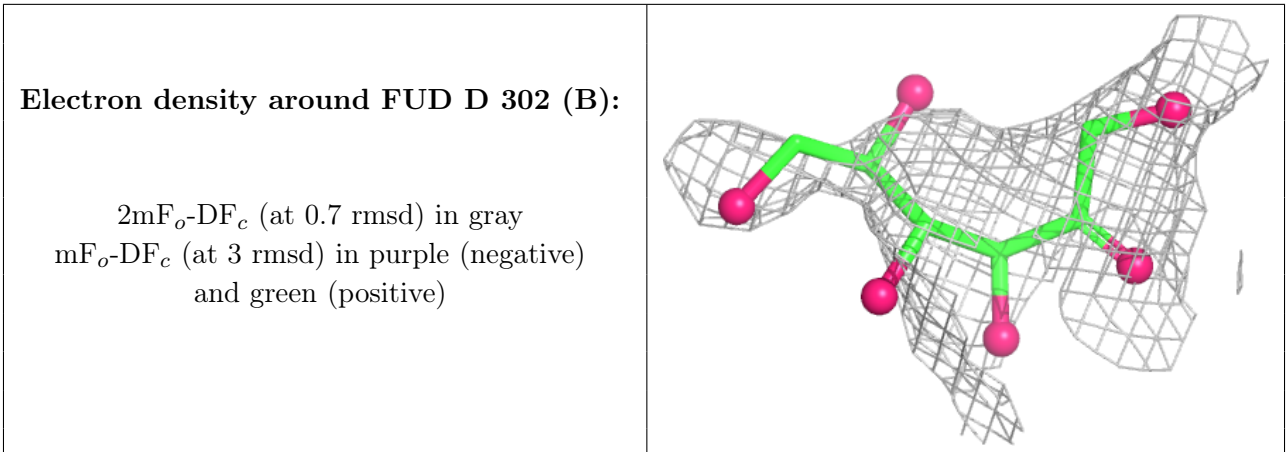
Electron density around MG P 303:

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



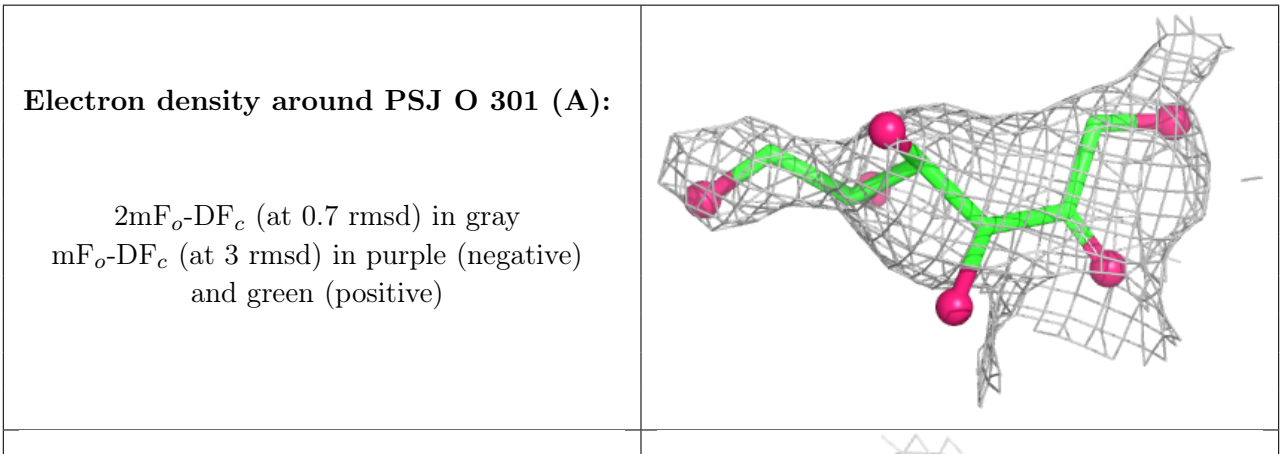
Electron density around FUD D 302 (B):

