



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:16 am BST

PDB ID : 1VCR
Title : An icosahedral assembly of light-harvesting chlorophyll a/b protein complex from pea thylakoid membranes
Authors : Hino, T.; Kanamori, E.; Shen, J.-R.; Kouyama, T.
Deposited on : 2004-03-10
Resolution : 9.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

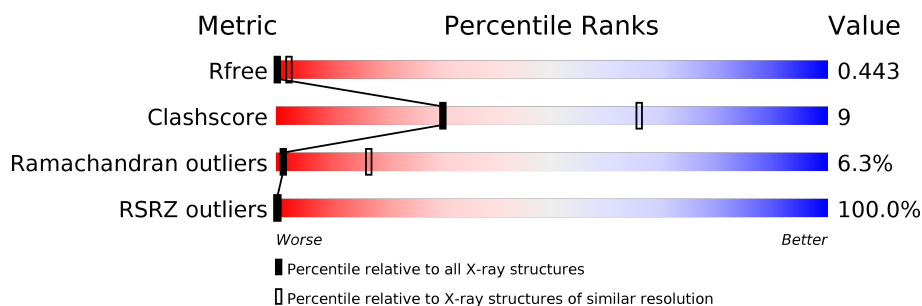
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.50 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}	130704	1005 (11.50-3.90)
Clashscore	141614	1071 (15.00-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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 on 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 $\leq 5\%$. 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	232	<div> <div>44%</div> <div>36%</div> <div>6%</div> <div>56%</div> </div>

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
2	CLA	A	251	X	-	-	X
2	CLA	A	252	X	-	-	X
2	CLA	A	253	X	-	-	X
2	CLA	A	254	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	A	255	X	-	-	X
2	CLA	A	256	X	-	-	X
2	CLA	A	257	X	-	-	X
3	CHL	A	261	X	-	-	X
3	CHL	A	262	X	-	-	X
3	CHL	A	263	X	-	-	X
3	CHL	A	265	X	-	-	X
3	CHL	A	266	X	-	-	X

2 Entry composition [i](#)

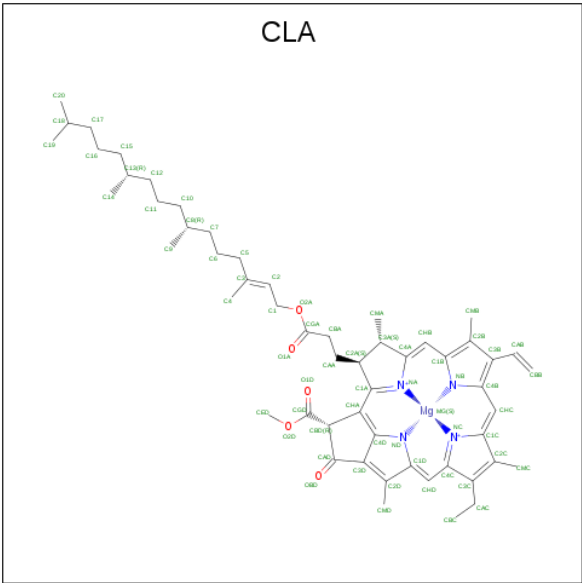
There are 3 unique types of molecules in this entry. The entry contains 796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll a-b binding protein AB80.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	0	0
			496	294	101	101		

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



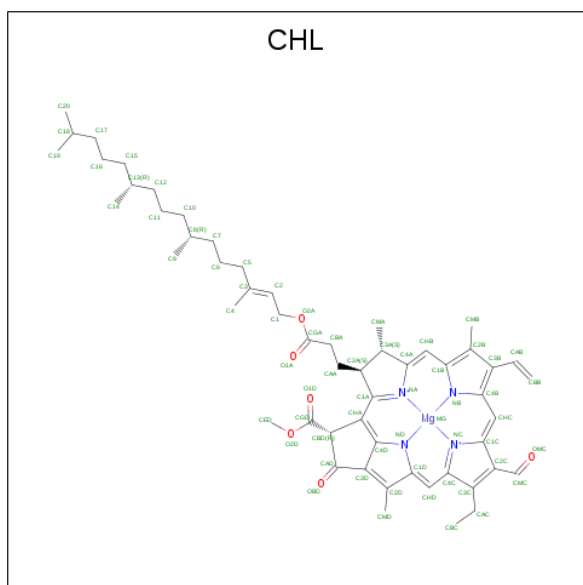
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 25	C 20	Mg 1	N 4	0	0
2	A	1	Total 25	C 20	Mg 1	N 4	0	0

- Molecule 3 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).

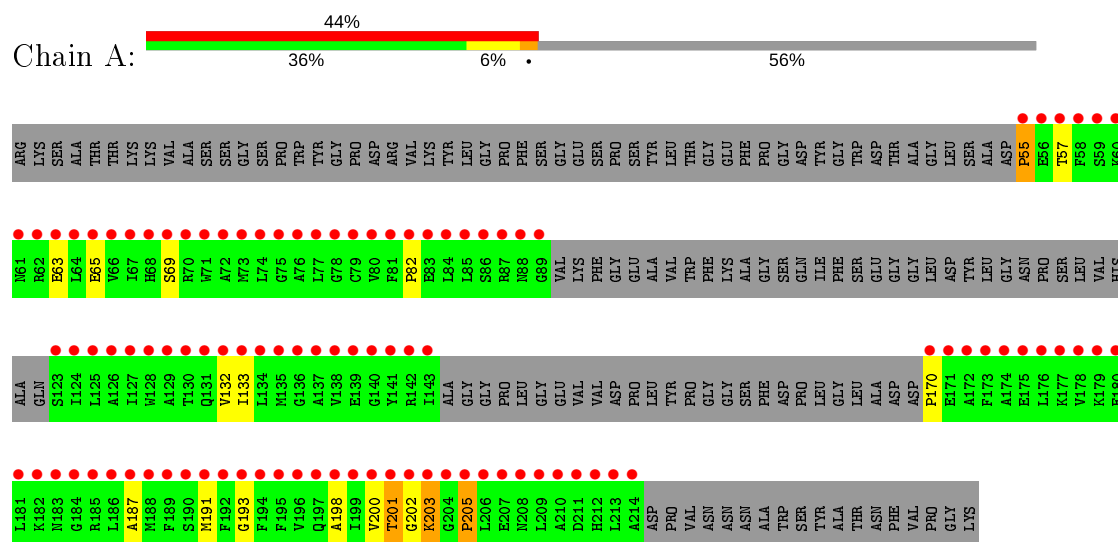


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 25	C 20	Mg 1	N 4	0	0
3	A	1	Total 25	C 20	Mg 1	N 4	0	0
3	A	1	Total 25	C 20	Mg 1	N 4	0	0
3	A	1	Total 25	C 20	Mg 1	N 4	0	0
3	A	1	Total 25	C 20	Mg 1	N 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Chlorophyll a-b binding protein AB80



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	360.65Å 360.65Å 360.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 9.50 208.22 – 9.50	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-9.50) 99.7 (208.22-9.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.13 (at 9.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.379 , 0.353 0.427 , 0.443	Depositor DCC
R_{free} test set	241 reflections (9.52%)	wwPDB-VP
Wilson B-factor (Å ²)	281.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , -110.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.16$, $\langle L^2 \rangle = 0.04$	Xtriage
Estimated twinning fraction	0.459 for k,h,-l	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	796	wwPDB-VP
Average B, all atoms (Å ²)	296.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CHL, CLA

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	0.34	0/493	0.63	4/680 (0.6%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	55	PRO	N-CA-CB	5.58	109.99	103.30
1	A	205	PRO	N-CA-CB	5.56	109.98	103.30
1	A	170	PRO	N-CA-CB	5.49	109.89	103.30
1	A	82	PRO	N-CA-CB	5.46	109.85	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	496	0	239	10	0
2	A	175	0	21	0	0
3	A	125	0	15	0	0
All	All	796	0	275	10	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 9.

