



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:18 AM UTC

PDB ID : 7KLS / pdb\_00007kls  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H59A mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2020-10-31  
Resolution : 2.59 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

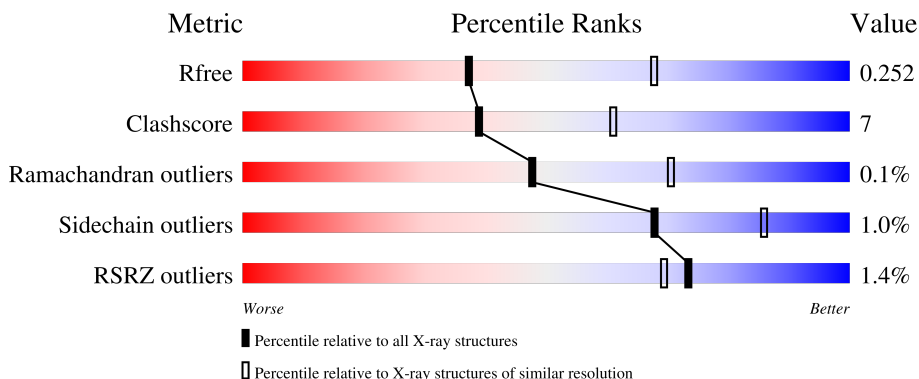
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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.



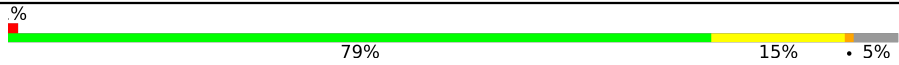
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	 81% 14% 5%
1	B	310	 79% 16% 5%
1	C	310	 80% 15% 5%
1	D	310	 77% 18% 5%
1	E	310	 81% 14% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment representing 79%, a yellow segment representing 15%, and a grey segment representing 5%. A small red square is at the beginning of the bar, and a '%' symbol is above it.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	2250	1431	369	437	13	0	1	0
1	B	296	2266	1441	375	437	13	0	0	0
1	C	295	2259	1437	373	436	13	0	0	0
1	D	296	2255	1433	372	437	13	0	0	0
1	E	296	2266	1441	375	437	13	0	0	0
1	F	296	2270	1446	374	437	13	0	1	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	59	ALA	HIS	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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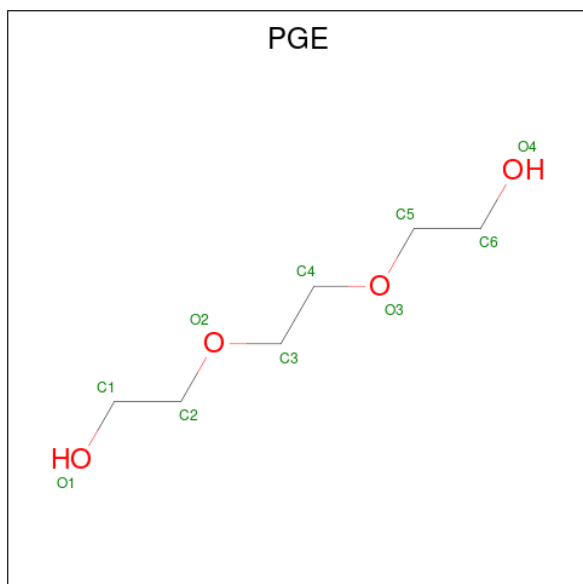
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	59	ALA	HIS	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	59	ALA	HIS	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	59	ALA	HIS	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	59	ALA	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	59	ALA	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

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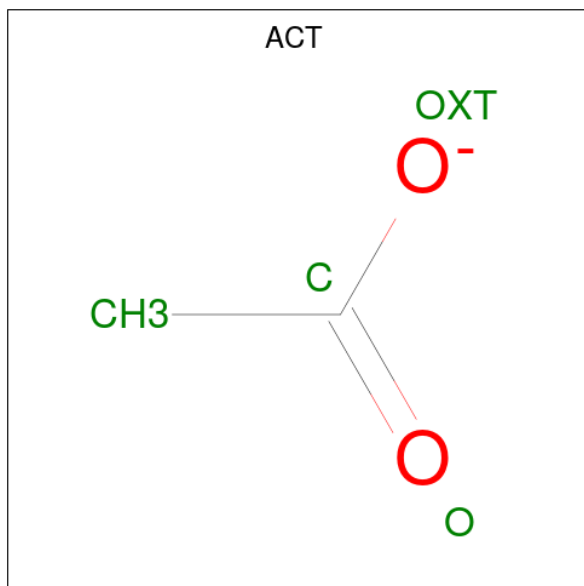
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0

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

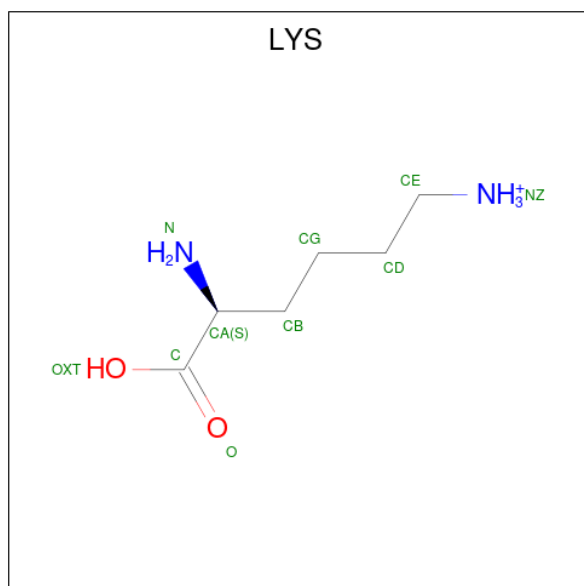
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is LYSINE (CCD ID: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

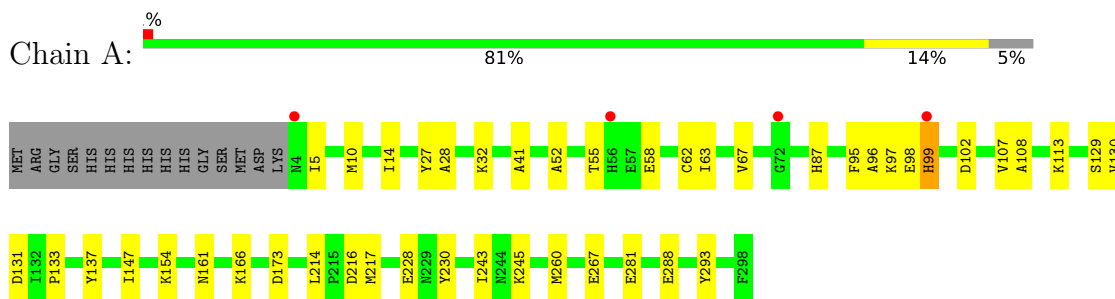
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	39	Total	O	0	0
			39	39		
6	C	47	Total	O	0	0
			47	47		
6	D	43	Total	O	0	0
			43	43		
6	E	45	Total	O	0	0
			45	45		
6	F	50	Total	O	0	0
			50	50		

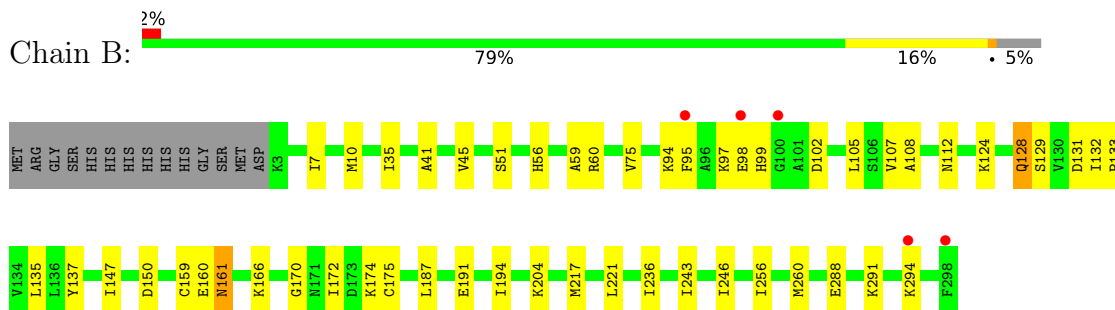
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

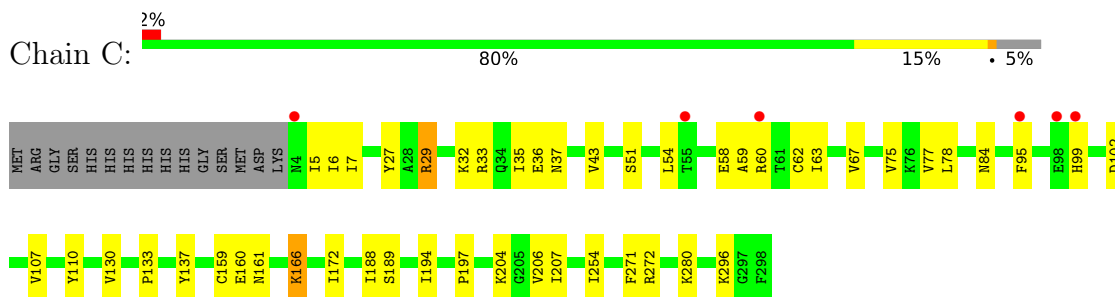
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



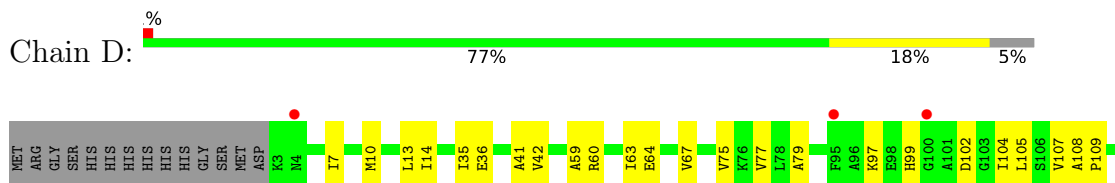
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

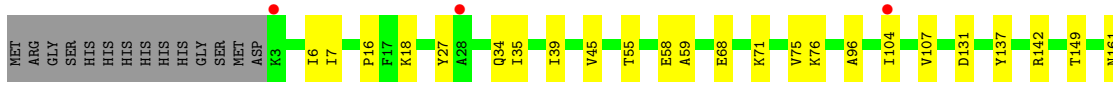
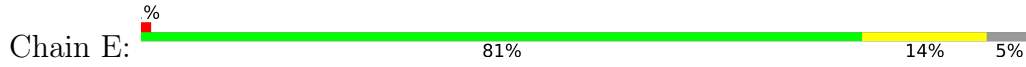


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

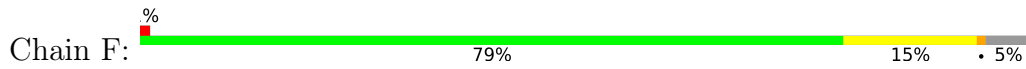




- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.08Å 231.29Å 201.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.59 49.70 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.70-2.59) 99.5 (49.70-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.211 , 0.253 0.214 , 0.252	Depositor DCC
$R_{free}$ test set	3097 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.58	0/2276	0.58	5/3083 (0.2%)
1	B	0.39	1/2289 (0.0%)	0.48	0/3097
1	C	0.44	2/2282 (0.1%)	0.52	1/3088 (0.0%)
1	D	0.54	1/2278 (0.0%)	0.55	0/3086
1	E	0.36	0/2289	0.47	2/3097 (0.1%)
1	F	0.54	1/2297 (0.0%)	0.51	0/3109
All	All	0.48	5/13711 (0.0%)	0.52	8/18560 (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	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	ILE	C-O	-6.25	1.17	1.24
1	B	159	CYS	CA-C	-6.18	1.45	1.52
1	D	285	LYS	C-O	-5.29	1.17	1.24
1	F	182	GLU	C-O	-5.13	1.18	1.24
1	C	159	CYS	C-O	-5.04	1.18	1.24

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	HIS	N-CA-C	9.89	123.99	112.72
1	A	5	ILE	N-CA-C	6.87	118.60	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLU	CB-CA-C	-5.78	101.77	110.90
1	E	230	TYR	N-CA-C	5.64	118.19	111.71
1	E	68	GLU	CB-CA-C	-5.47	101.55	110.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	166	KPI	Mainchain

## 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	2250	0	2265	35	0
1	B	2266	0	2295	34	0
1	C	2259	0	2286	32	0
1	D	2255	0	2264	34	1
1	E	2266	0	2295	25	0
1	F	2270	0	2293	32	1
2	A	10	0	14	0	0
2	B	10	0	14	1	0
2	C	10	0	14	0	0
2	D	10	0	14	0	0
2	E	10	0	14	0	0
2	F	10	0	14	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	4	0	3	0	0
4	C	8	0	6	1	0
4	D	4	0	3	1	0
4	E	4	0	3	0	0
4	F	8	0	6	0	0
5	A	10	0	12	1	0
5	B	10	0	12	1	0
5	C	10	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	12	0	0
5	E	10	0	12	0	0
5	F	10	0	12	1	0
6	A	44	0	0	3	0
6	B	39	0	0	0	0
6	C	47	0	0	1	0
6	D	43	0	0	0	0
6	E	45	0	0	1	0
6	F	50	0	0	0	0
All	All	13985	0	13875	188	1

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 7.

The worst 5 of 188 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:A:95:PHE:CE2	1:A:99:HIS:CD2	2.13	1.37
1:A:95:PHE:HE2	1:A:99:HIS:NE2	1.57	1.03
1:A:95:PHE:CD2	1:A:99:HIS:CD2	2.47	1.02
1:A:95:PHE:CE2	1:A:99:HIS:CG	2.56	0.93
1:A:95:PHE:HE2	1:A:99:HIS:CD2	1.71	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:PHE:O	1:F:184:ARG:NH2[3_655]	2.17	0.03

## 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	293/310 (94%)	283 (97%)	10 (3%)	0	100	100
1	B	293/310 (94%)	283 (97%)	10 (3%)	0	100	100
1	C	292/310 (94%)	284 (97%)	8 (3%)	0	100	100
1	D	293/310 (94%)	282 (96%)	11 (4%)	0	100	100
1	E	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	F	294/310 (95%)	284 (97%)	9 (3%)	1 (0%)	36	58
All	All	1758/1860 (94%)	1700 (97%)	57 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	268	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/259 (94%)	241 (99%)	2 (1%)	73	88
1	B	245/259 (95%)	242 (99%)	3 (1%)	63	83
1	C	244/259 (94%)	243 (100%)	1 (0%)	84	93
1	D	242/259 (93%)	239 (99%)	3 (1%)	63	83
1	E	245/259 (95%)	244 (100%)	1 (0%)	84	93
1	F	245/259 (95%)	242 (99%)	3 (1%)	63	83
All	All	1464/1554 (94%)	1451 (99%)	13 (1%)	68	87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	288	GLU
1	D	292	LYS
1	F	288	GLU
1	F	26	SER

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Mol	Chain	Res	Type
1	F	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	161	ASN
1	B	99	HIS
1	D	37	ASN
1	E	229	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KPI	B	166	1	11,13,14	1.98	2 (18%)	9,15,17	3.86	5 (55%)
1	KPI	D	166	1	11,13,14	0.93	1 (9%)	9,15,17	3.61	4 (44%)
1	KPI	E	166	1	11,13,14	1.61	2 (18%)	9,15,17	3.28	3 (33%)
1	KPI	F	166	1	11,13,14	0.90	1 (9%)	9,15,17	3.50	4 (44%)
1	KPI	A	166	1	11,13,14	1.96	2 (18%)	9,15,17	3.83	4 (44%)
1	KPI	C	166	1	11,13,14	1.99	2 (18%)	9,15,17	4.08	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	B	166	1	-	1/13/14/16	-
1	KPI	D	166	1	-	2/13/14/16	-
1	KPI	E	166	1	-	2/13/14/16	-
1	KPI	F	166	1	-	1/13/14/16	-
1	KPI	A	166	1	-	1/13/14/16	-
1	KPI	C	166	1	-	1/13/14/16	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	KPI	O2-CX2	5.74	1.36	1.22
1	C	166	KPI	O2-CX2	5.67	1.36	1.22
1	A	166	KPI	O2-CX2	5.60	1.36	1.22
1	E	166	KPI	O-C	4.37	1.36	1.20
1	A	166	KPI	O1-CX2	-2.56	1.23	1.30