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



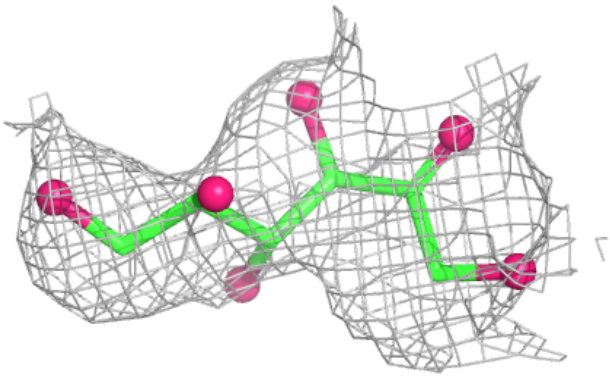
Electron density around PSJ O 301 (A):

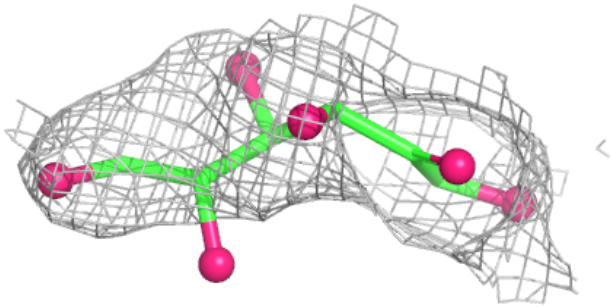
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

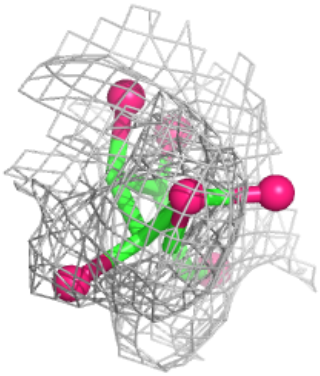


Electron density around PSJ G 301 (A):

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

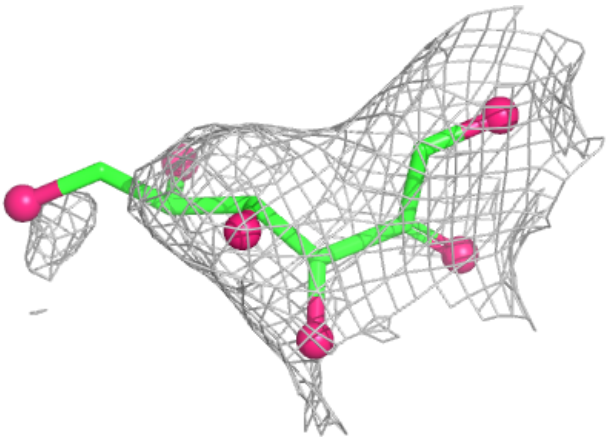


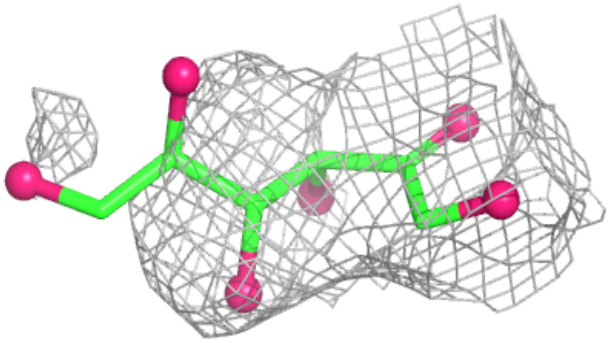


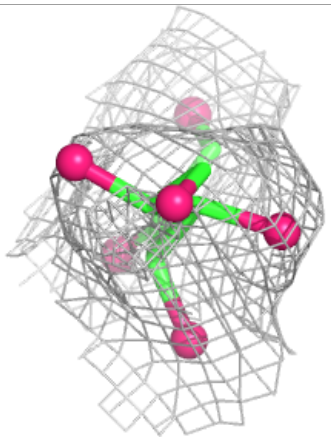


Electron density around FUD E 302 (B):