All (10) 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:63:GLU:C	1:A:65:GLU:H	1.97	0.66
1:A:55:PRO:C	1:A:57:THR:H	2.03	0.62
1:A:200:VAL:O	1:A:201:THR:CB	2.50	0.58
1:A:198:ALA:HA	1:A:203:LYS:O	2.10	0.52
1:A:63:GLU:C	1:A:65:GLU:N	2.63	0.51
1:A:191:MET:C	1:A:193:GLY:H	2.13	0.50
1:A:55:PRO:C	1:A:57:THR:N	2.67	0.47
1:A:187:ALA:O	1:A:191:MET:N	2.49	0.46
1:A:65:GLU:O	1:A:69:SER:N	2.44	0.46
1:A:191:MET:C	1:A:193:GLY:N	2.73	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	95/232 (41%)	79 (83%)	10 (10%)	6 (6%)	1 17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	THR
1	A	203	LYS
1	A	205	PRO
1	A	132	VAL
1	A	202	GLY
1	A	133	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands 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	$\# Z > 2$
2	CLA	A	257	-	22,32,73	3.15	10 (45%)	26,54,113	2.01	7 (26%)
2	CLA	A	256	-	22,32,73	3.18	10 (45%)	26,54,113	1.94	7 (26%)
2	CLA	A	253	-	22,32,73	3.23	11 (50%)	26,54,113	1.99	7 (26%)
3	CHL	A	263	-	22,32,74	3.20	11 (50%)	26,54,114	1.95	7 (26%)
2	CLA	A	252	-	22,32,73	3.21	11 (50%)	26,54,113	1.96	7 (26%)
2	CLA	A	255	-	22,32,73	3.20	11 (50%)	26,54,113	1.95	7 (26%)
3	CHL	A	266	-	22,32,74	3.13	9 (40%)	26,54,114	1.98	7 (26%)
2	CLA	A	251	-	22,32,73	3.15	10 (45%)	26,54,113	1.97	7 (26%)
3	CHL	A	262	-	22,32,74	3.20	11 (50%)	26,54,114	1.95	7 (26%)
3	CHL	A	265	-	22,32,74	3.20	11 (50%)	26,54,114	1.96	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	A	254	-	22,32,73	3.13	11 (50%)	26,54,113	2.00	7 (26%)
3	CHL	A	261	-	22,32,74	3.15	9 (40%)	26,54,114	1.98	7 (26%)

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	CLA	A	257	-	3/3/7/25	-	-
2	CLA	A	256	-	3/3/7/25	-	-
2	CLA	A	253	-	3/3/7/25	-	-
3	CHL	A	263	-	3/3/7/26	-	-
2	CLA	A	252	-	3/3/7/25	-	-
2	CLA	A	255	-	3/3/7/25	-	-
3	CHL	A	266	-	3/3/7/26	-	-
2	CLA	A	251	-	3/3/7/25	-	-
3	CHL	A	262	-	3/3/7/26	-	-
3	CHL	A	265	-	3/3/7/26	-	-
2	CLA	A	254	-	3/3/7/25	-	-
3	CHL	A	261	-	3/3/7/26	-	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	254	CLA	C3C-C2C	8.64	1.54	1.35
2	A	253	CLA	C3C-C2C	8.56	1.54	1.35
2	A	252	CLA	C3C-C2C	8.50	1.54	1.35
2	A	255	CLA	C3C-C2C	8.48	1.54	1.35
3	A	261	CHL	C3C-C2C	8.47	1.54	1.35
3	A	263	CHL	C3C-C2C	8.46	1.54	1.35
3	A	262	CHL	C3C-C2C	8.45	1.54	1.35
2	A	256	CLA	C3C-C2C	8.42	1.54	1.35
3	A	265	CHL	C3C-C2C	8.40	1.53	1.35
2	A	251	CLA	C3C-C2C	8.40	1.53	1.35
3	A	266	CHL	C3C-C2C	8.38	1.53	1.35
2	A	257	CLA	C3C-C2C	8.36	1.53	1.35
2	A	256	CLA	CHB-C4A	6.07	1.39	1.34
3	A	265	CHL	CHB-C4A	6.01	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	253	CLA	CHB-C4A	6.00	1.39	1.34
2	A	251	CLA	CHB-C4A	5.93	1.39	1.34
3	A	263	CHL	CHB-C4A	5.90	1.39	1.34
2	A	252	CLA	CHB-C4A	5.90	1.39	1.34
2	A	255	CLA	CHB-C4A	5.89	1.39	1.34
3	A	262	CHL	CHB-C4A	5.87	1.39	1.34
2	A	257	CLA	CHB-C4A	5.77	1.39	1.34
3	A	266	CHL	CHB-C4A	5.74	1.39	1.34
2	A	257	CLA	MG-NA	5.71	2.19	2.06
2	A	253	CLA	MG-NA	5.68	2.19	2.06
2	A	252	CLA	MG-NA	5.65	2.19	2.06
2	A	255	CLA	MG-NA	5.63	2.19	2.06
3	A	262	CHL	MG-NA	5.62	2.19	2.06
3	A	261	CHL	CHB-C4A	5.61	1.39	1.34
3	A	263	CHL	MG-NA	5.60	2.19	2.06
3	A	261	CHL	MG-NA	5.60	2.19	2.06
3	A	266	CHL	C3B-C4B	5.56	1.49	1.39
3	A	265	CHL	MG-NA	5.55	2.19	2.06
2	A	255	CLA	C3B-C4B	5.50	1.49	1.39
2	A	254	CLA	MG-NA	5.49	2.19	2.06
2	A	252	CLA	C3B-C4B	5.49	1.49	1.39
3	A	262	CHL	C3B-C4B	5.45	1.49	1.39
3	A	263	CHL	C3B-C4B	5.45	1.49	1.39
3	A	265	CHL	C3B-C4B	5.44	1.49	1.39
2	A	256	CLA	MG-NA	5.38	2.19	2.06
2	A	251	CLA	MG-NA	5.38	2.19	2.06
2	A	251	CLA	C3B-C4B	5.38	1.49	1.39
2	A	256	CLA	C3B-C4B	5.34	1.49	1.39
2	A	254	CLA	C3B-C4B	5.33	1.49	1.39
3	A	266	CHL	MG-NA	5.31	2.18	2.06
2	A	253	CLA	C3B-C4B	5.26	1.49	1.39
3	A	261	CHL	C3B-C4B	5.24	1.49	1.39
2	A	257	CLA	C3B-C4B	5.21	1.49	1.39
2	A	254	CLA	CHB-C4A	4.94	1.38	1.34
3	A	261	CHL	C2B-C1B	3.87	1.46	1.39
2	A	256	CLA	C2B-C1B	3.81	1.46	1.39
3	A	265	CHL	C2B-C1B	3.80	1.46	1.39
3	A	262	CHL	C2B-C1B	3.80	1.46	1.39
2	A	251	CLA	C2B-C1B	3.76	1.46	1.39
2	A	255	CLA	C2B-C1B	3.76	1.46	1.39
2	A	252	CLA	C2B-C1B	3.76	1.46	1.39
3	A	263	CHL	C2B-C1B	3.74	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	253	CLA	C2B-C1B	3.71	1.46	1.39
3	A	266	CHL	C2B-C1B	3.68	1.46	1.39
2	A	257	CLA	C2B-C1B	3.55	1.46	1.39
2	A	254	CLA	C2B-C1B	3.47	1.46	1.39
2	A	253	CLA	C2C-C1C	2.96	1.50	1.43
2	A	254	CLA	C3C-C4C	2.96	1.50	1.43
3	A	263	CHL	C2C-C1C	2.92	1.50	1.43
2	A	253	CLA	C3C-C4C	2.91	1.50	1.43
2	A	252	CLA	C2C-C1C	2.88	1.49	1.43
3	A	262	CHL	C2C-C1C	2.88	1.49	1.43
2	A	255	CLA	C2C-C1C	2.86	1.49	1.43
3	A	261	CHL	C2C-C1C	2.85	1.49	1.43
2	A	257	CLA	C2C-C1C	2.83	1.49	1.43
3	A	263	CHL	C3C-C4C	2.82	1.49	1.43
3	A	266	CHL	C2C-C1C	2.81	1.49	1.43
2	A	252	CLA	C3C-C4C	2.80	1.49	1.43
3	A	261	CHL	C3C-C4C	2.79	1.49	1.43
3	A	266	CHL	C4B-CHC	-2.78	1.38	1.43
2	A	255	CLA	C3C-C4C	2.77	1.49	1.43
3	A	262	CHL	C3C-C4C	2.75	1.49	1.43
2	A	256	CLA	C3C-C4C	2.73	1.49	1.43
3	A	265	CHL	C2C-C1C	2.72	1.49	1.43
2	A	254	CLA	C2C-C1C	2.72	1.49	1.43
2	A	256	CLA	C2C-C1C	2.71	1.49	1.43
2	A	251	CLA	C4B-CHC	-2.71	1.38	1.43
3	A	265	CHL	C3C-C4C	2.70	1.49	1.43
2	A	256	CLA	C4B-CHC	-2.70	1.38	1.43
2	A	257	CLA	C3C-C4C	2.66	1.49	1.43
2	A	251	CLA	C2C-C1C	2.64	1.49	1.43
3	A	265	CHL	C4B-CHC	-2.64	1.38	1.43
2	A	254	CLA	C4B-CHC	-2.62	1.38	1.43
3	A	262	CHL	C4B-CHC	-2.57	1.38	1.43
3	A	266	CHL	C3C-C4C	2.57	1.49	1.43
2	A	255	CLA	C4B-CHC	-2.56	1.38	1.43
2	A	252	CLA	C4B-CHC	-2.53	1.38	1.43
3	A	263	CHL	C4B-CHC	-2.52	1.38	1.43
2	A	251	CLA	C3C-C4C	2.50	1.49	1.43
2	A	253	CLA	C4B-CHC	-2.48	1.38	1.43
3	A	261	CHL	C4B-CHC	-2.42	1.39	1.43
2	A	257	CLA	C4B-CHC	-2.40	1.39	1.43
2	A	257	CLA	C1B-NB	2.40	1.37	1.35
2	A	254	CLA	C1B-CHB	-2.34	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	253	CLA	C1B-NB	2.21	1.37	1.35
2	A	254	CLA	C1B-NB	2.19	1.37	1.35
2	A	256	CLA	C3A-C2A	2.18	1.58	1.52
3	A	263	CHL	C1B-NB	2.17	1.37	1.35
2	A	253	CLA	C4C-NC	2.17	1.40	1.37
2	A	253	CLA	C3A-C2A	2.17	1.58	1.52
2	A	251	CLA	C3A-C2A	2.16	1.58	1.52
2	A	254	CLA	C4C-NC	2.15	1.40	1.37
2	A	252	CLA	C3A-C2A	2.15	1.58	1.52
2	A	257	CLA	C3A-C2A	2.15	1.58	1.52
3	A	265	CHL	C1B-NB	2.14	1.37	1.35
3	A	263	CHL	C3A-C2A	2.14	1.58	1.52
3	A	261	CHL	C1B-NB	2.13	1.37	1.35
2	A	255	CLA	C3A-C2A	2.13	1.58	1.52
3	A	265	CHL	C3A-C2A	2.13	1.58	1.52
3	A	262	CHL	C3A-C2A	2.12	1.58	1.52
3	A	266	CHL	C3A-C2A	2.12	1.58	1.52
2	A	252	CLA	C1B-NB	2.12	1.37	1.35
3	A	265	CHL	C4C-NC	2.09	1.40	1.37
3	A	262	CHL	C1B-NB	2.07	1.37	1.35
3	A	263	CHL	C4C-NC	2.07	1.40	1.37
2	A	255	CLA	C1B-NB	2.07	1.37	1.35
3	A	262	CHL	C4C-NC	2.07	1.40	1.37
2	A	255	CLA	C4C-NC	2.06	1.40	1.37
2	A	251	CLA	C1B-NB	2.04	1.37	1.35
2	A	252	CLA	C4C-NC	2.04	1.40	1.37
2	A	256	CLA	C1B-NB	2.01	1.37	1.35