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	-8.75	109.86	118.11
1	D	166	KPI	C1-CX1-CX2	-8.36	110.23	118.11
1	A	166	KPI	C1-CX1-CX2	-7.77	110.79	118.11
1	F	166	KPI	C1-CX1-CX2	-7.58	110.96	118.11
1	B	166	KPI	C1-CX1-CX2	-7.42	111.11	118.11

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	166	KPI	C-CA-CB-CG
1	A	166	KPI	C1-CX1-NZ-CE
1	B	166	KPI	C1-CX1-NZ-CE
1	C	166	KPI	C1-CX1-NZ-CE
1	D	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	166	KPI	1	0
1	C	166	KPI	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	PGE	D	301	-	9,9,9	0.32	0	8,8,8	0.24	0
2	PGE	F	301	-	9,9,9	0.31	0	8,8,8	0.37	0
2	PGE	A	301	-	9,9,9	0.32	0	8,8,8	0.27	0
4	ACT	C	303	-	3,3,3	1.43	1 (33%)	3,3,3	1.50	0
2	PGE	E	301	-	9,9,9	0.32	0	8,8,8	0.30	0
4	ACT	D	302	-	3,3,3	1.45	1 (33%)	3,3,3	1.48	0
5	LYS	C	305	-	8,9,9	0.85	1 (12%)	7,10,10	1.10	1 (14%)
4	ACT	C	304	-	3,3,3	1.48	1 (33%)	3,3,3	1.35	0
5	LYS	D	303	-	8,9,9	0.85	1 (12%)	7,10,10	1.11	1 (14%)
5	LYS	A	304	-	8,9,9	1.15	1 (12%)	7,10,10	1.52	1 (14%)
2	PGE	B	301	-	9,9,9	0.32	0	8,8,8	0.23	0
5	LYS	E	304	-	8,9,9	0.84	1 (12%)	7,10,10	1.01	1 (14%)
4	ACT	E	303	-	3,3,3	1.40	1 (33%)	3,3,3	1.52	0
2	PGE	C	301	-	9,9,9	0.34	0	8,8,8	0.20	0
4	ACT	F	303	-	3,3,3	1.31	0	3,3,3	1.36	0
4	ACT	F	302	-	3,3,3	1.43	1 (33%)	3,3,3	1.36	0
4	ACT	A	303	-	3,3,3	1.30	0	3,3,3	1.44	0
5	LYS	F	304	-	8,9,9	0.85	1 (12%)	7,10,10	1.07	1 (14%)
5	LYS	B	302	-	8,9,9	0.87	1 (12%)	7,10,10	1.14	1 (14%)

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	PGE	D	301	-	-	3/7/7/7	-
5	LYS	A	304	-	-	4/9/9/9	-
2	PGE	F	301	-	-	6/7/7/7	-
2	PGE	B	301	-	-	0/7/7/7	-
2	PGE	A	301	-	-	1/7/7/7	-
2	PGE	E	301	-	-	2/7/7/7	-
5	LYS	C	305	-	-	3/9/9/9	-
5	LYS	F	304	-	-	0/9/9/9	-
5	LYS	E	304	-	-	2/9/9/9	-
5	LYS	D	303	-	-	2/9/9/9	-
2	PGE	C	301	-	-	1/7/7/7	-
5	LYS	B	302	-	-	3/9/9/9	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	LYS	OXT-C	-2.95	1.21	1.30
5	B	302	LYS	OXT-C	-2.26	1.23	1.30
5	E	304	LYS	OXT-C	-2.23	1.23	1.30
5	F	304	LYS	OXT-C	-2.22	1.23	1.30
4	C	304	ACT	CH3-C	2.22	1.57	1.49

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	LYS	OXT-C-O	-3.73	115.61	124.08
5	B	302	LYS	OXT-C-O	-2.96	117.37	124.08
5	C	305	LYS	OXT-C-O	-2.78	117.76	124.08
5	D	303	LYS	OXT-C-O	-2.76	117.81	124.08
5	F	304	LYS	OXT-C-O	-2.72	117.91	124.08

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	LYS	C-CA-CB-CG

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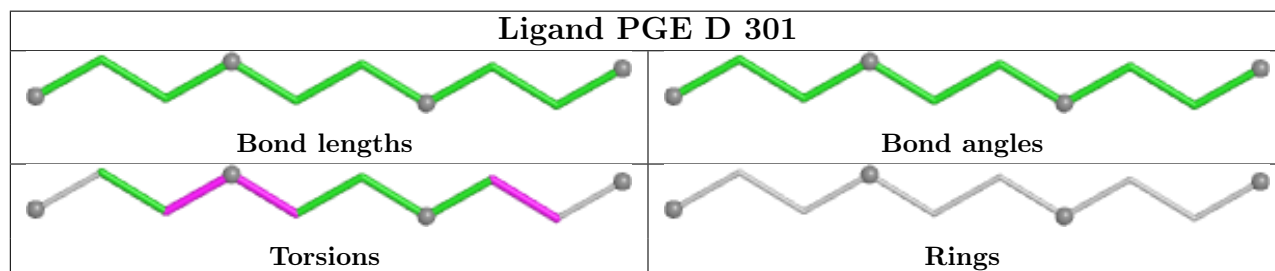
Mol	Chain	Res	Type	Atoms
5	D	303	LYS	C-CA-CB-CG
2	A	301	PGE	O1-C1-C2-O2
2	F	301	PGE	O3-C5-C6-O4
5	A	304	LYS	CG-CD-CE-NZ

There are no ring outliers.

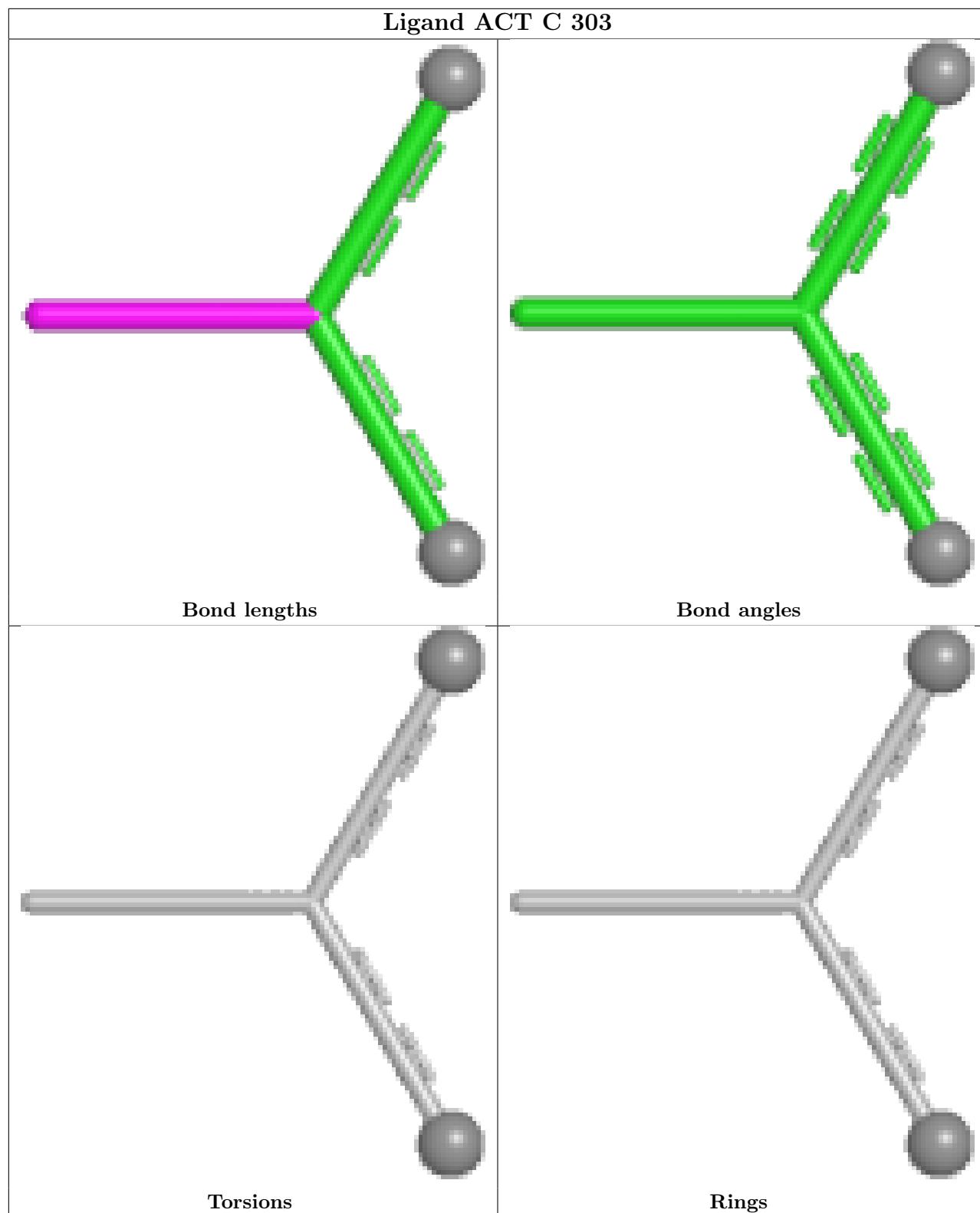
8 monomers are involved in 10 short contacts:

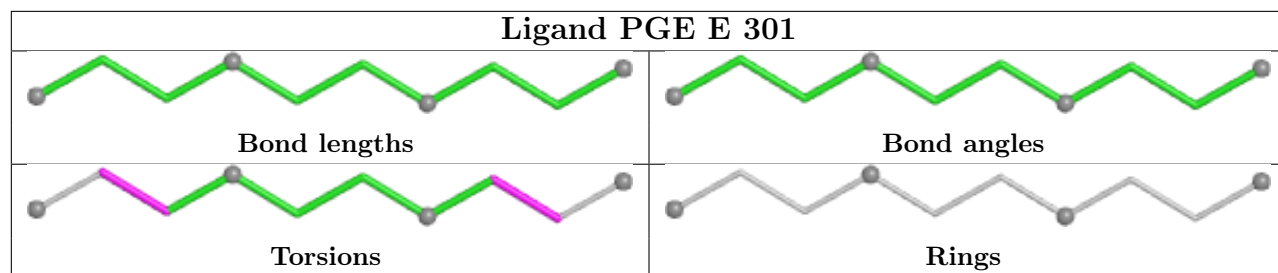
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	PGE	2	0
4	C	303	ACT	1	0
4	D	302	ACT	1	0
5	C	305	LYS	2	0
5	A	304	LYS	1	0
2	B	301	PGE	1	0
5	F	304	LYS	1	0
5	B	302	LYS	1	0

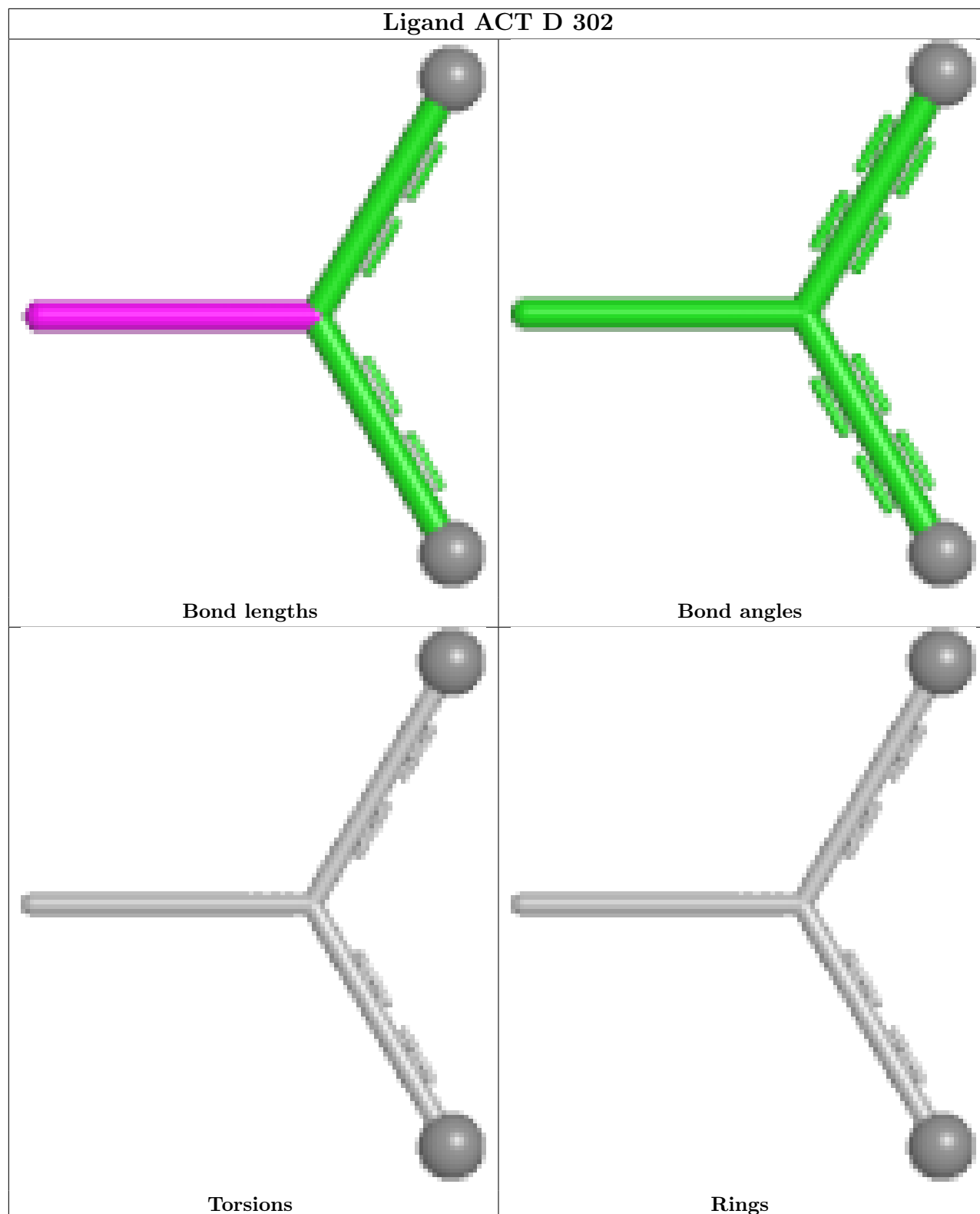
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