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

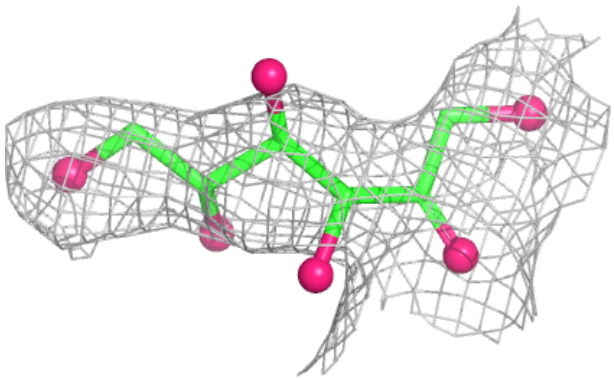


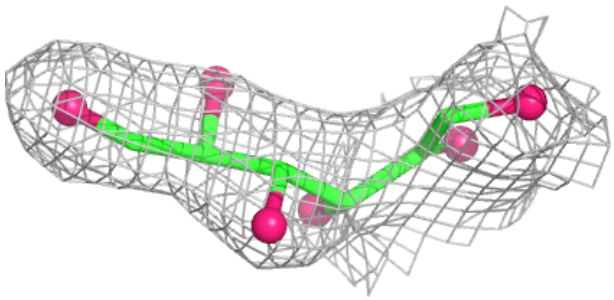


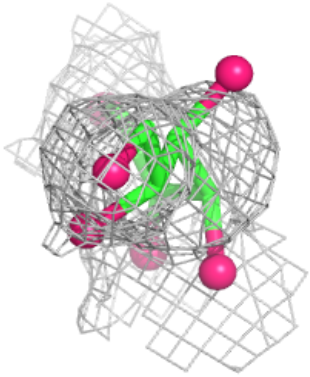


Electron density around PSJ J 302 (A):

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

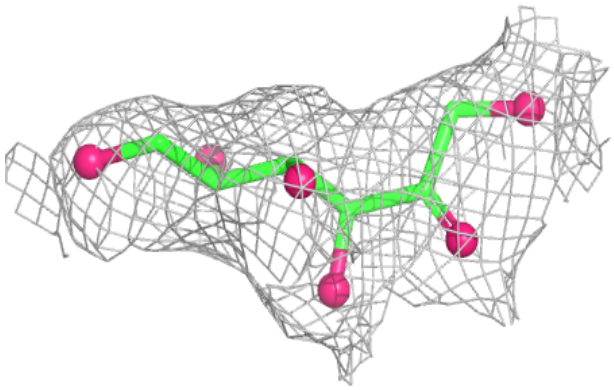


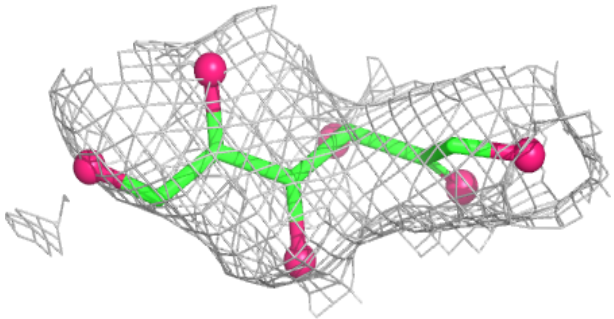


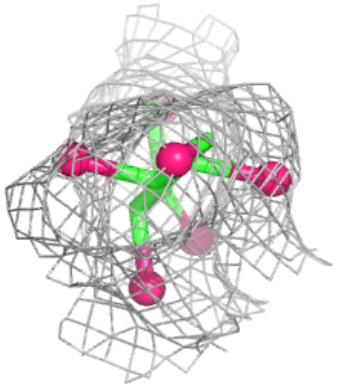


Electron density around FUD K 302 (B):