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	253	CLA	C3C-C2C-C1C	-4.55	101.76	107.21
2	A	257	CLA	C3C-C2C-C1C	-4.49	101.84	107.21
2	A	251	CLA	C3C-C2C-C1C	-4.46	101.87	107.21
3	A	261	CHL	C3C-C2C-C1C	-4.45	101.87	107.21
2	A	256	CLA	C3C-C2C-C1C	-4.41	101.93	107.21
3	A	263	CHL	C3C-C2C-C1C	-4.39	101.95	107.21
2	A	254	CLA	C3C-C2C-C1C	-4.39	101.95	107.21
2	A	252	CLA	C3C-C2C-C1C	-4.38	101.97	107.21
2	A	255	CLA	C3C-C2C-C1C	-4.37	101.98	107.21
3	A	262	CHL	C3C-C2C-C1C	-4.35	102.00	107.21
3	A	266	CHL	C3C-C2C-C1C	-4.35	102.00	107.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	265	CHL	C3C-C2C-C1C	-4.23	102.15	107.21
2	A	251	CLA	C3D-C2D-C1D	-3.86	102.98	106.30
2	A	253	CLA	C3D-C2D-C1D	-3.86	102.98	106.30
3	A	261	CHL	C3D-C2D-C1D	-3.84	102.99	106.30
2	A	257	CLA	C3D-C2D-C1D	-3.84	103.00	106.30
3	A	266	CHL	C3D-C2D-C1D	-3.78	103.04	106.30
3	A	265	CHL	C3D-C2D-C1D	-3.78	103.05	106.30
2	A	254	CLA	C3D-C2D-C1D	-3.73	103.09	106.30
3	A	263	CHL	C3D-C2D-C1D	-3.71	103.10	106.30
3	A	262	CHL	C3D-C2D-C1D	-3.70	103.11	106.30
2	A	252	CLA	C3D-C2D-C1D	-3.70	103.12	106.30
2	A	256	CLA	C3D-C2D-C1D	-3.69	103.12	106.30
2	A	255	CLA	C3D-C2D-C1D	-3.65	103.16	106.30
2	A	254	CLA	C2D-C3D-C4D	3.57	109.38	106.30
2	A	257	CLA	C2D-C3D-C4D	3.49	109.31	106.30
3	A	266	CHL	C2D-C3D-C4D	3.48	109.30	106.30
2	A	253	CLA	C2D-C3D-C4D	3.47	109.29	106.30
2	A	251	CLA	C2D-C3D-C4D	3.41	109.24	106.30
3	A	262	CHL	C2D-C3D-C4D	3.38	109.21	106.30
3	A	265	CHL	C2D-C3D-C4D	3.35	109.19	106.30
2	A	252	CLA	C2D-C3D-C4D	3.31	109.16	106.30
2	A	256	CLA	C2D-C3D-C4D	3.28	109.13	106.30
3	A	263	CHL	C2D-C3D-C4D	3.28	109.12	106.30
2	A	255	CLA	C2D-C3D-C4D	3.27	109.12	106.30
2	A	254	CLA	C3A-C4A-NA	3.16	116.55	109.92
3	A	261	CHL	C2D-C3D-C4D	3.08	108.96	106.30
3	A	261	CHL	C3A-C4A-NA	3.05	116.32	109.92
2	A	252	CLA	C3A-C4A-NA	3.00	116.22	109.92
2	A	257	CLA	C3A-C4A-NA	3.00	116.21	109.92
3	A	265	CHL	C3A-C4A-NA	3.00	116.21	109.92
2	A	255	CLA	C3A-C4A-NA	2.97	116.16	109.92
3	A	263	CHL	C3A-C4A-NA	2.97	116.14	109.92
3	A	262	CHL	C3A-C4A-NA	2.95	116.11	109.92
2	A	253	CLA	C3A-C4A-NA	2.95	116.11	109.92
2	A	251	CLA	C3A-C4A-NA	2.95	116.10	109.92
2	A	256	CLA	C3A-C4A-NA	2.91	116.03	109.92
3	A	266	CHL	C3A-C4A-NA	2.89	115.98	109.92
2	A	253	CLA	C2C-C1C-NC	2.78	114.23	109.51
3	A	266	CHL	C3B-C4B-NB	-2.77	107.68	110.11
2	A	254	CLA	C2C-C1C-NC	2.75	114.17	109.51
2	A	257	CLA	C2C-C1C-NC	2.74	114.16	109.51
2	A	256	CLA	C2C-C1C-NC	2.72	114.12	109.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	257	CLA	C3B-C4B-NB	-2.68	107.75	110.11
3	A	261	CHL	C1C-NC-C4C	2.68	107.91	106.71
2	A	254	CLA	C1C-NC-C4C	2.65	107.90	106.71
2	A	252	CLA	C2C-C1C-NC	2.65	114.00	109.51
2	A	251	CLA	C2C-C1C-NC	2.65	114.00	109.51
3	A	262	CHL	C2C-C1C-NC	2.64	113.99	109.51
3	A	263	CHL	C2C-C1C-NC	2.64	113.98	109.51
2	A	255	CLA	C2C-C1C-NC	2.63	113.96	109.51
3	A	261	CHL	C2C-C1C-NC	2.61	113.93	109.51
3	A	265	CHL	C2C-C1C-NC	2.59	113.90	109.51
2	A	253	CLA	C3B-C4B-NB	-2.53	107.89	110.11
3	A	266	CHL	C1C-NC-C4C	2.53	107.84	106.71
3	A	266	CHL	C2C-C1C-NC	2.51	113.76	109.51
3	A	262	CHL	C3B-C4B-NB	-2.49	107.92	110.11
3	A	263	CHL	C1C-NC-C4C	2.49	107.83	106.71
2	A	255	CLA	C1C-NC-C4C	2.49	107.82	106.71
2	A	255	CLA	C3B-C4B-NB	-2.47	107.94	110.11
2	A	251	CLA	C1C-NC-C4C	2.47	107.81	106.71
3	A	265	CHL	C3B-C4B-NB	-2.46	107.95	110.11
2	A	254	CLA	C3B-C4B-NB	-2.45	107.96	110.11
3	A	263	CHL	C3B-C4B-NB	-2.44	107.96	110.11
3	A	265	CHL	C1C-NC-C4C	2.44	107.80	106.71
2	A	252	CLA	C3B-C4B-NB	-2.43	107.97	110.11
2	A	252	CLA	C1C-NC-C4C	2.32	107.75	106.71
2	A	256	CLA	C3B-C4B-NB	-2.29	108.09	110.11
2	A	253	CLA	C1C-NC-C4C	2.28	107.73	106.71
2	A	251	CLA	C3B-C4B-NB	-2.26	108.12	110.11
2	A	256	CLA	C1C-NC-C4C	2.23	107.71	106.71
3	A	262	CHL	C1C-NC-C4C	2.22	107.70	106.71
3	A	261	CHL	C3B-C4B-NB	-2.21	108.17	110.11
2	A	257	CLA	C1C-NC-C4C	2.02	107.62	106.71