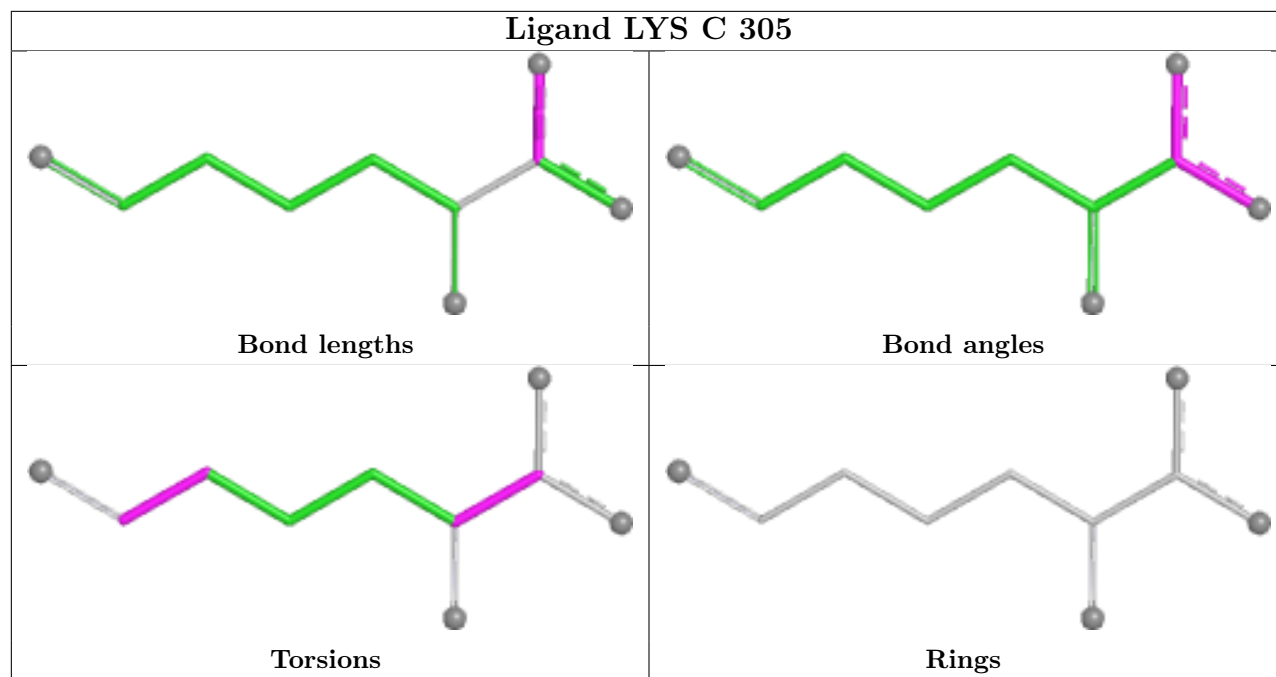


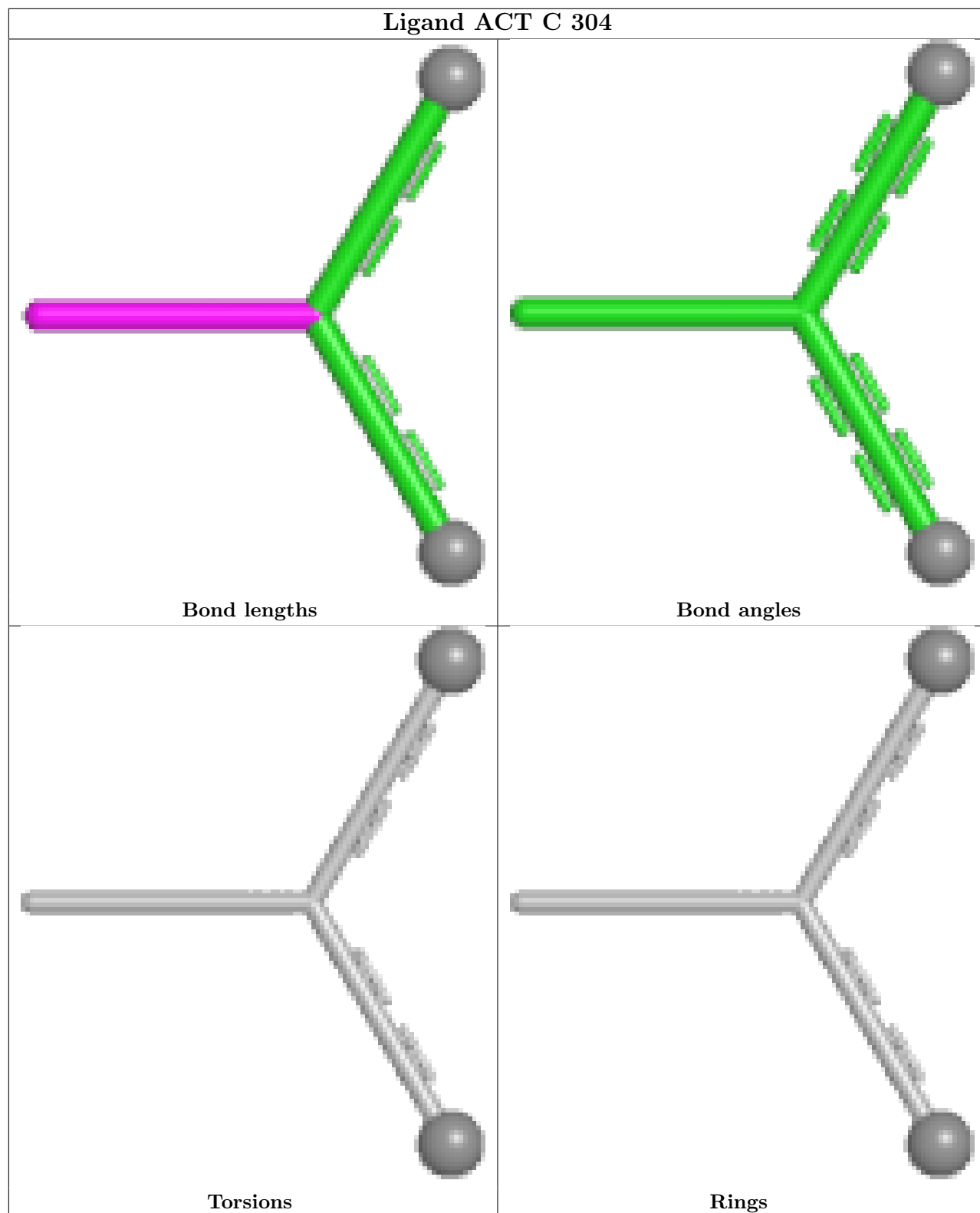


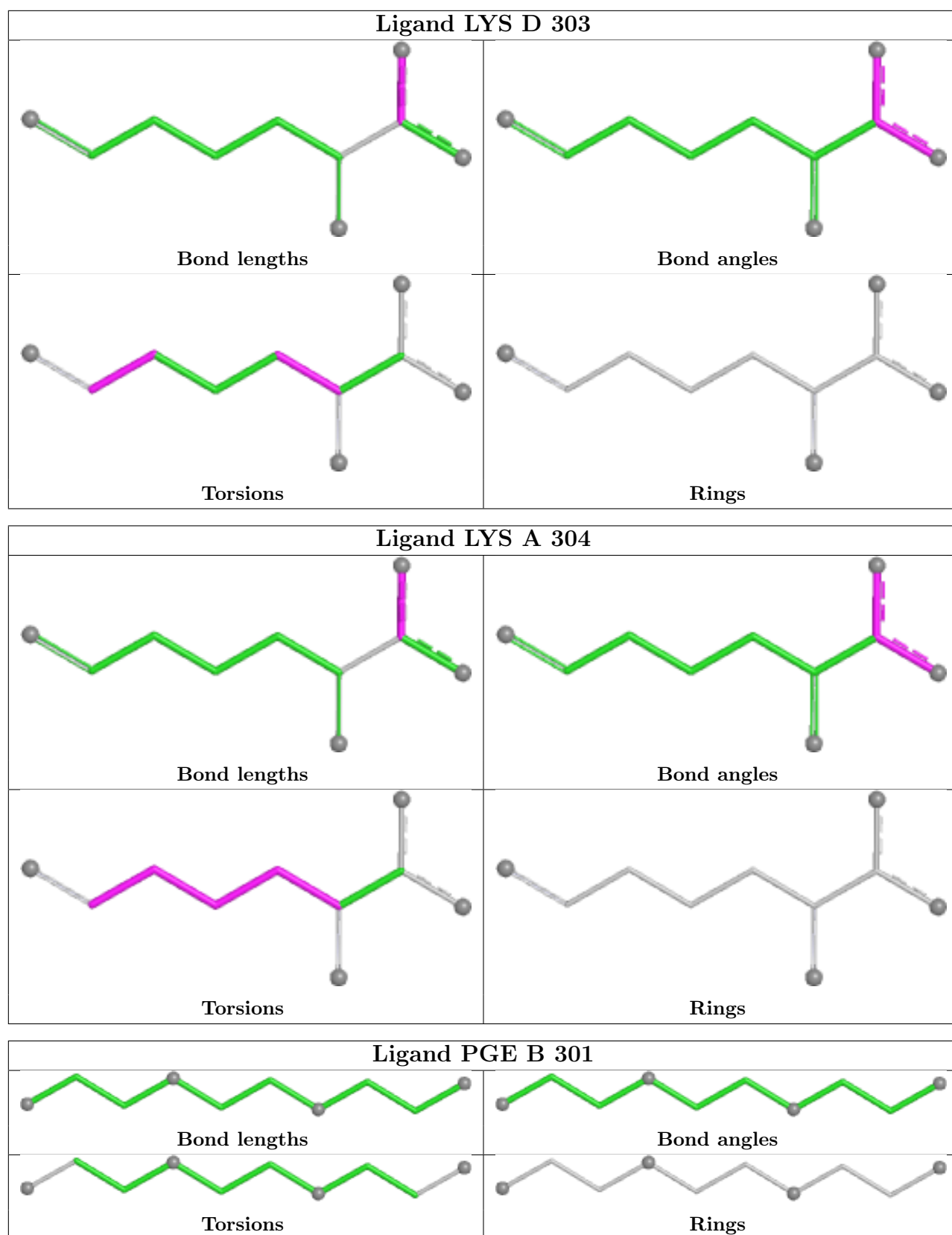


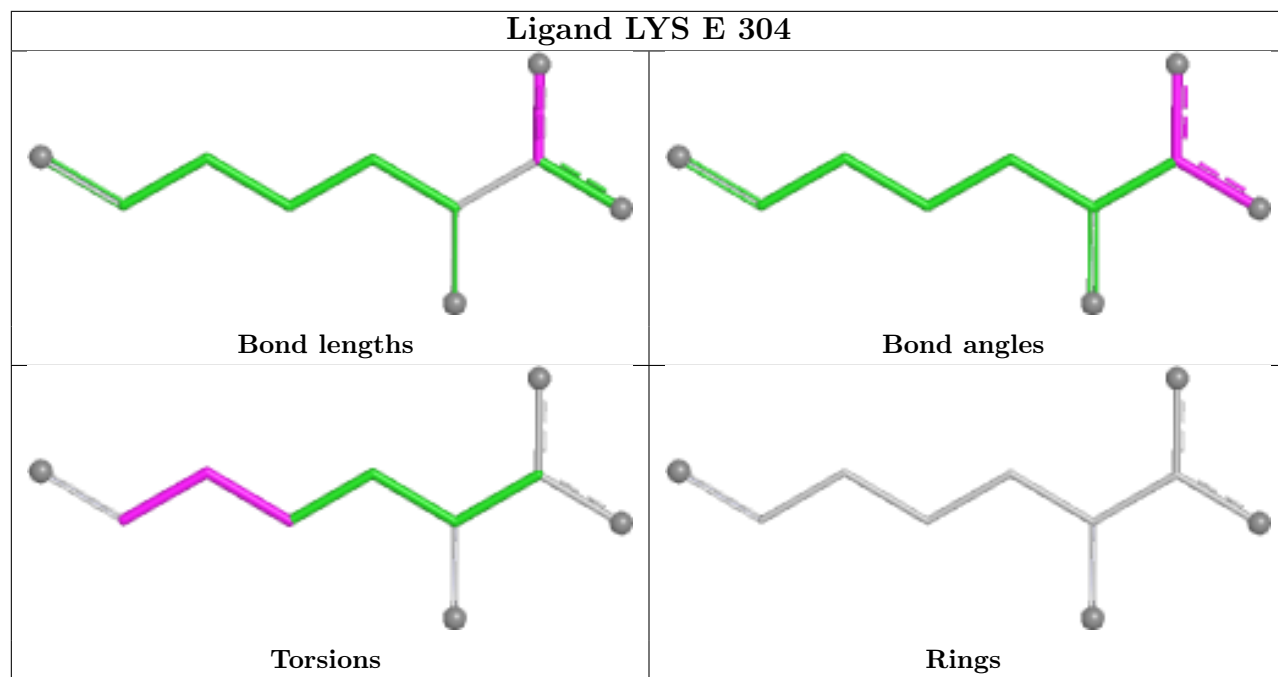


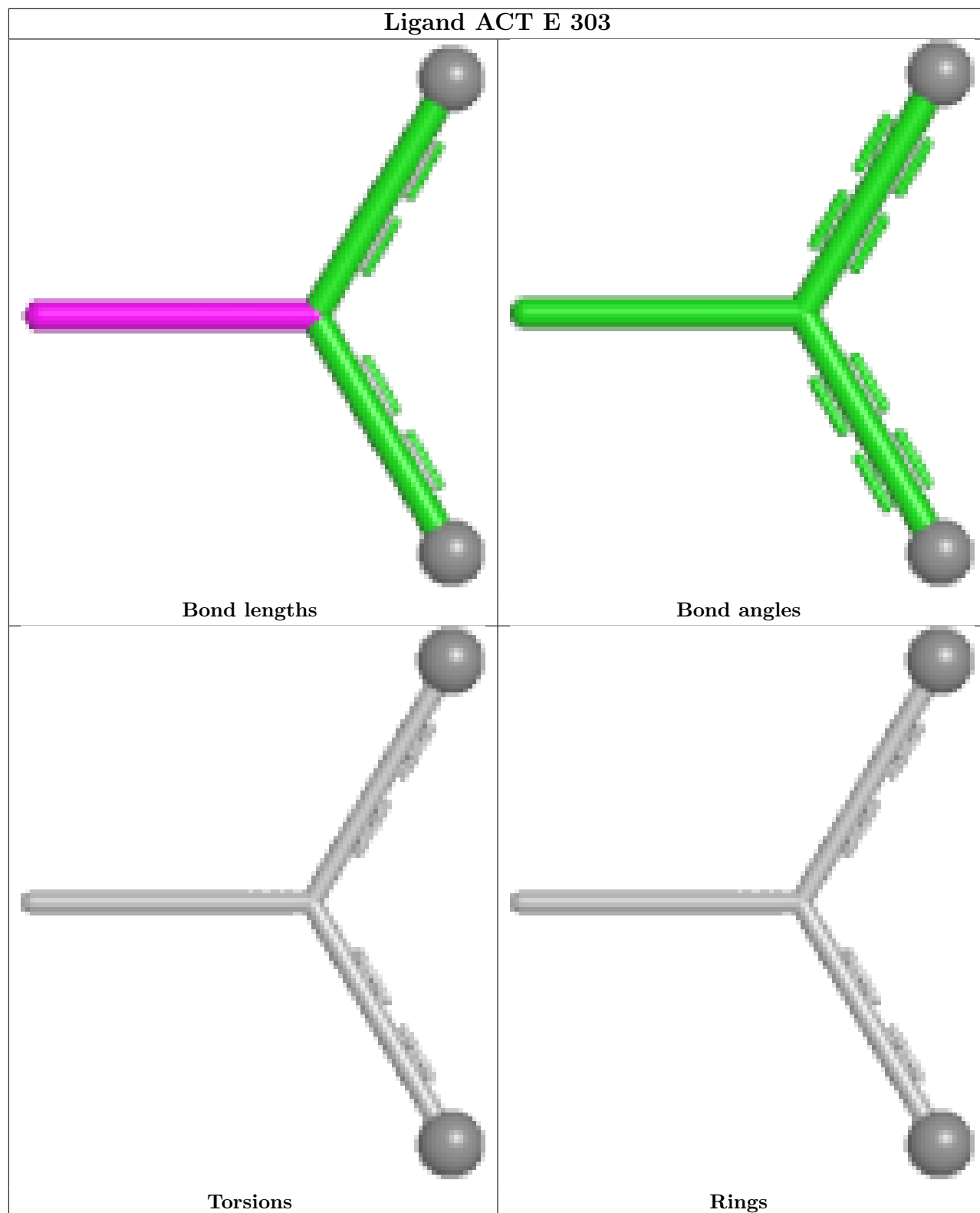


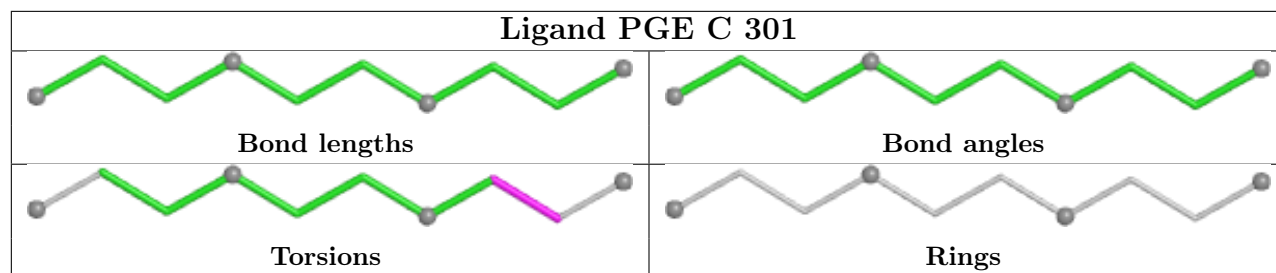


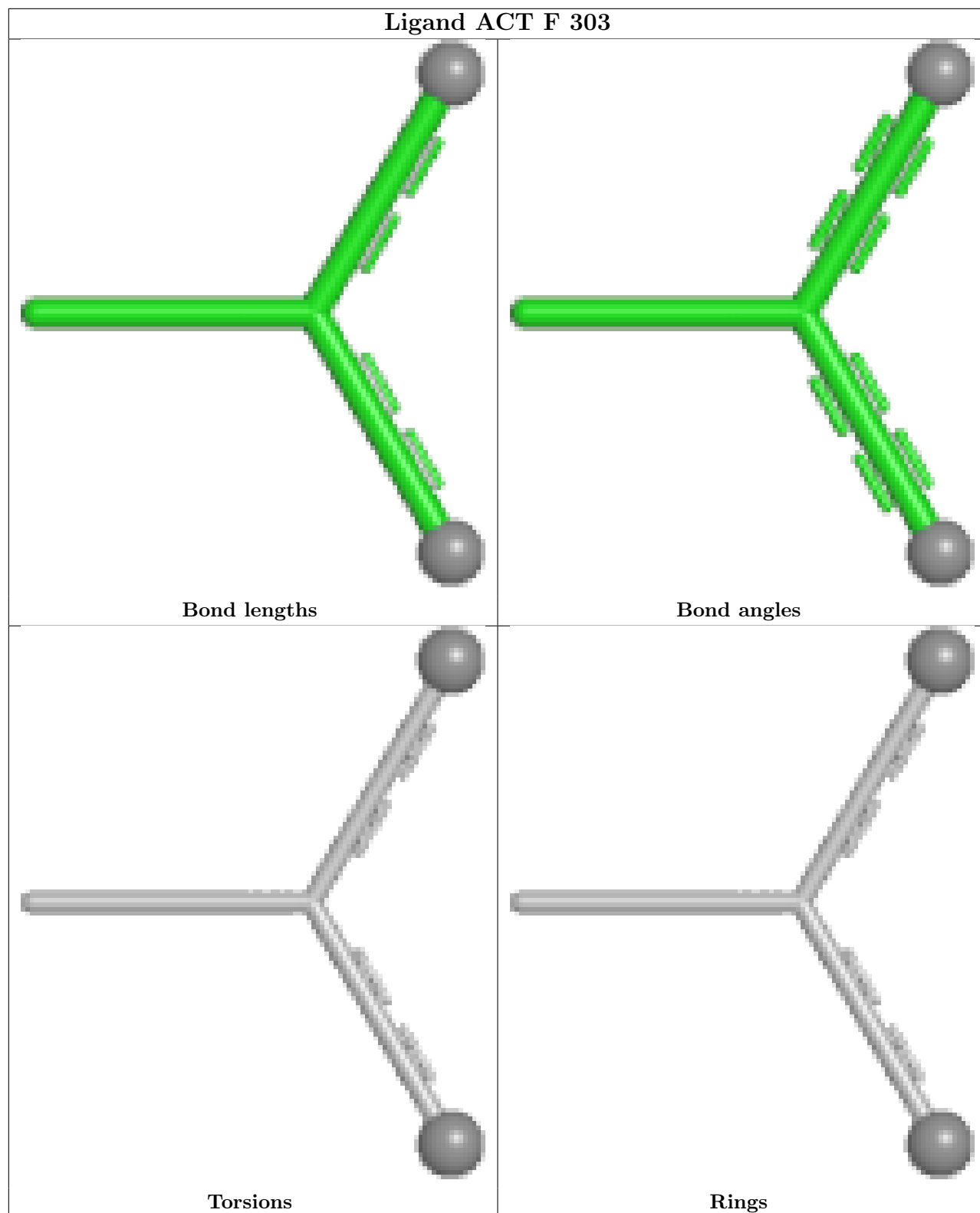


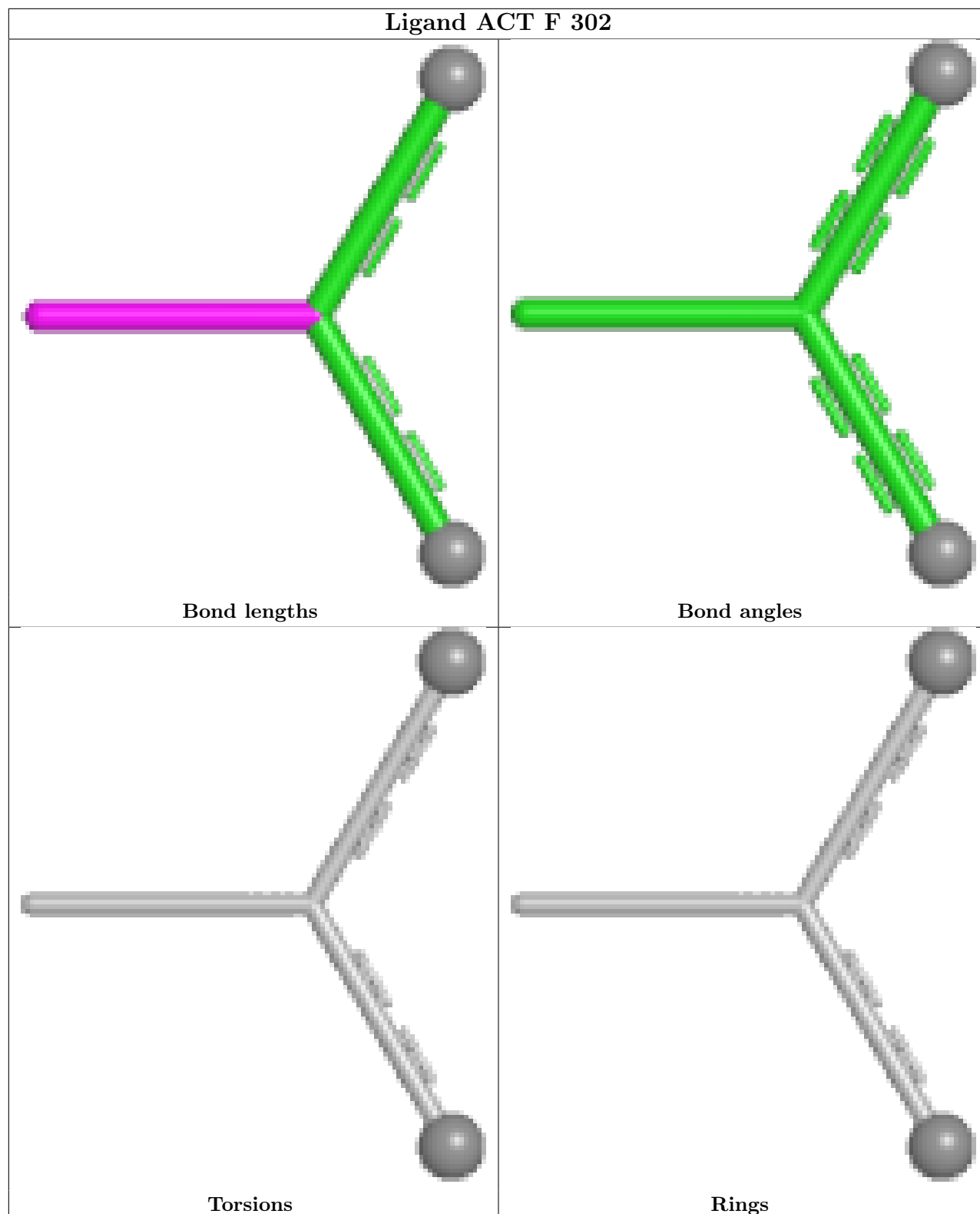


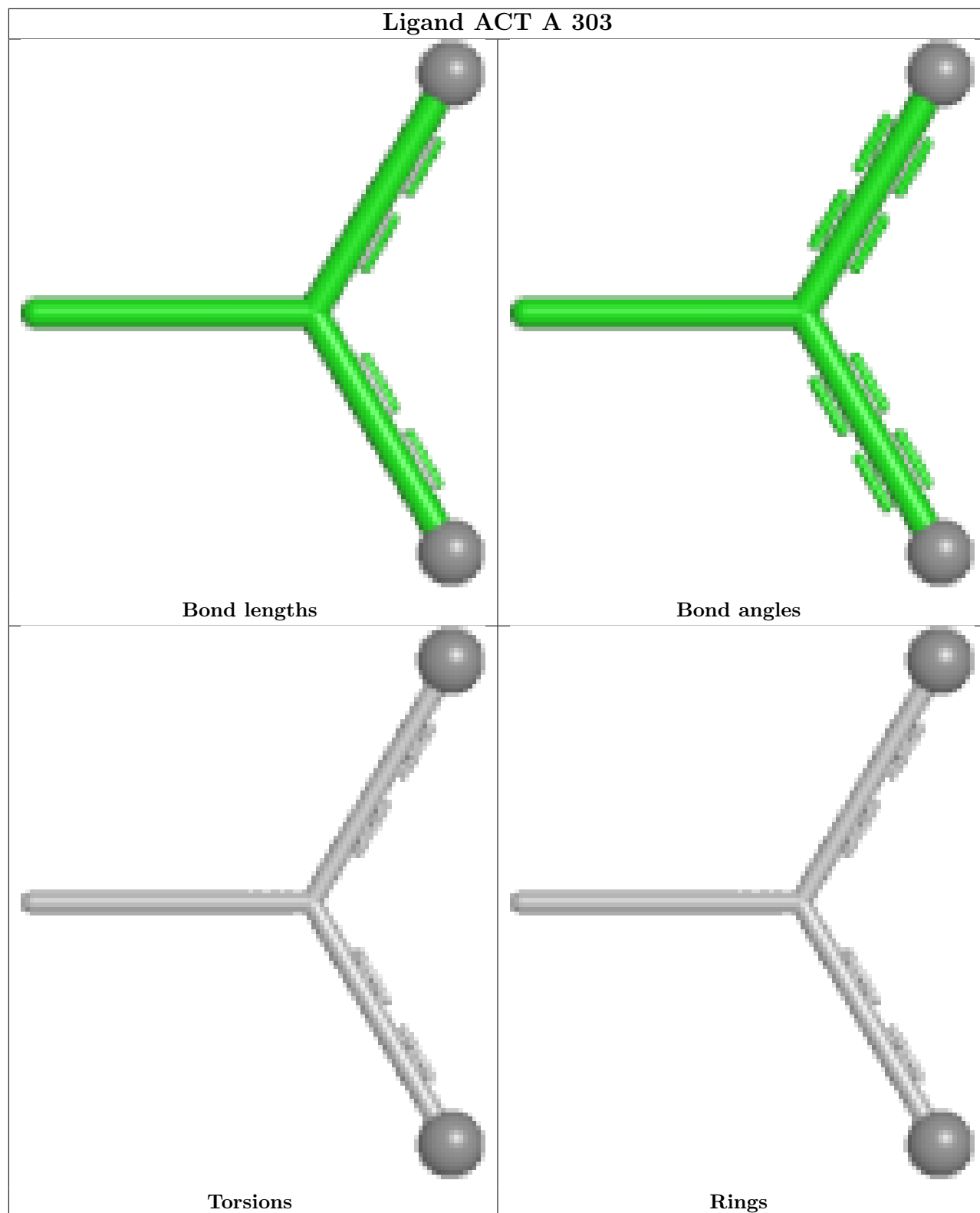


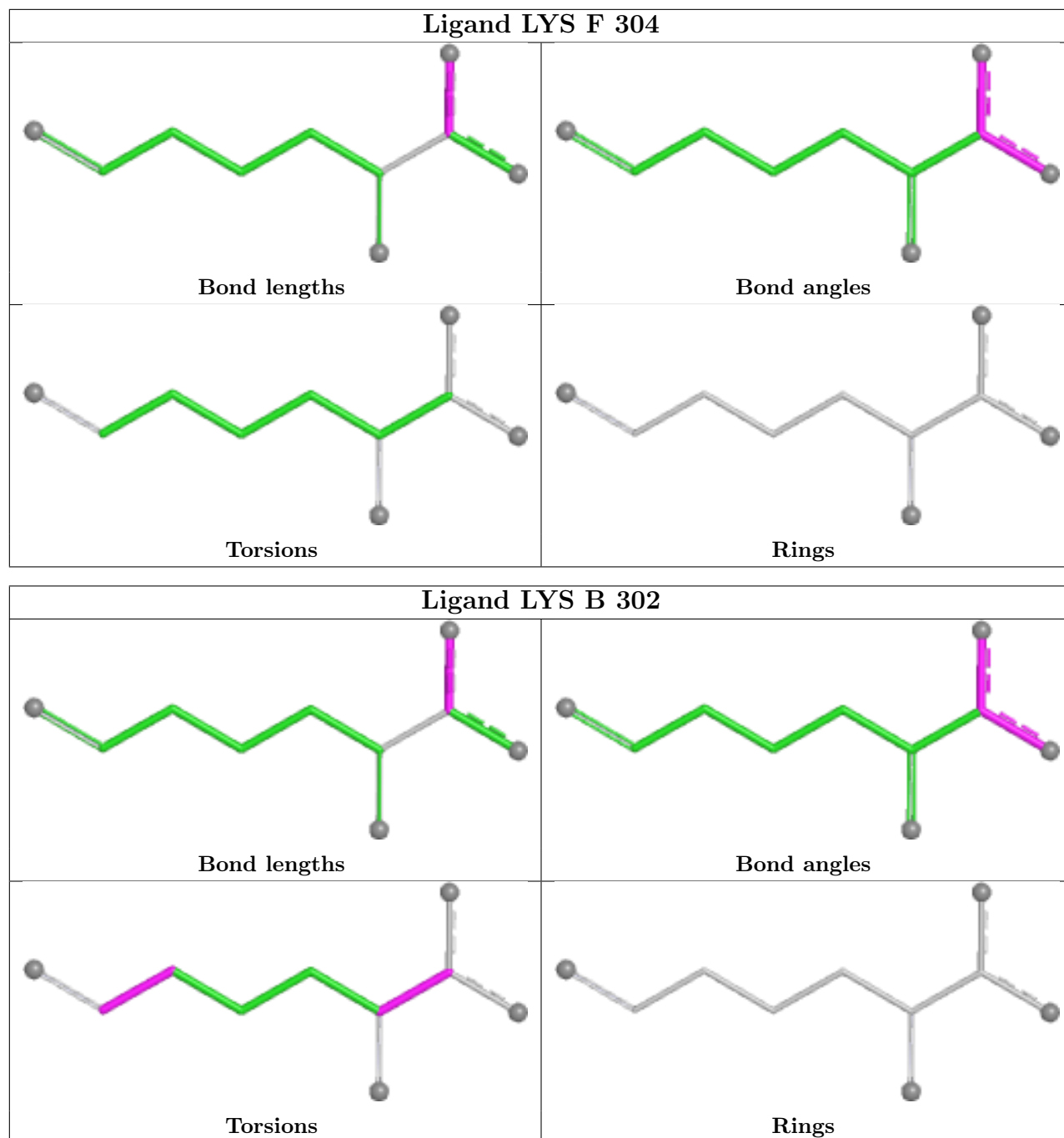












## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	294/310 (94%)	0.24	4 (1%) 73 69	33, 43, 59, 71	1 (0%)
1	B	295/310 (95%)	0.10	5 (1%) 69 64	32, 40, 55, 67	0
1	C	294/310 (94%)	0.22	6 (2%) 65 60	33, 41, 60, 72	0
1	D	295/310 (95%)	0.26	4 (1%) 73 69	34, 42, 60, 73	0
1	E	295/310 (95%)	0.17	3 (1%) 79 76	34, 40, 55, 67	0
1	F	295/310 (95%)	0.27	3 (1%) 79 76	34, 43, 60, 70	1 (0%)
All	All	1768/1860 (95%)	0.21	25 (1%) 73 69	32, 42, 59, 73	2 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	95[A]	PHE	4.6
1	C	60	ARG	3.7
1	C	95	PHE	3.7
1	C	99	HIS	3.0
1	D	95	PHE	3.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KPI	A	166	14/15	0.90	0.10	38,39,43,45	0
1	KPI	B	166	14/15	0.90	0.10	31,34,40,40	0
1	KPI	C	166	14/15	0.90	0.10	34,35,46,48	0
1	KPI	D	166	14/15	0.90	0.10	39,42,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	F	166	14/15	0.92	0.09	37,39,44,46	0
1	KPI	E	166	14/15	0.94	0.08	35,38,43,43	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