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

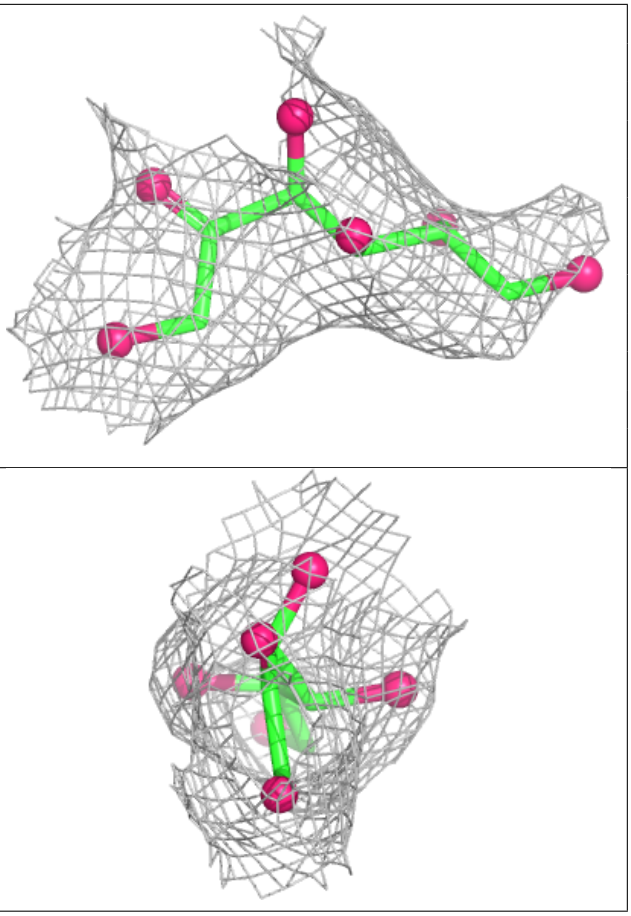






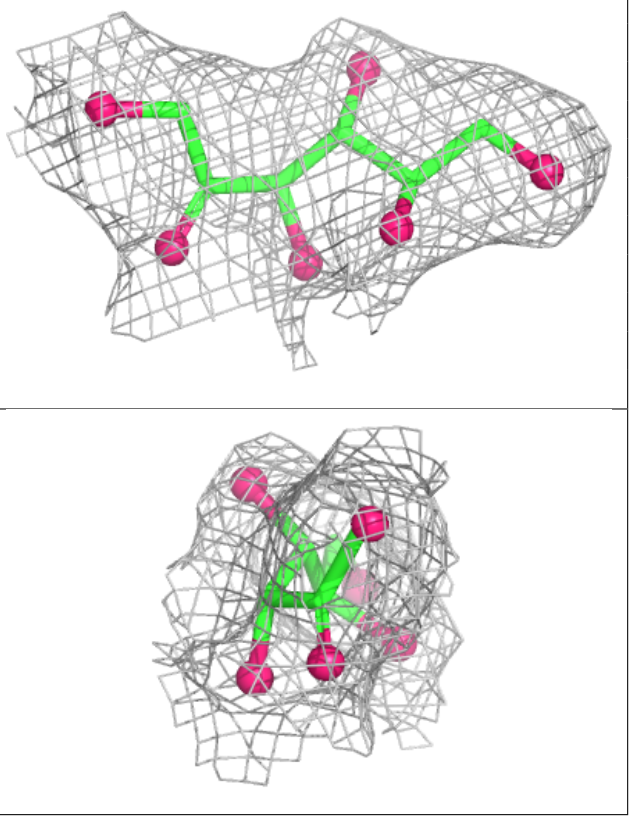
Electron density around FUD A 302 (B):