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	257	CLA	NC
2	A	257	CLA	ND
2	A	257	CLA	NA
2	A	256	CLA	NC
2	A	256	CLA	ND
2	A	256	CLA	NA
2	A	253	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	A	253	CLA	ND
2	A	253	CLA	NA
3	A	263	CHL	NC
3	A	263	CHL	ND
3	A	263	CHL	NA
2	A	252	CLA	NC
2	A	252	CLA	ND
2	A	252	CLA	NA
2	A	255	CLA	NC
2	A	255	CLA	ND
2	A	255	CLA	NA
3	A	266	CHL	NC
3	A	266	CHL	ND
3	A	266	CHL	NA
2	A	251	CLA	NC
2	A	251	CLA	ND
2	A	251	CLA	NA
3	A	262	CHL	NC
3	A	262	CHL	ND
3	A	262	CHL	NA
3	A	265	CHL	NC
3	A	265	CHL	ND
3	A	265	CHL	NA
2	A	254	CLA	NC
2	A	254	CLA	ND
2	A	254	CLA	NA
3	A	261	CHL	NC
3	A	261	CHL	ND
3	A	261	CHL	NA

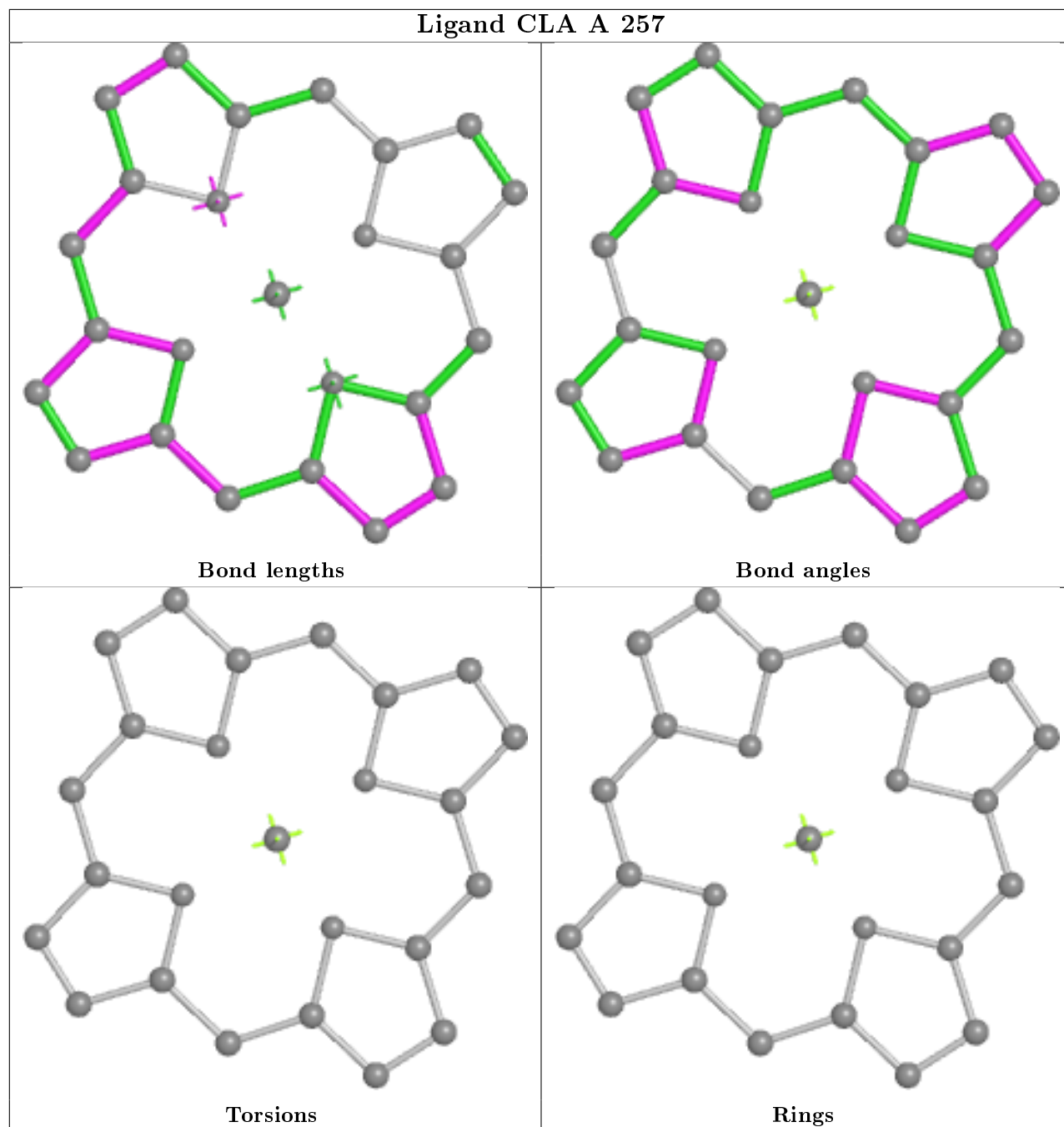
There are no torsion outliers.

There are no ring outliers.

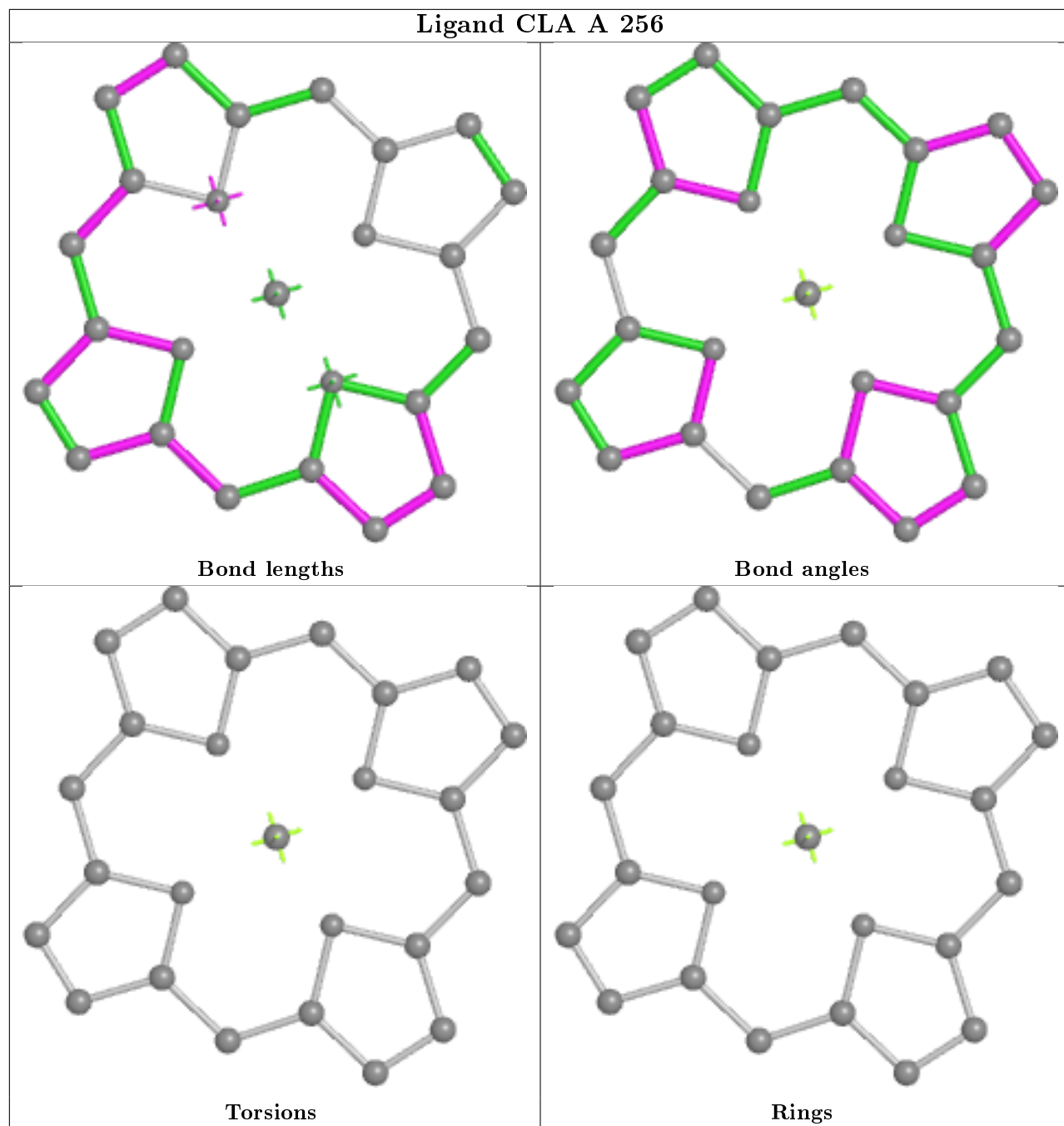
No monomer is involved in short contacts.