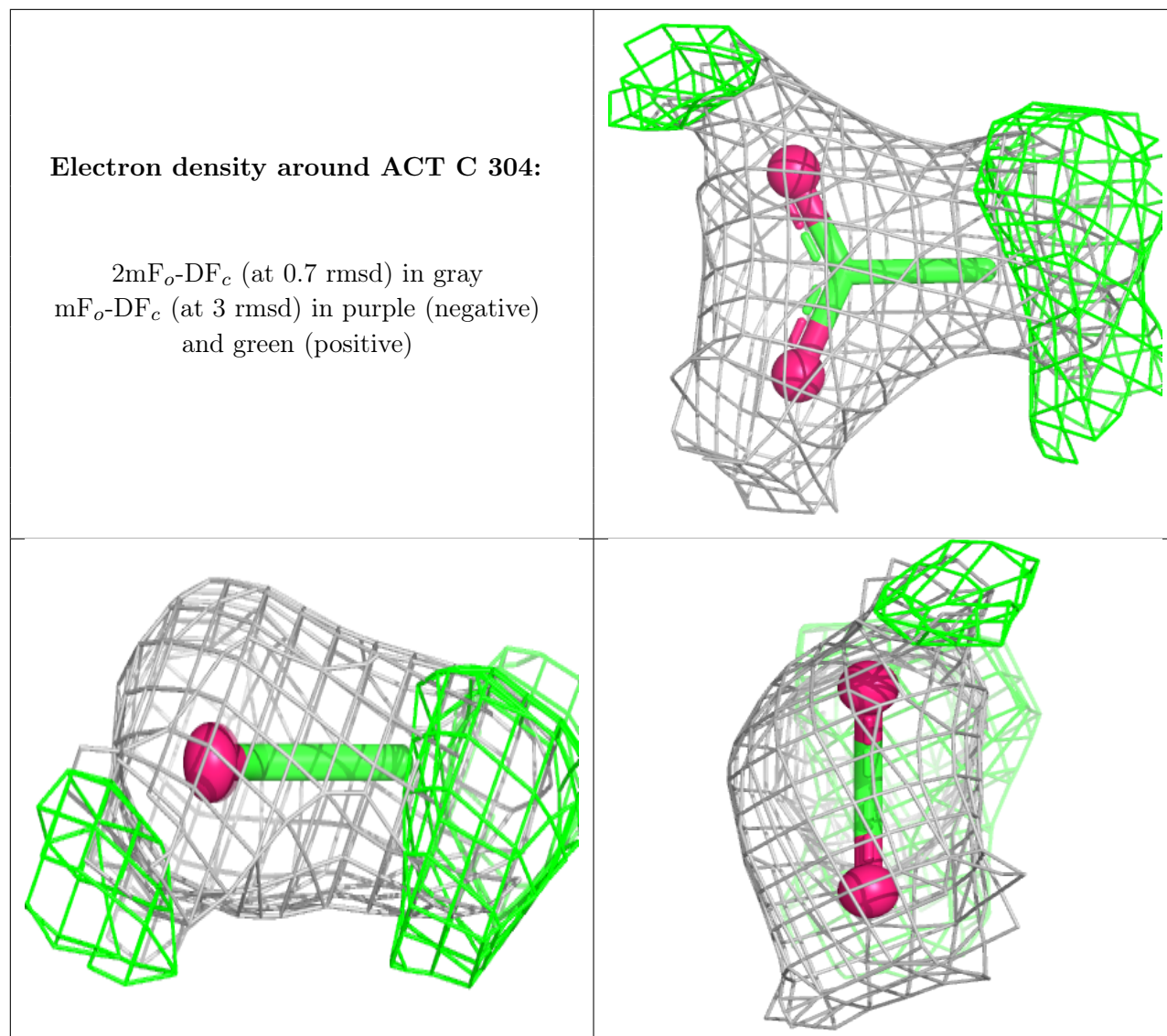
### 6.4 Ligands [i](#)

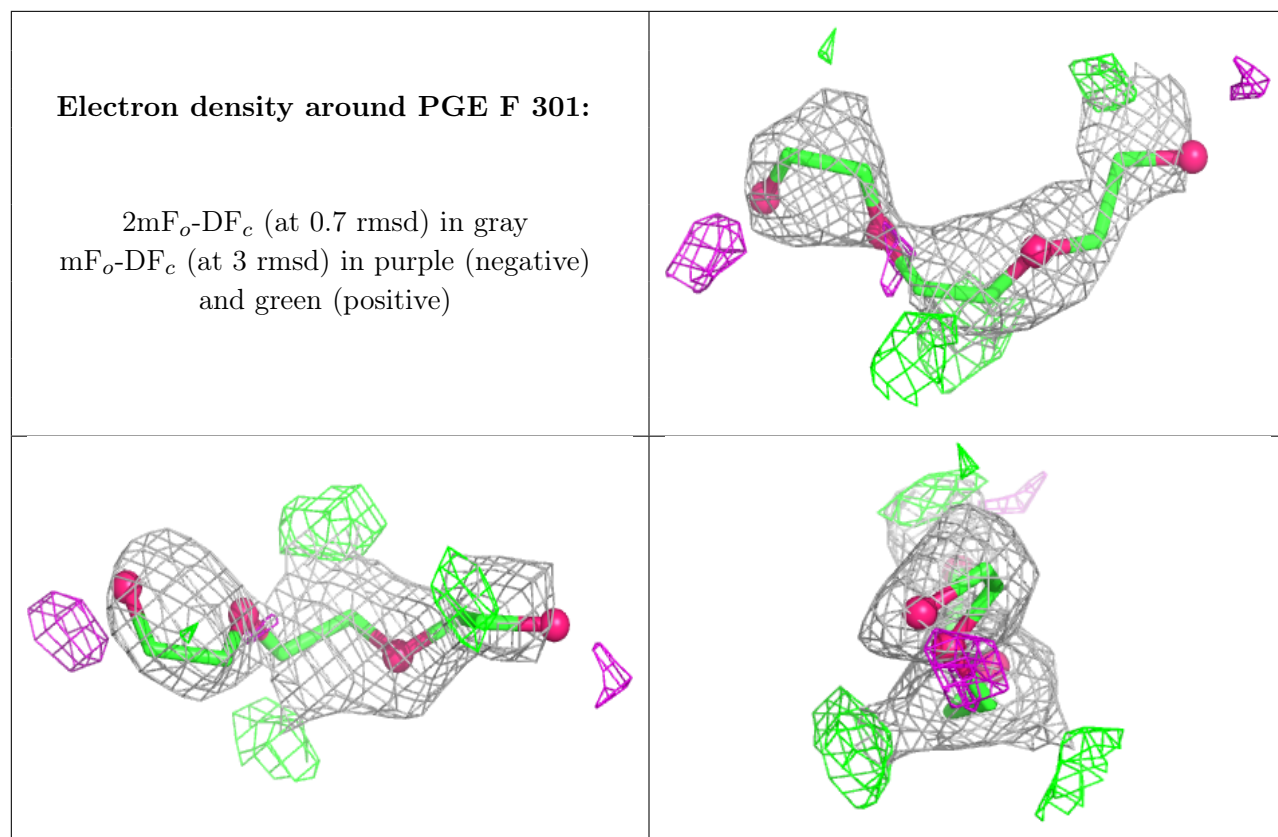
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACT	C	304	4/4	0.59	0.21	44,48,49,51	0
2	PGE	F	301	10/10	0.68	0.18	50,55,58,60	0
3	MG	E	302	1/1	0.76	0.27	48,48,48,48	0
4	ACT	D	302	4/4	0.77	0.17	46,46,49,51	0
4	ACT	F	302	4/4	0.82	0.12	44,44,52,52	0
5	LYS	B	302	10/10	0.83	0.13	40,44,49,50	0
4	ACT	C	303	4/4	0.84	0.14	42,45,46,50	0
2	PGE	C	301	10/10	0.85	0.12	40,41,43,44	0
4	ACT	E	303	4/4	0.85	0.12	41,42,44,44	0
3	MG	A	302	1/1	0.86	0.07	50,50,50,50	0
4	ACT	A	303	4/4	0.87	0.14	38,42,45,46	0
5	LYS	A	304	10/10	0.89	0.17	20,20,20,20	0
5	LYS	C	305	10/10	0.89	0.11	40,46,53,53	0
4	ACT	F	303	4/4	0.90	0.13	45,48,48,49	0
2	PGE	D	301	10/10	0.90	0.11	44,46,50,51	0
2	PGE	E	301	10/10	0.91	0.10	41,44,49,51	0
2	PGE	B	301	10/10	0.91	0.11	42,45,53,54	0
5	LYS	D	303	10/10	0.91	0.11	43,47,50,54	0
5	LYS	E	304	10/10	0.91	0.10	40,44,50,52	0
5	LYS	F	304	10/10	0.91	0.11	44,46,52,57	0
2	PGE	A	301	10/10	0.94	0.08	44,49,51,52	0
3	MG	C	302	1/1	0.94	0.12	44,44,44,44	0

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

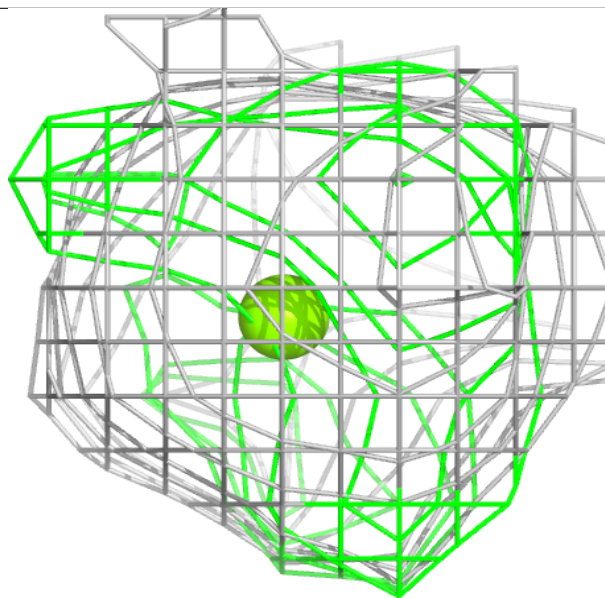
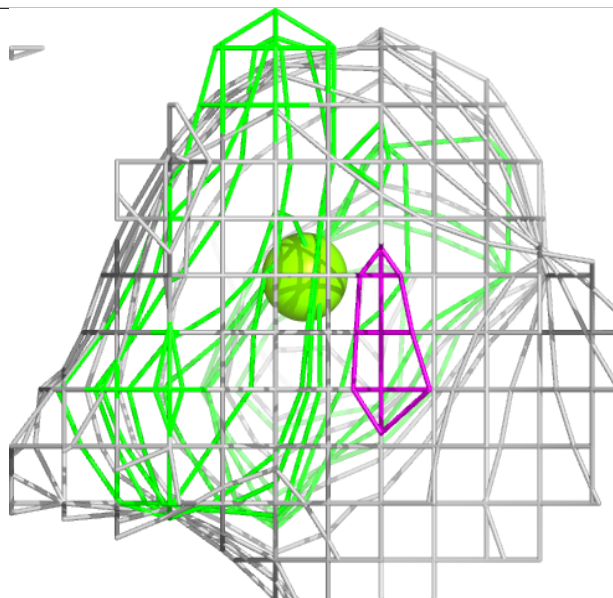
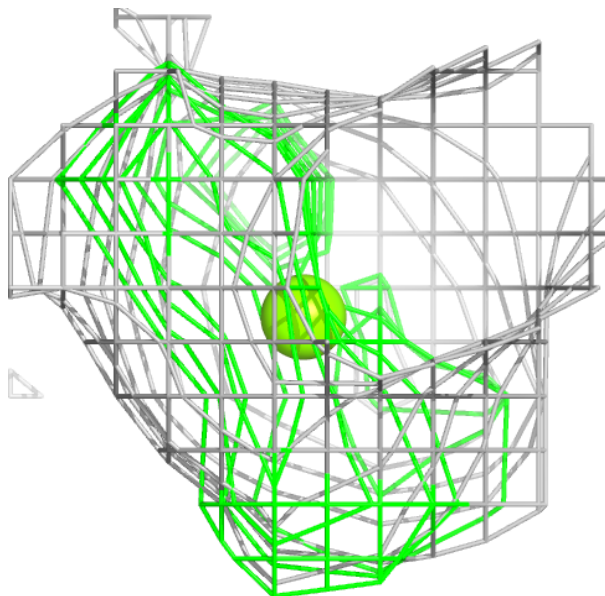
orientation to approximate a three-dimensional view.

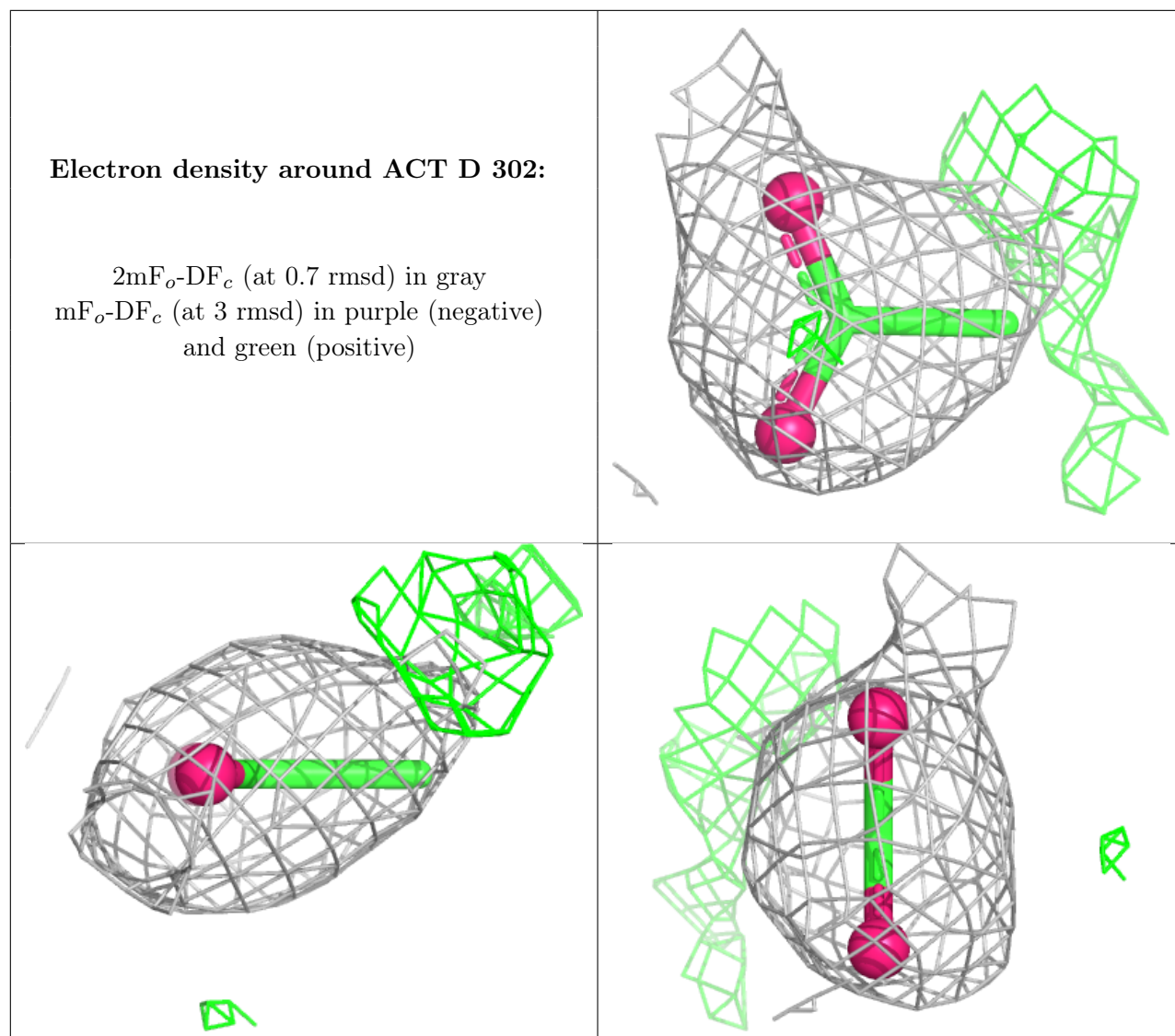




**Electron density around MG E 302:**

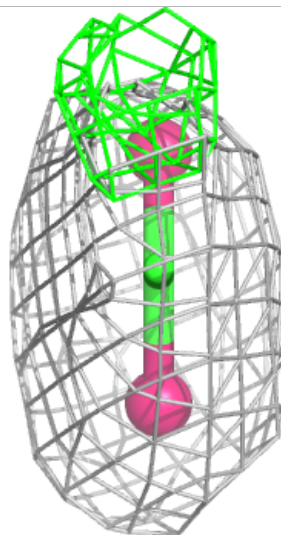
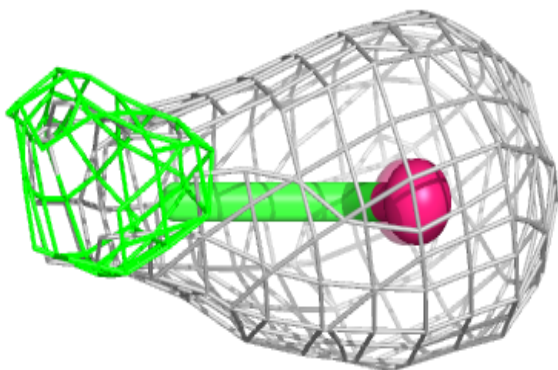
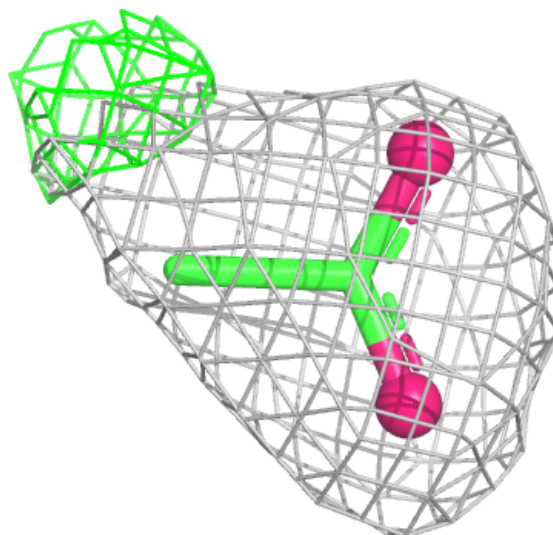
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