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



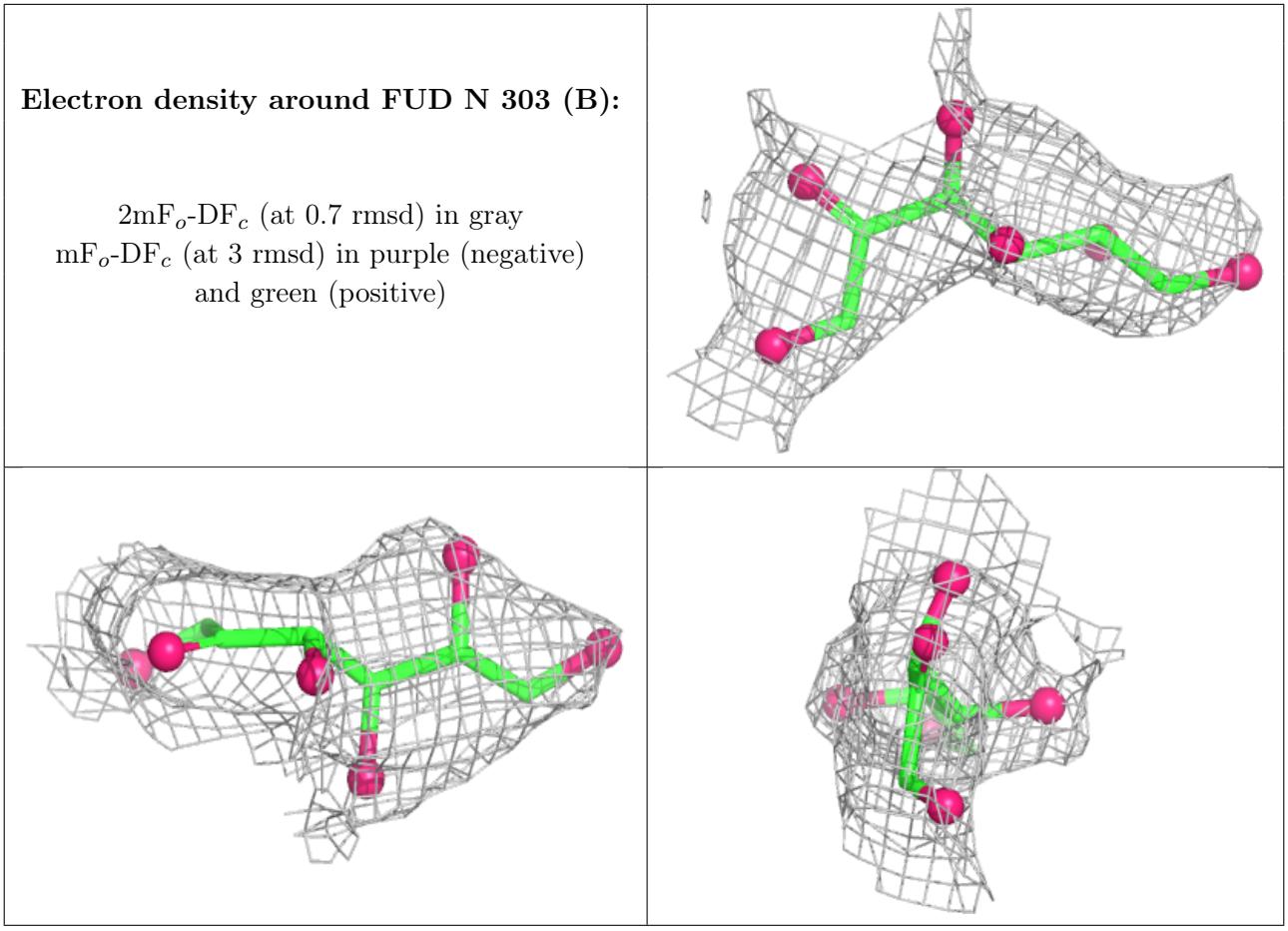
Electron density around PSJ K 301 (A):

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



Electron density around FUD N 303 (B):

$2mF_o$-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.