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

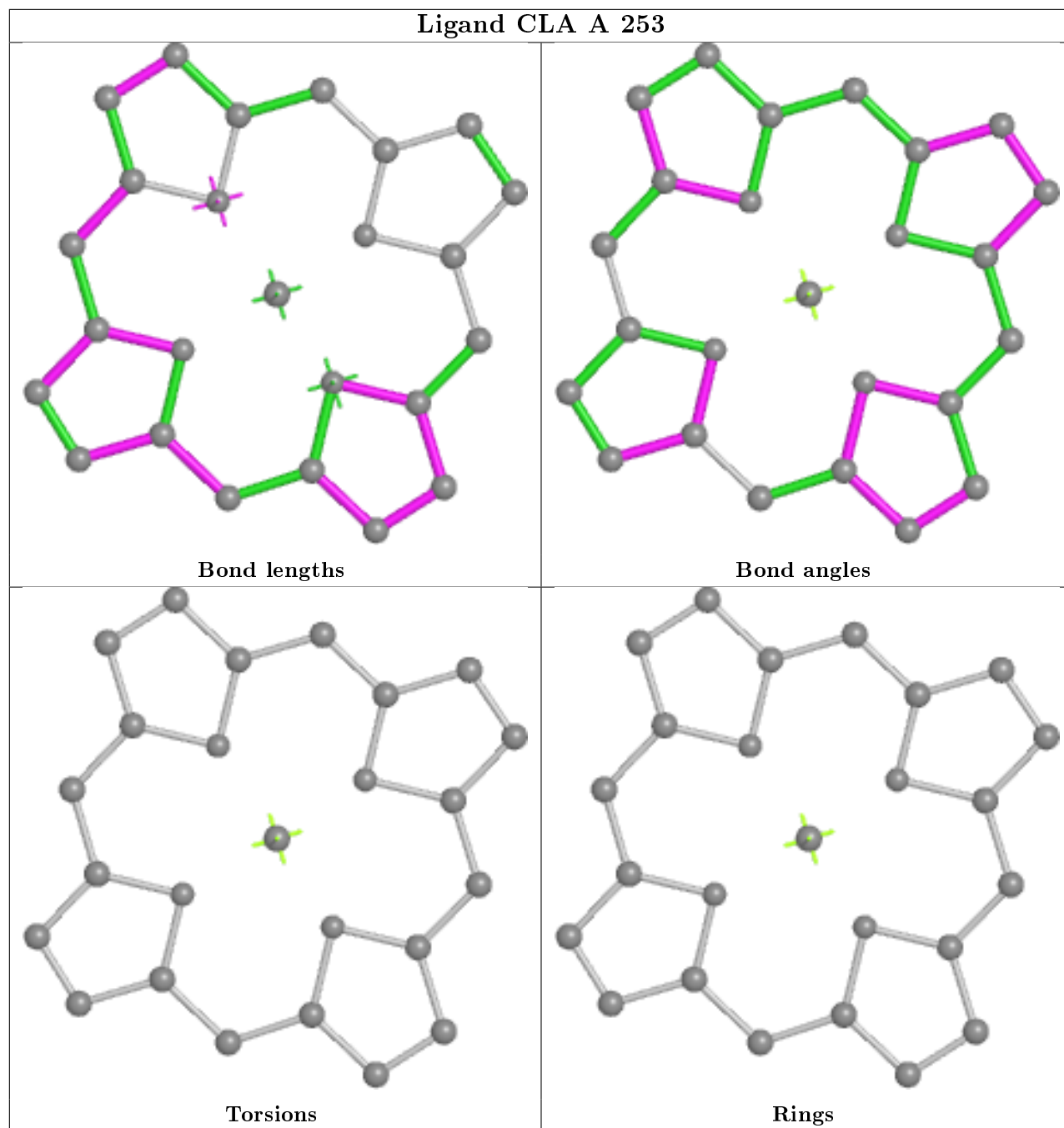
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