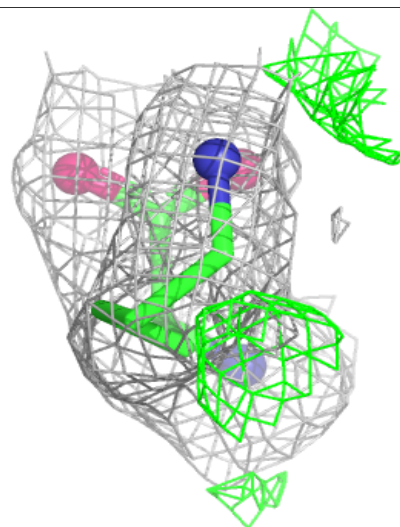
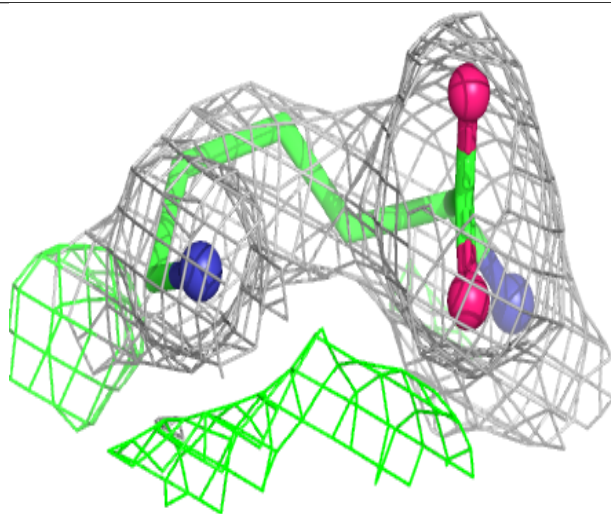
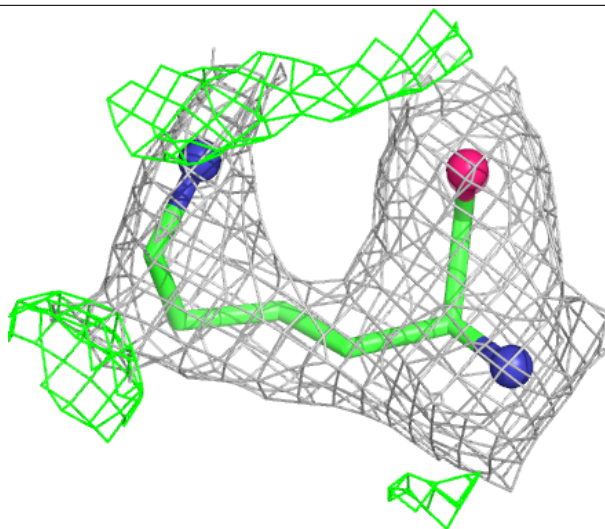
**Electron density around ACT F 302:**

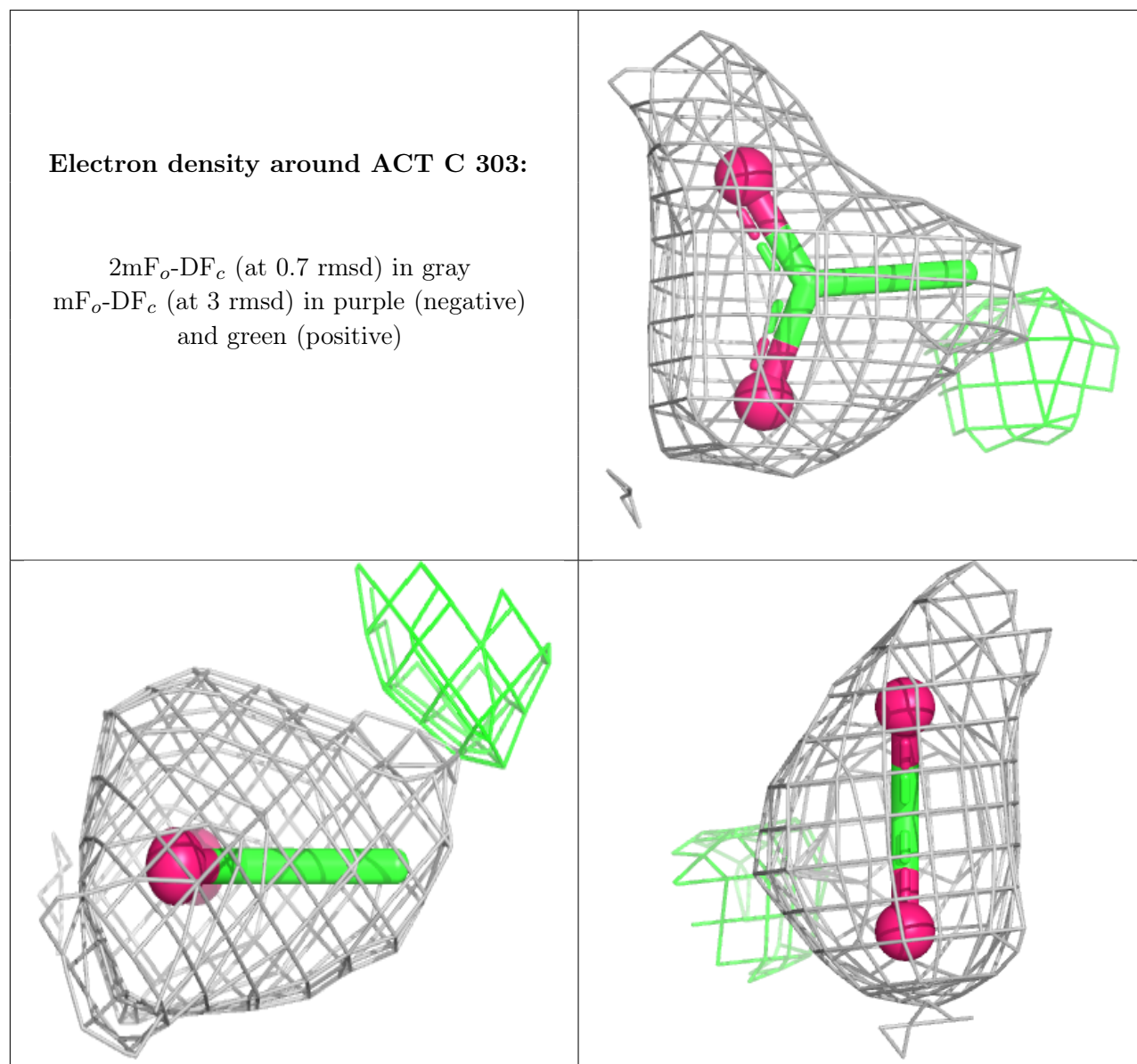
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

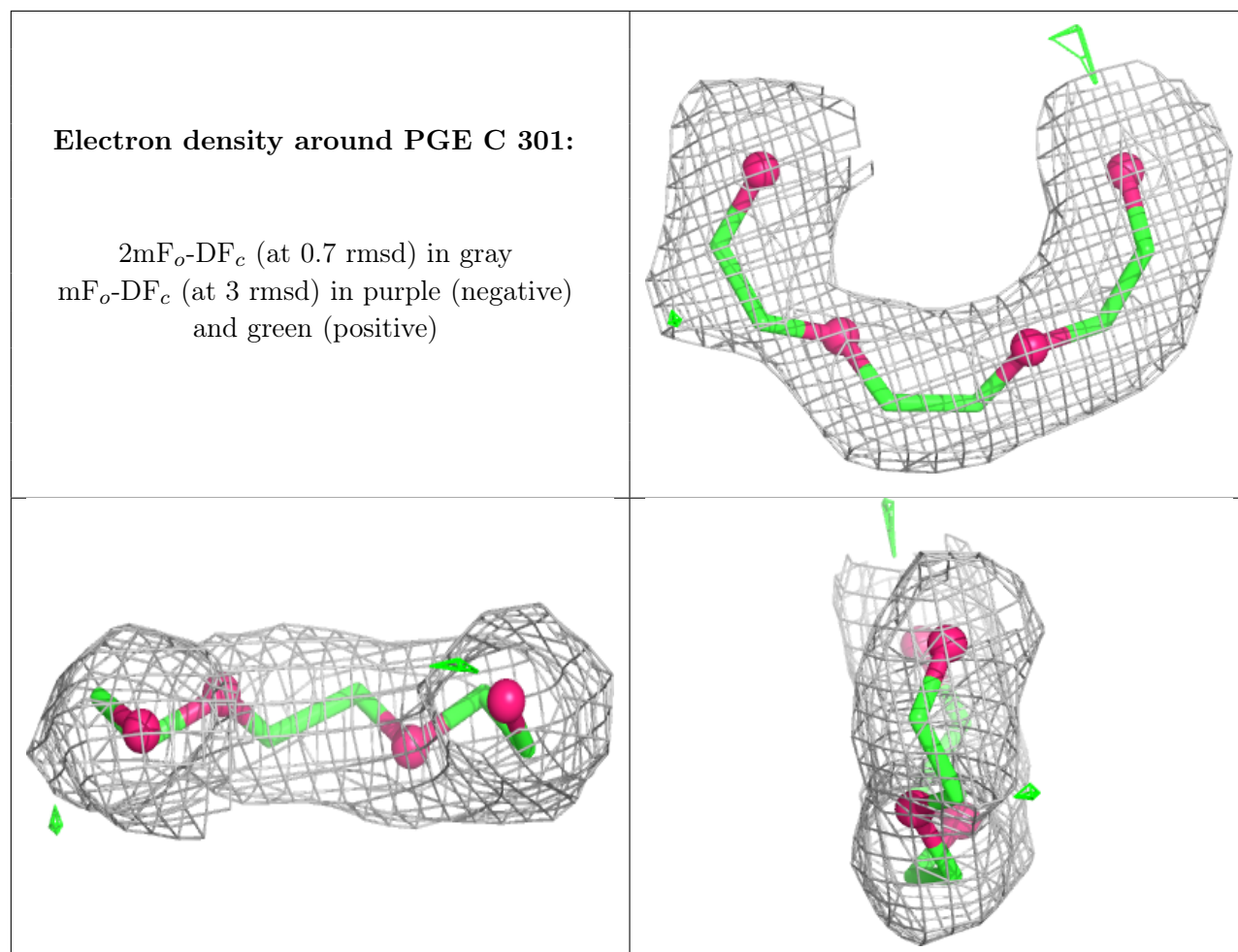


**Electron density around LYS B 302:**

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

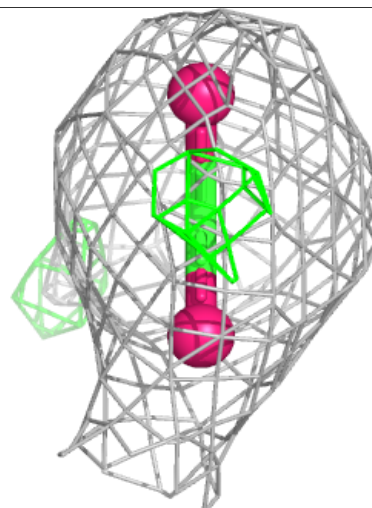
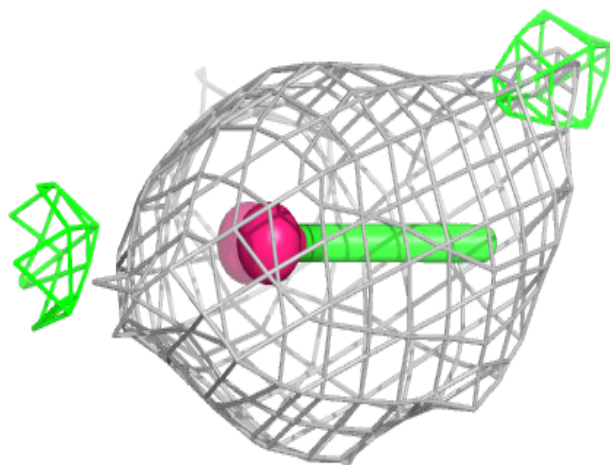
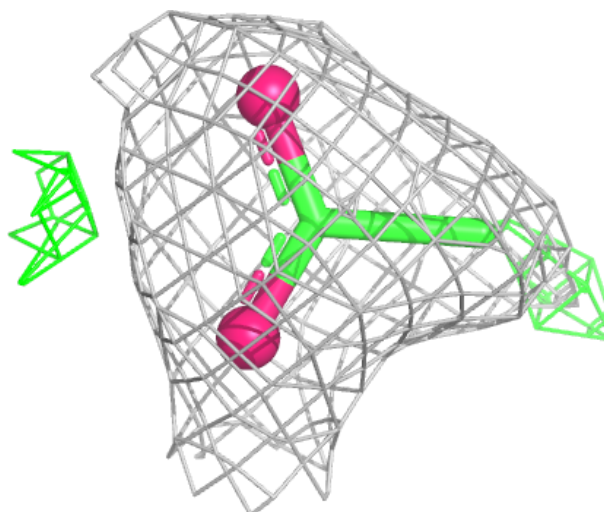






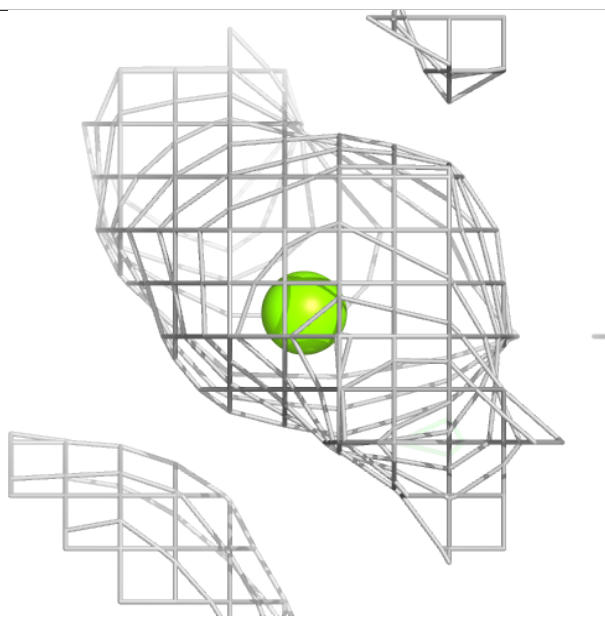
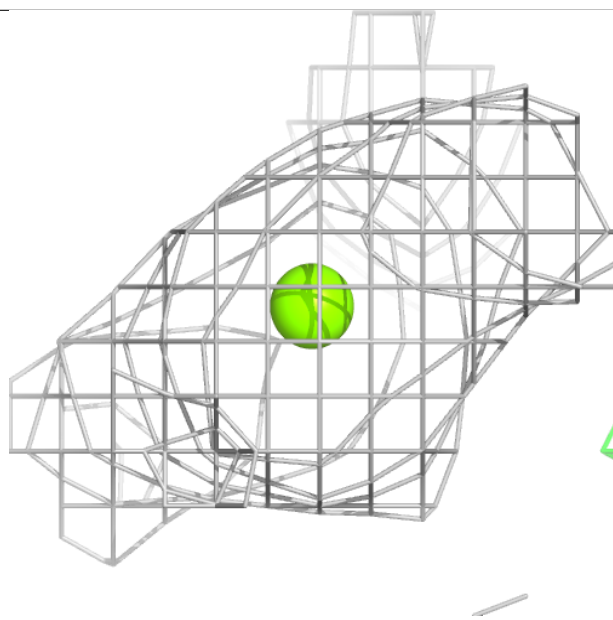
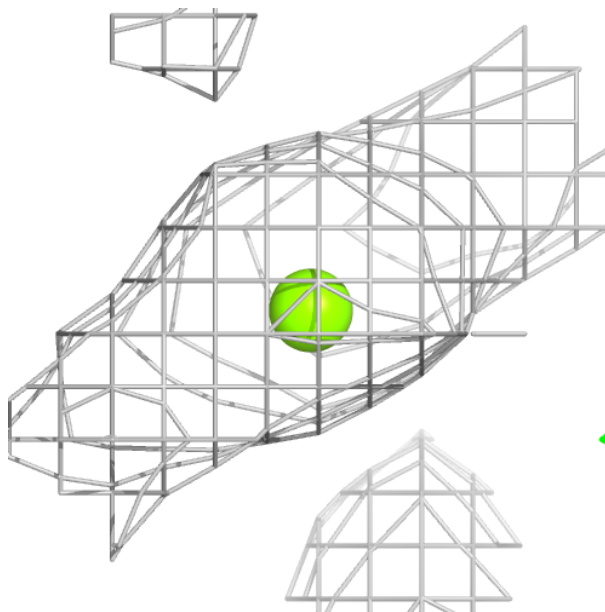
**Electron density around ACT E 303:**

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



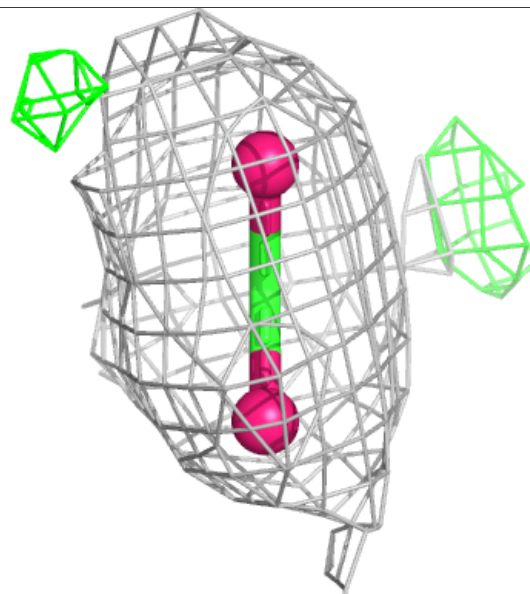
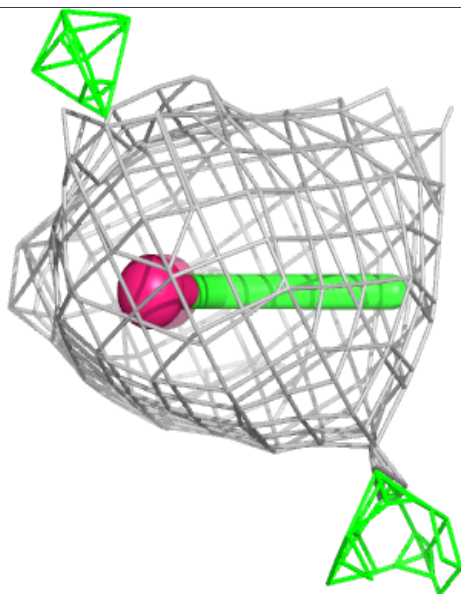
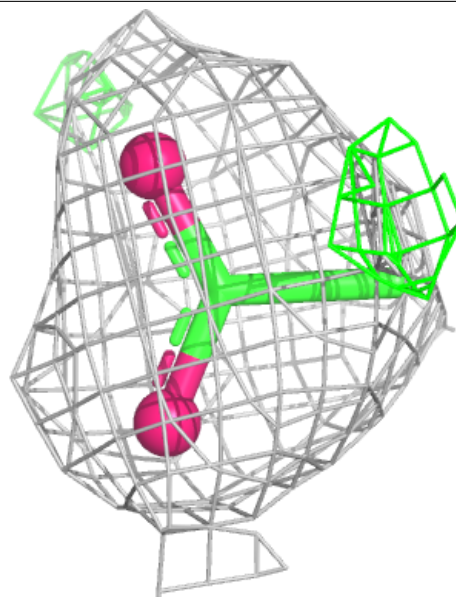
**Electron density around MG A 302:**

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



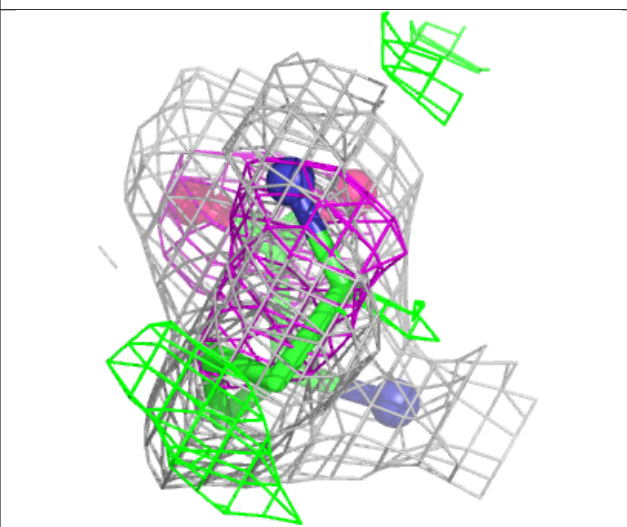
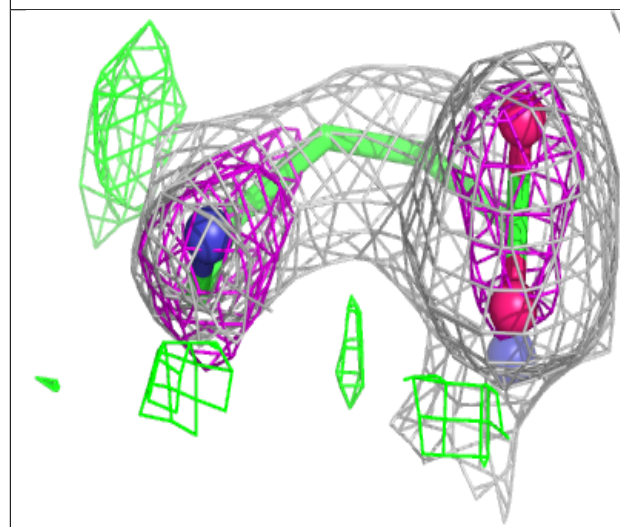
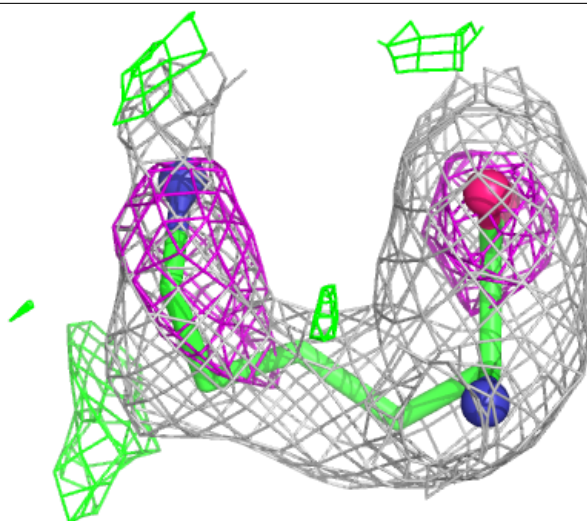
**Electron density around ACT A 303:**

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



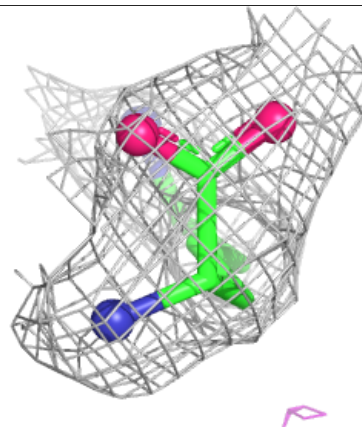
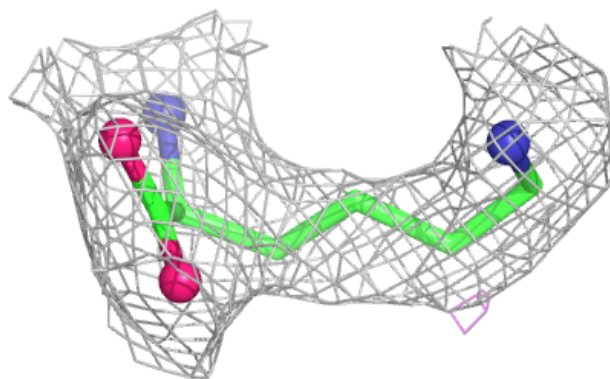
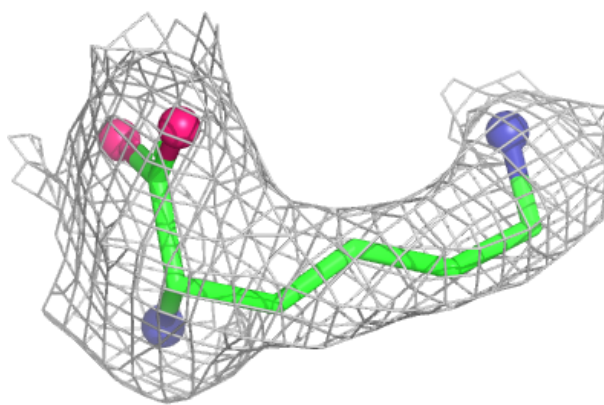
**Electron density around LYS A 304:**

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



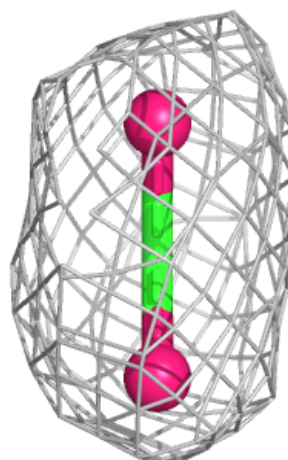
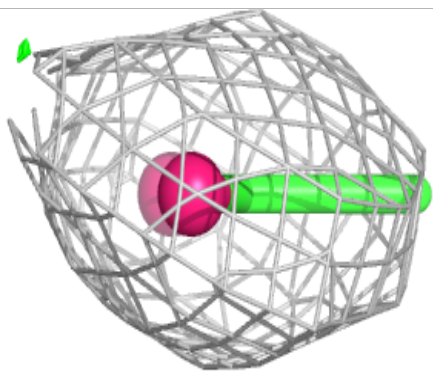
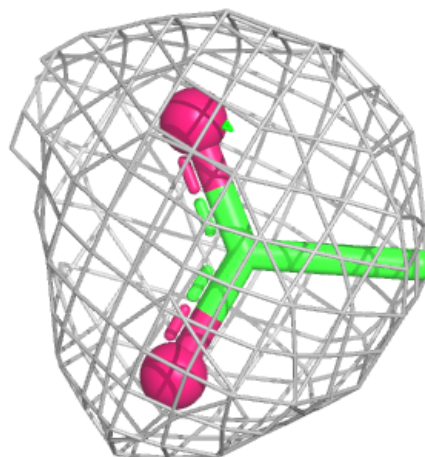
**Electron density around LYS C 305:**

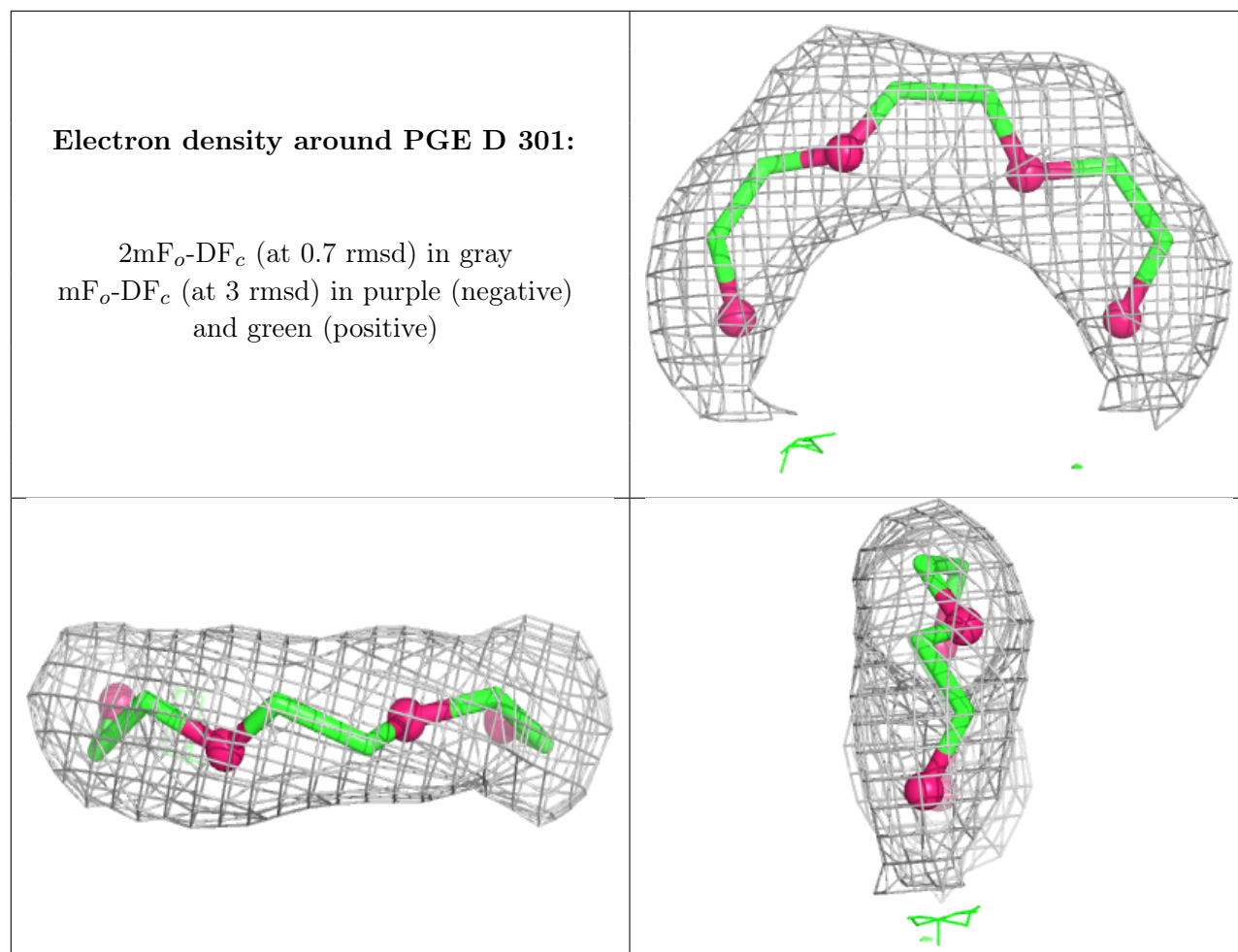
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ACT F 303:**