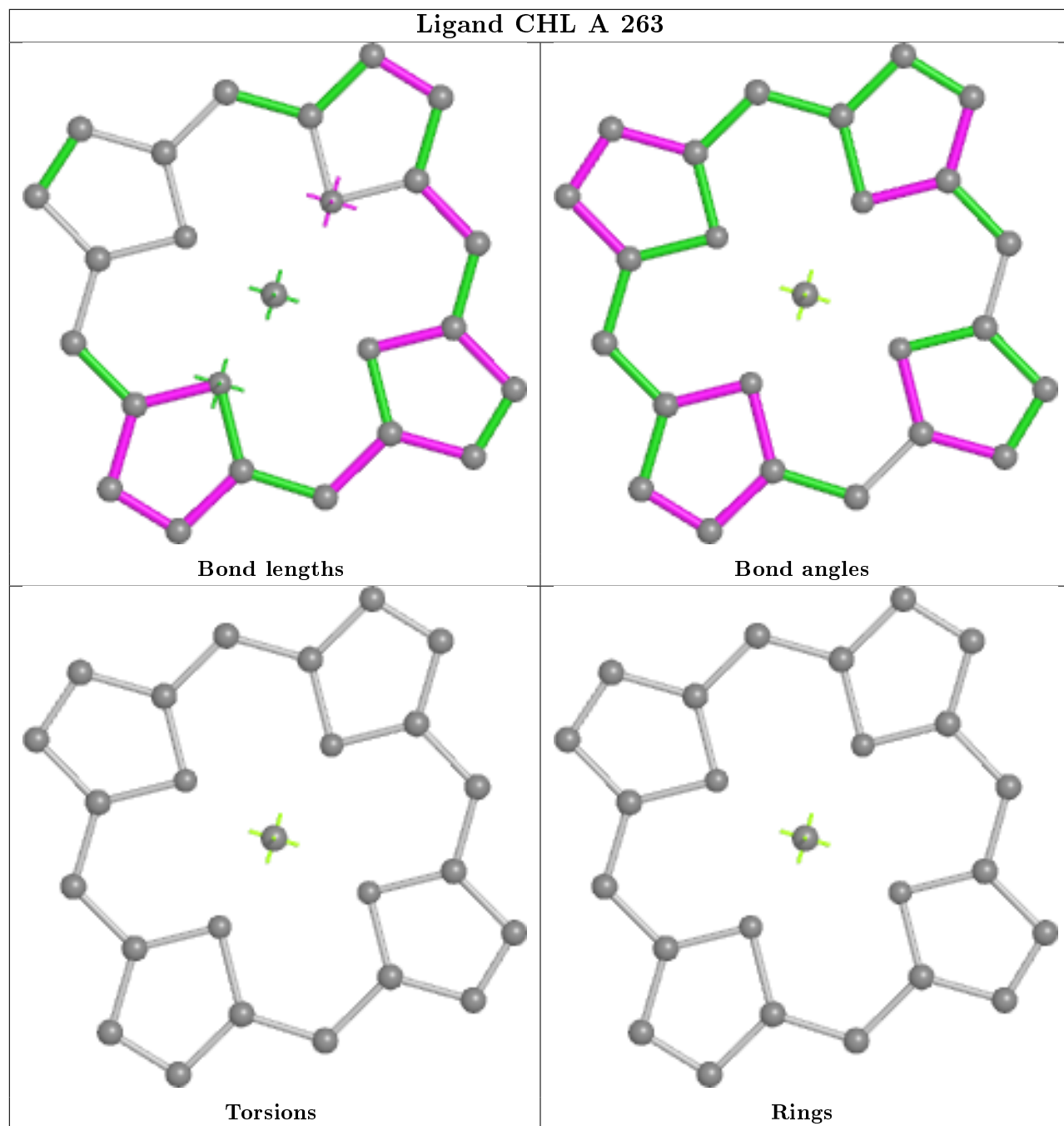
Ligand CLA A 256



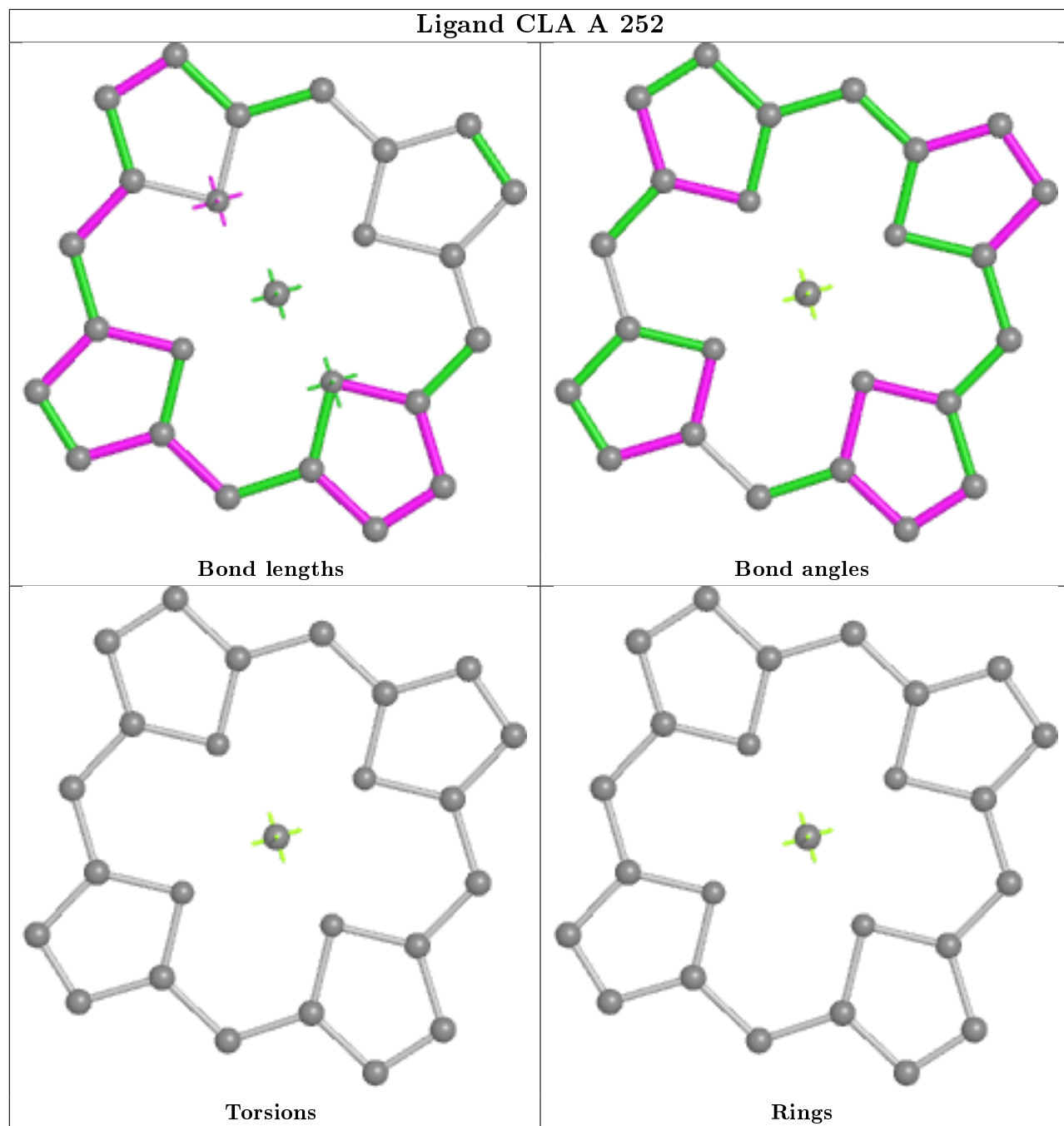
Ligand CLA A 253



Ligand CHL A 263



Ligand CLA A 252



Ligand CLA A 255

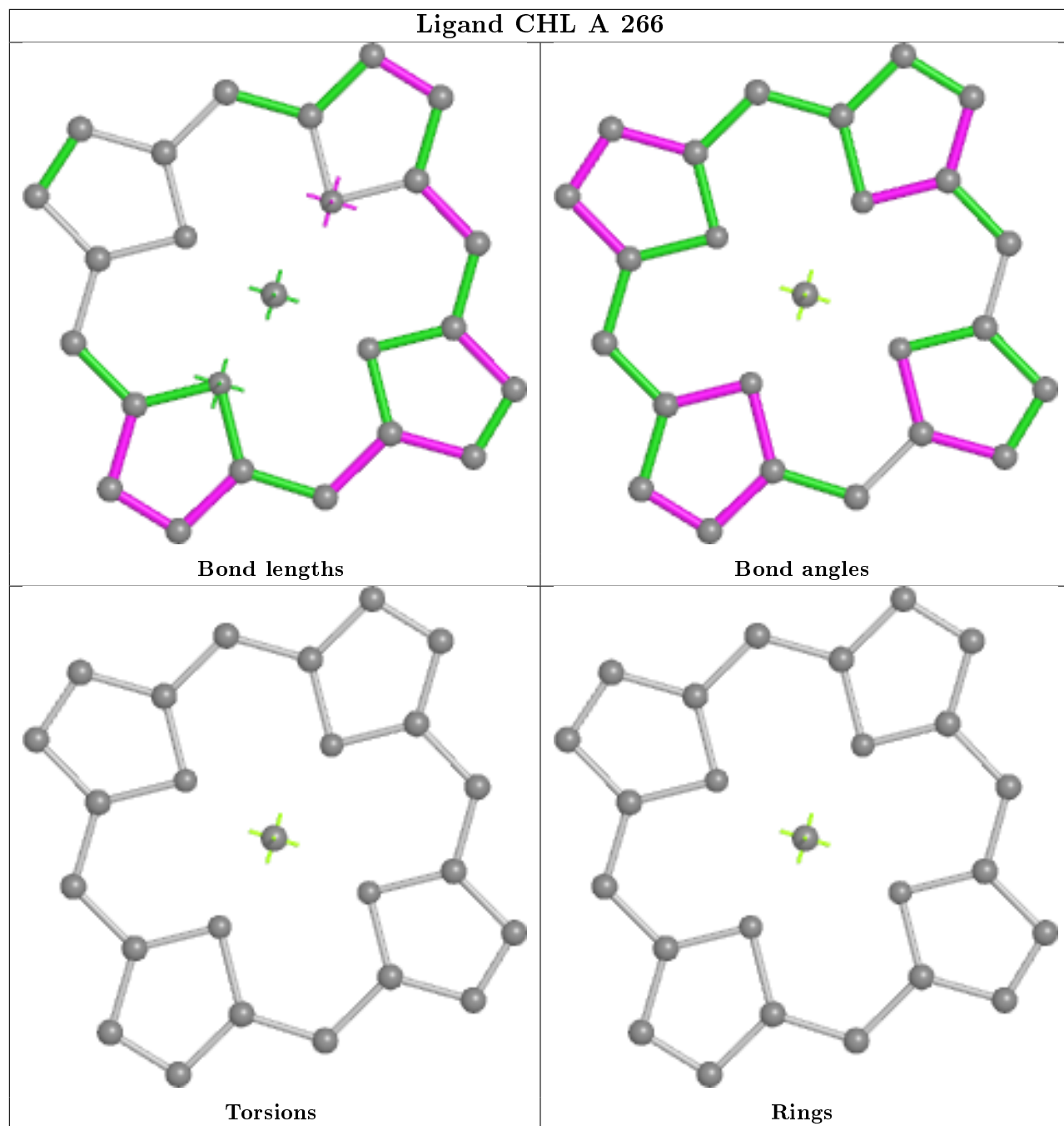
Bond lengths

Bond angles

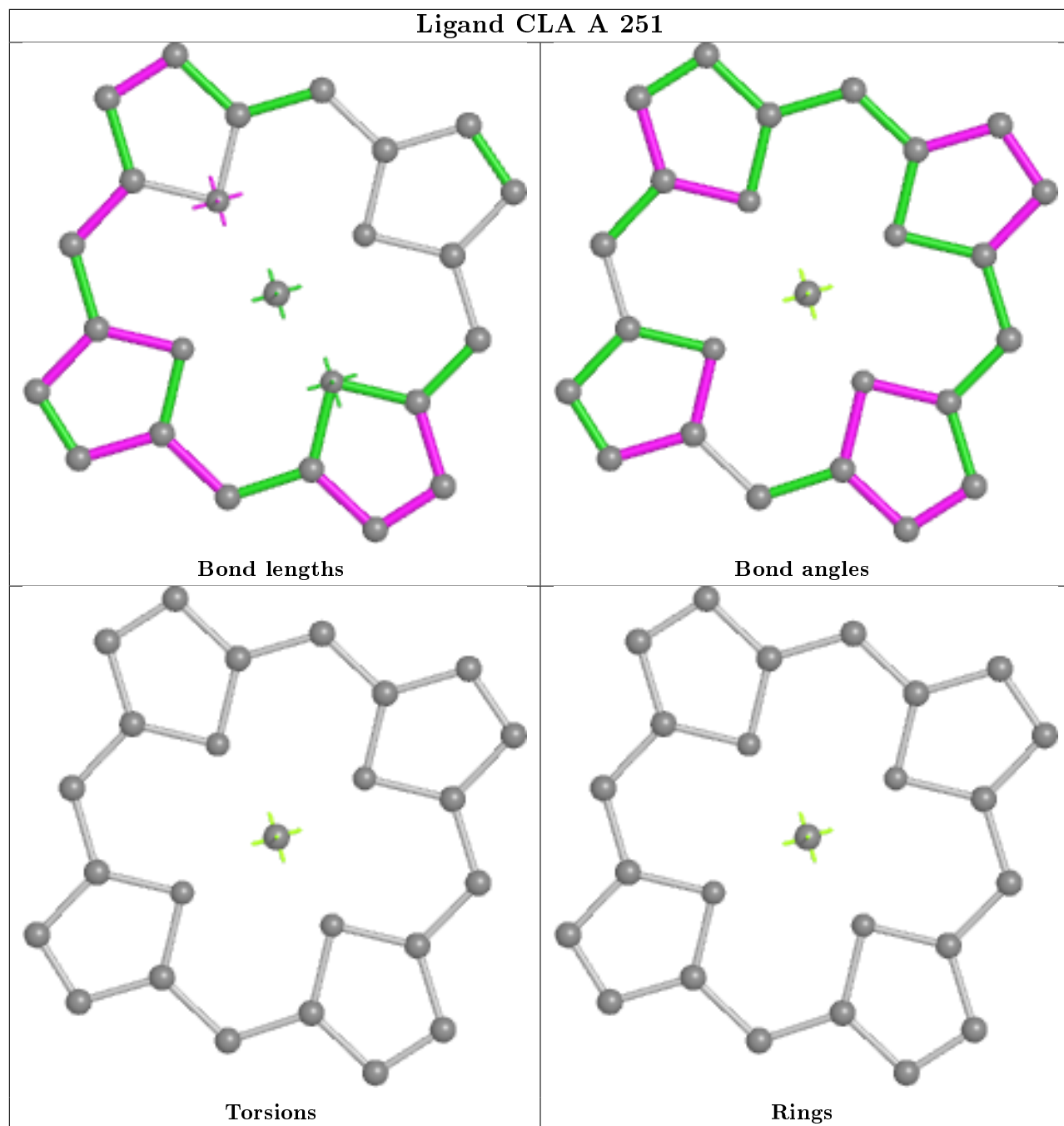
Torsions

Rings

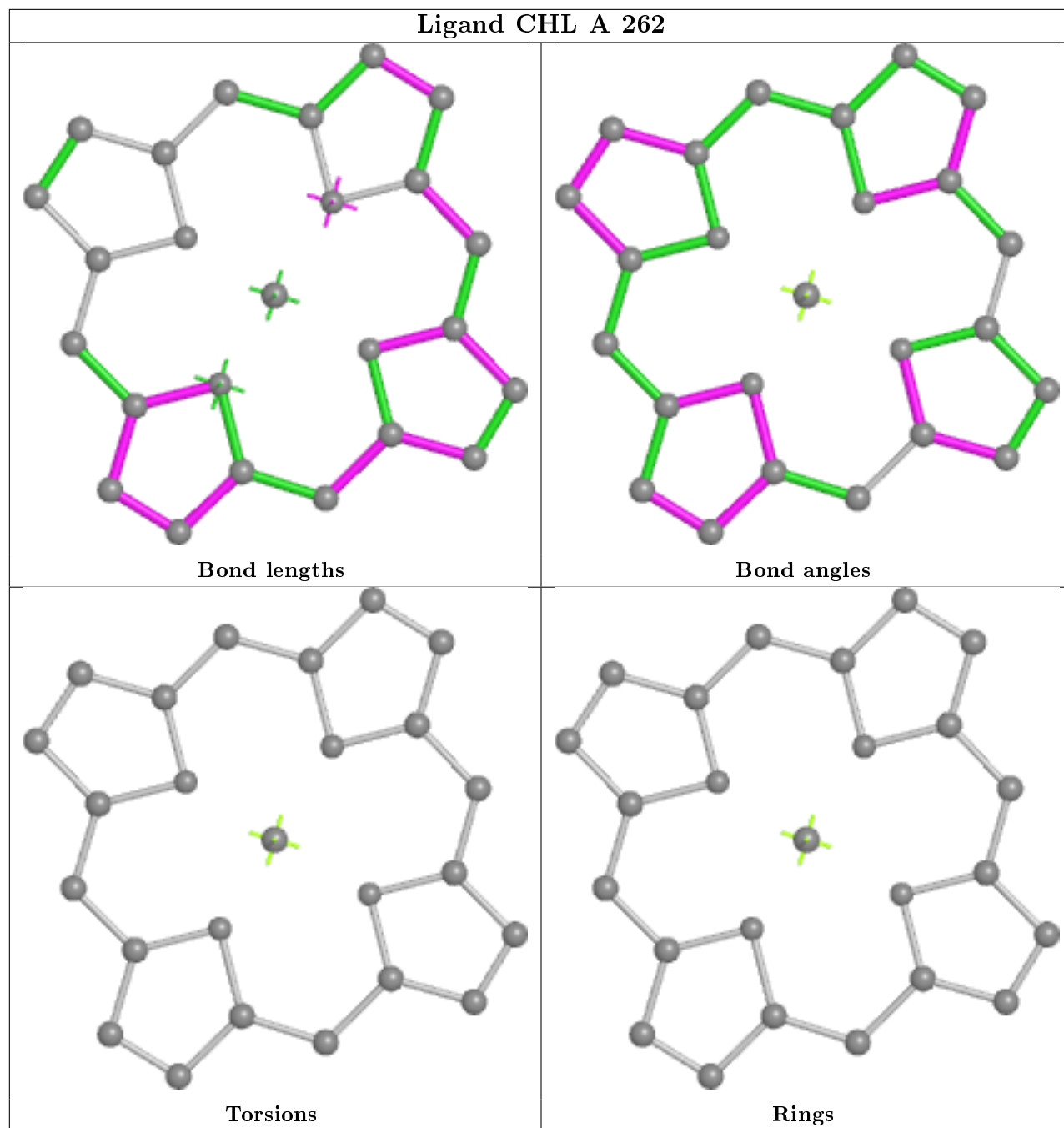
Ligand CHL A 266



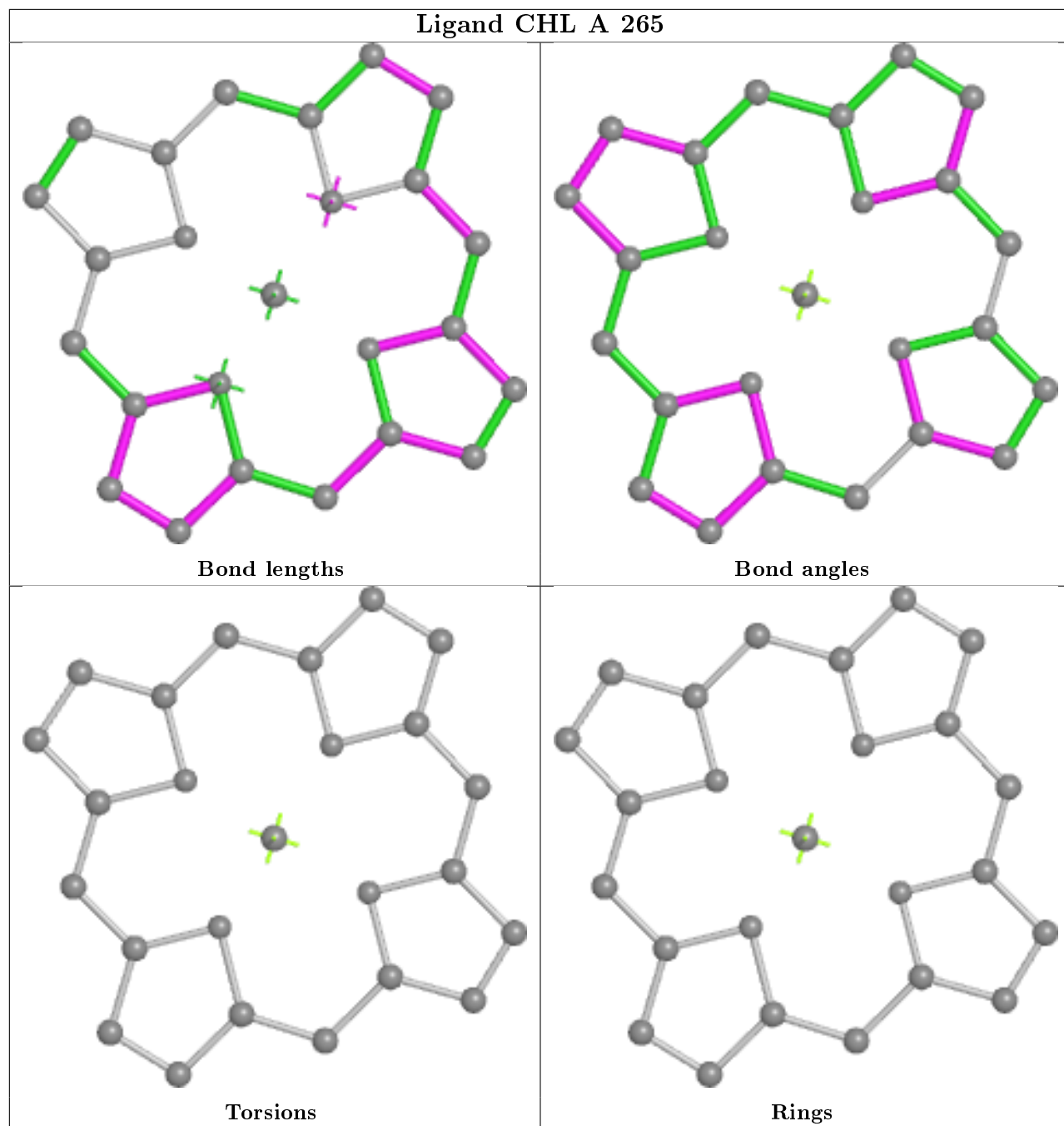
Ligand CLA A 251



Ligand CHL A 262



Ligand CHL A 265



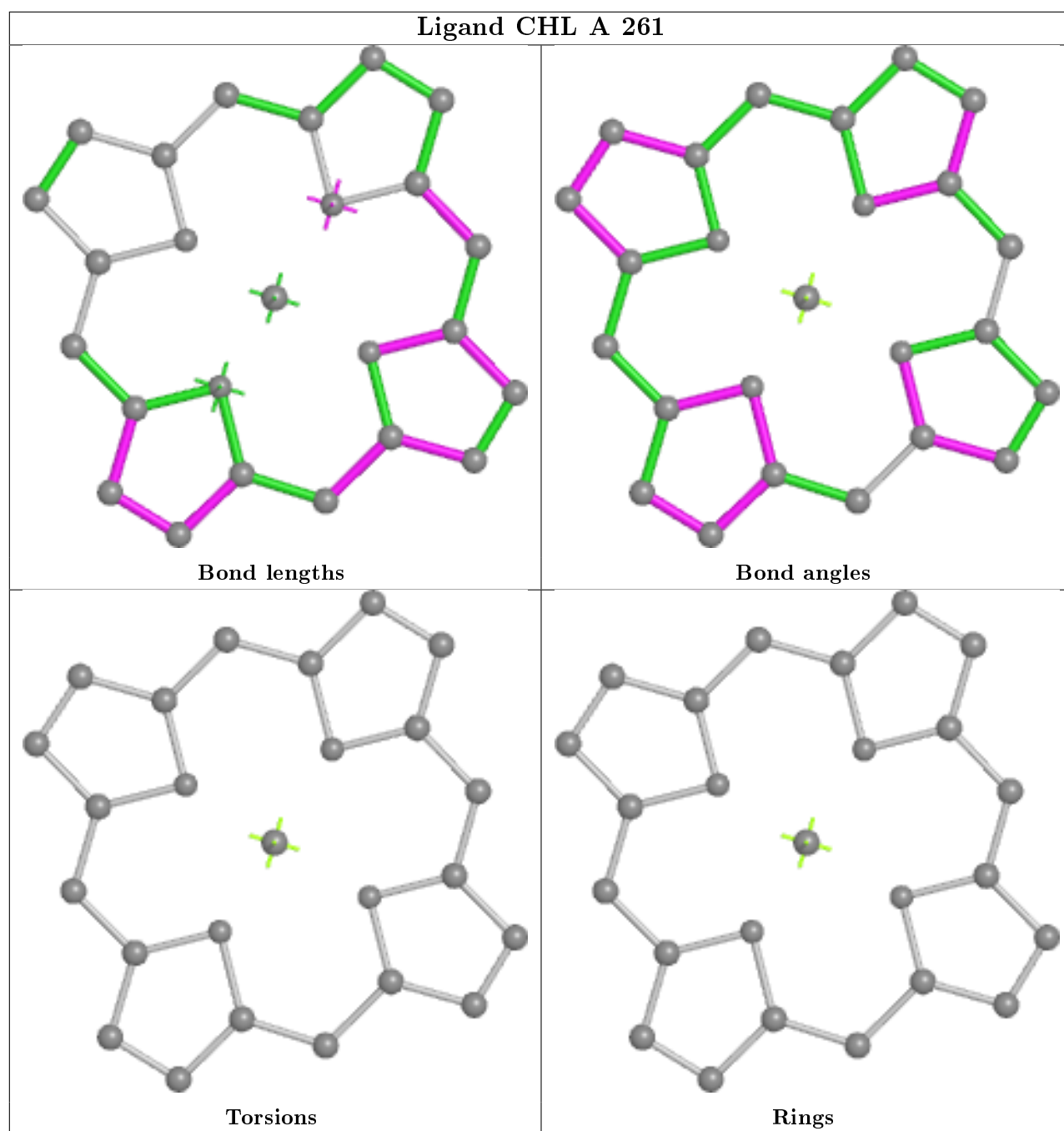
Ligand CLA A 254

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	101/232 (43%)	10.97	101 (100%) 0 0	295, 297, 297, 297	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	SER	25.2
1	A	87	ARG	22.9
1	A	175	GLU	22.9
1	A	171	GLU	21.5
1	A	135	MET	21.4
1	A	83	GLU	21.4
1	A	174	ALA	20.7
1	A	138	VAL	20.0
1	A	139	GLU	19.8
1	A	136	GLY	19.8
1	A	131	GLN	18.9
1	A	137	ALA	18.8
1	A	172	ALA	18.4
1	A	142	ARG	18.3
1	A	212	HIS	18.2
1	A	88	ASN	17.7
1	A	140	GLY	17.0
1	A	173	PHE	16.4
1	A	82	PRO	16.0
1	A	133	ILE	16.0
1	A	170	PRO	15.9
1	A	176	LEU	15.5
1	A	89	GLY	15.3
1	A	134	LEU	15.1
1	A	84	LEU	15.1
1	A	177	LYS	15.1
1	A	85	LEU	14.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	14.8
1	A	213	LEU	14.1
1	A	143	ILE	13.9
1	A	132	VAL	13.7
1	A	78	GLY	13.6
1	A	79	CYS	13.0
1	A	141	TYR	12.7
1	A	202	GLY	12.6
1	A	55	PRO	12.6
1	A	123	SER	12.1
1	A	57	THR	12.1
1	A	56	GLU	11.9
1	A	210	ALA	11.7
1	A	80	VAL	11.6
1	A	81	PHE	11.5
1	A	208	ASN	11.4
1	A	211	ASP	11.3
1	A	190	SER	11.1
1	A	124	ILE	11.0
1	A	127	ILE	10.2
1	A	179	LYS	10.1
1	A	130	THR	10.0
1	A	201	THR	9.6
1	A	207	GLU	9.4
1	A	77	LEU	9.3
1	A	129	ALA	9.2
1	A	128	TRP	8.9
1	A	75	GLY	8.8
1	A	205	PRO	8.8
1	A	59	SER	8.7
1	A	206	LEU	8.7