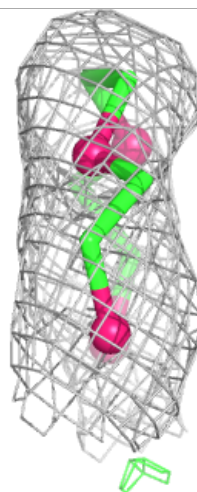
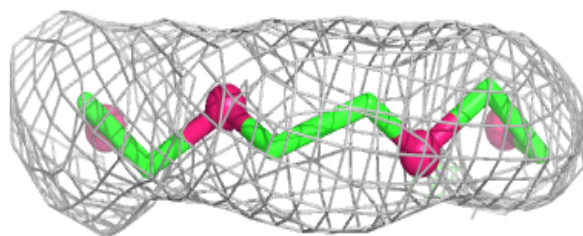
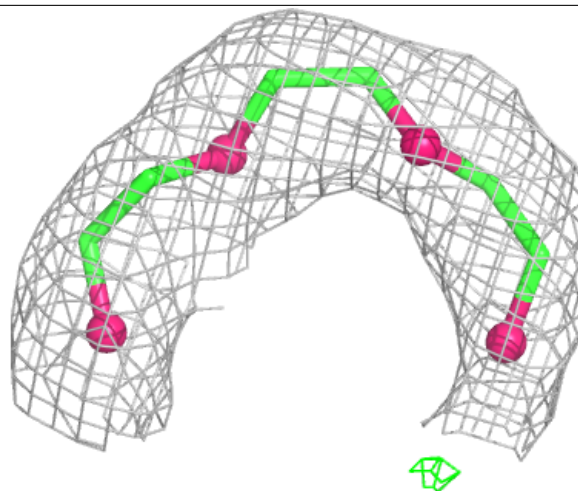
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





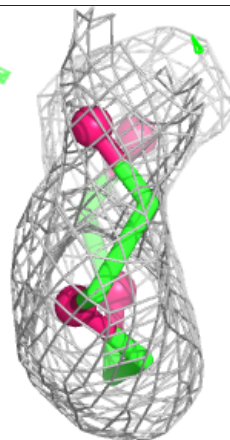
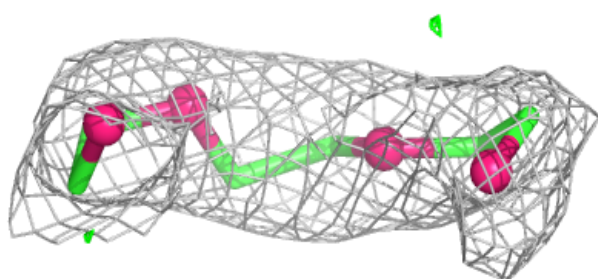
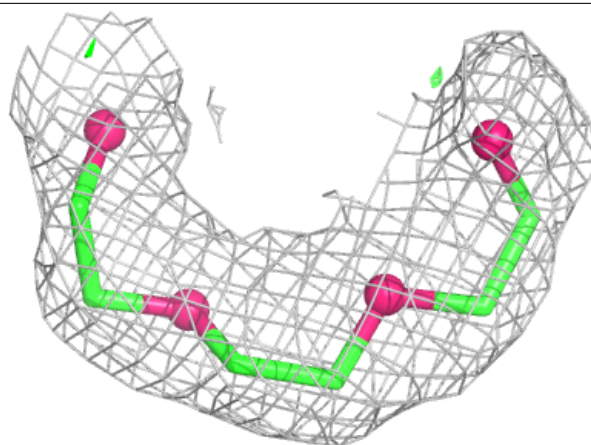
**Electron density around PGE E 301:**

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

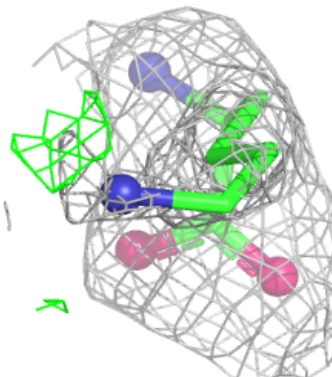
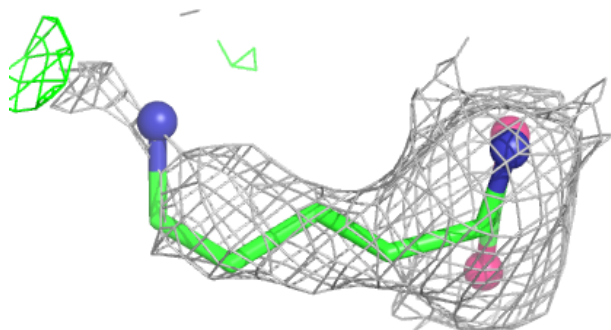
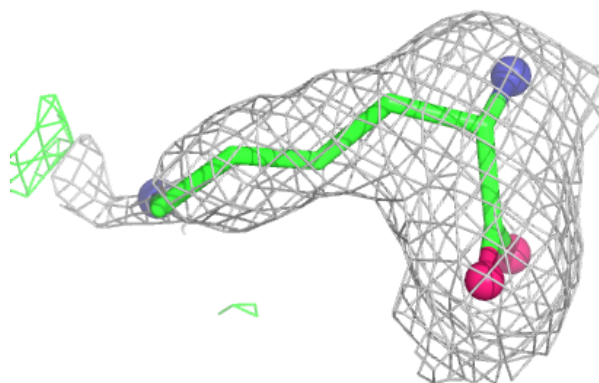


**Electron density around PGE B 301:**

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

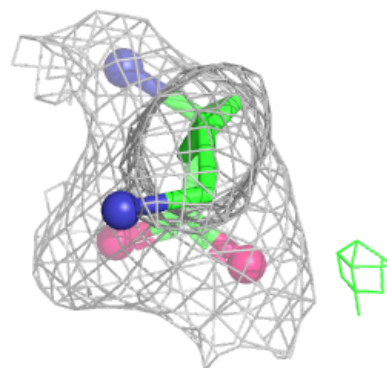
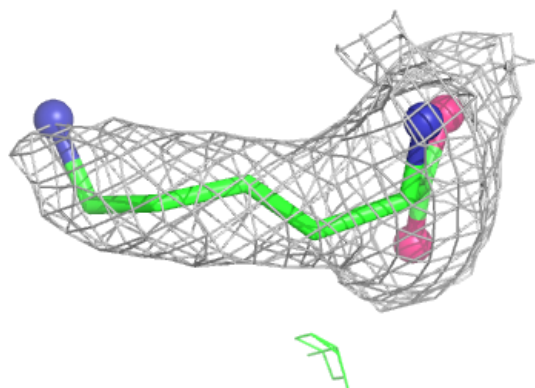
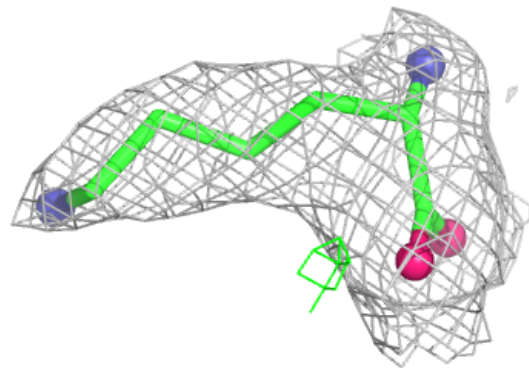
**Electron density around LYS D 303:**

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

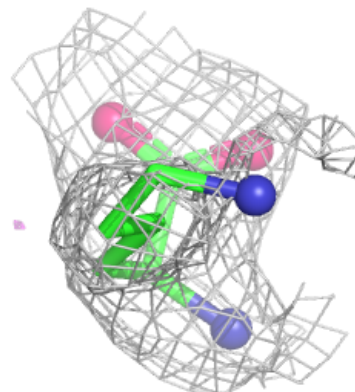
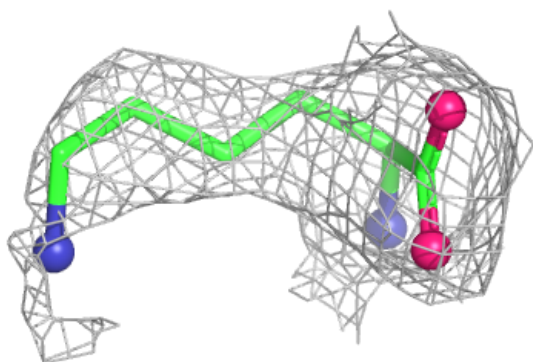
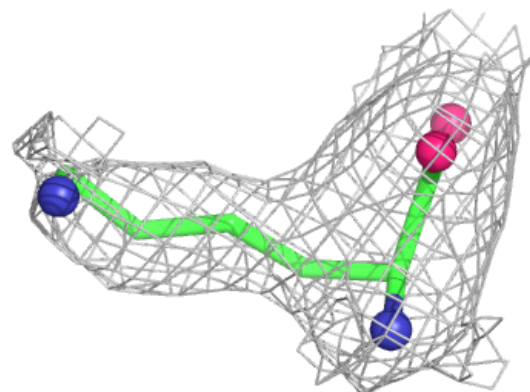


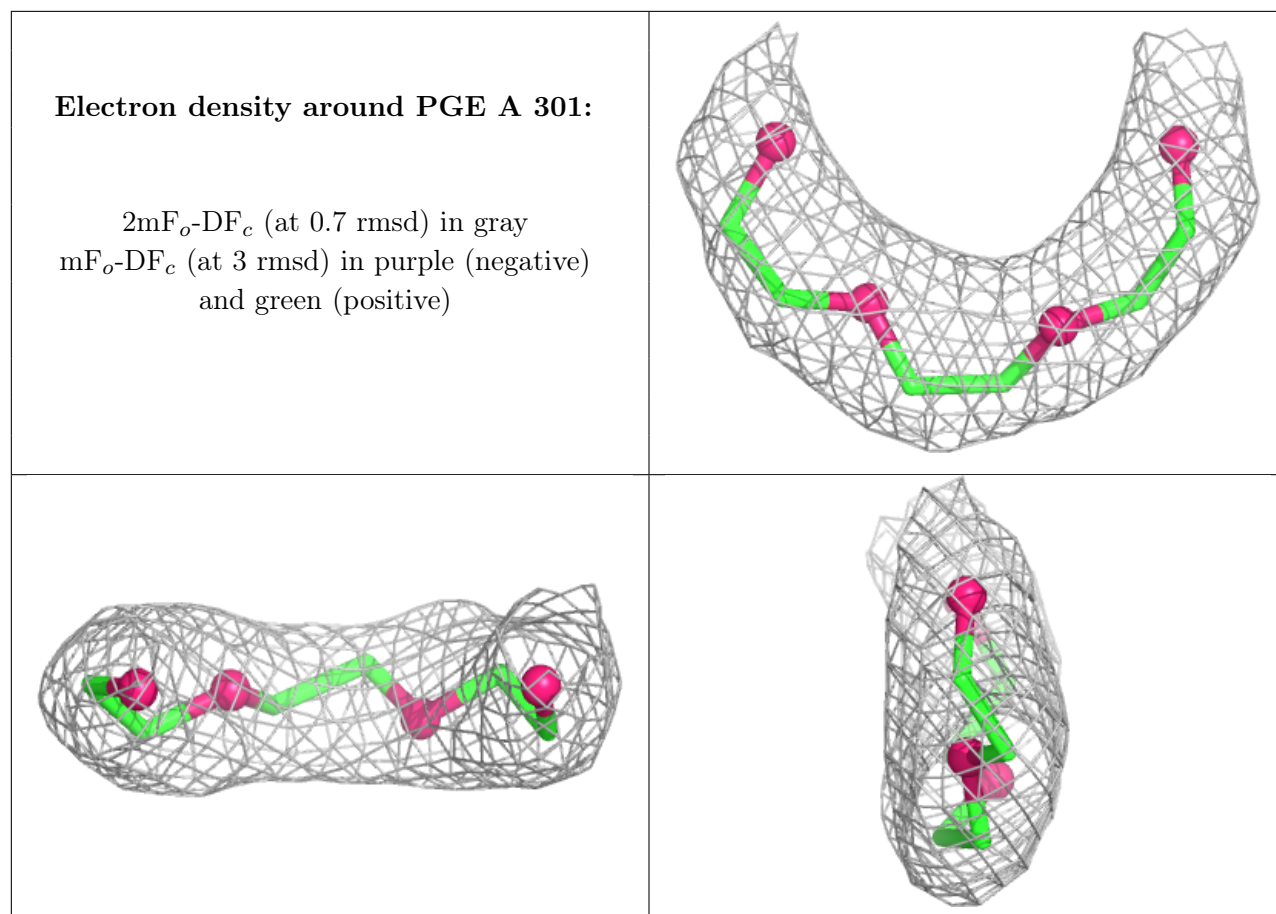
**Electron density around LYS E 304:**

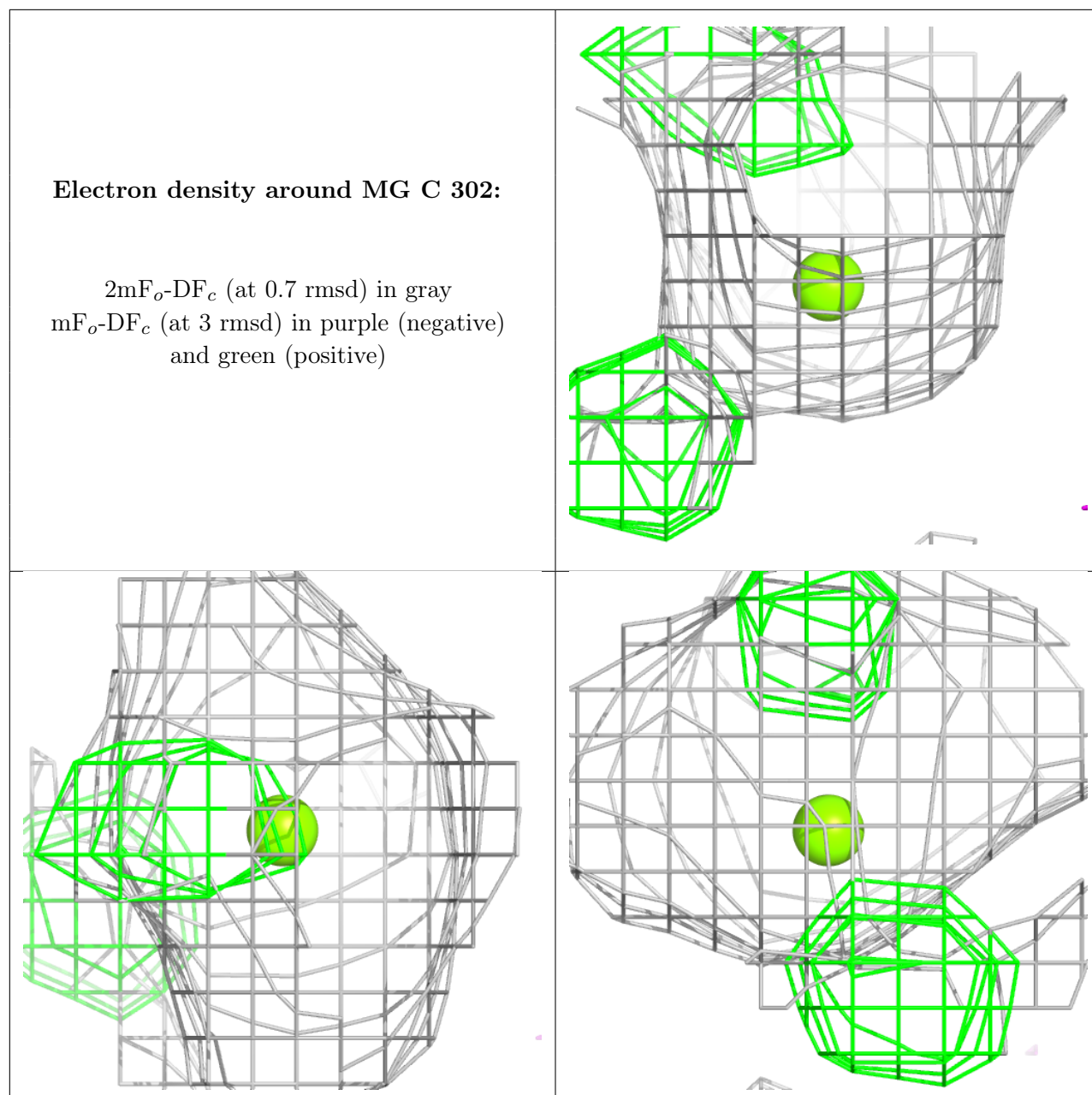
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LYS F 304:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.