1	A	204	GLY	8.6
1	A	178	VAL	8.5
1	A	180	GLU	8.5
1	A	209	LEU	8.4
1	A	125	LEU	8.4
1	A	200	VAL	8.2
1	A	58	PHE	8.1
1	A	76	ALA	7.9
1	A	203	LYS	7.8
1	A	183	ASN	7.7
1	A	126	ALA	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	7.3
1	A	70	ARG	7.1
1	A	187	ALA	7.0
1	A	189	PHE	6.9
1	A	60	LYS	6.8
1	A	186	LEU	6.8
1	A	74	LEU	6.8
1	A	191	MET	6.7
1	A	197	GLN	6.6
1	A	198	ALA	6.2
1	A	61	ASN	6.2
1	A	182	LYS	6.0
1	A	71	TRP	5.7
1	A	194	PHE	5.7
1	A	73	MET	5.3
1	A	66	VAL	5.3
1	A	188	MET	5.0
1	A	185	ARG	4.9
1	A	69	SER	4.9
1	A	67	ILE	4.8
1	A	64	LEU	4.6
1	A	195	PHE	4.5
1	A	181	LEU	4.3
1	A	199	ILE	4.3
1	A	62	ARG	4.3
1	A	72	ALA	4.2
1	A	65	GLU	4.1
1	A	184	GLY	4.1
1	A	63	GLU	3.8
1	A	68	HIS	3.8
1	A	196	VAL	3.6
1	A	192	PHE	3.5

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

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

6.3 Carbohydrates ⓘ

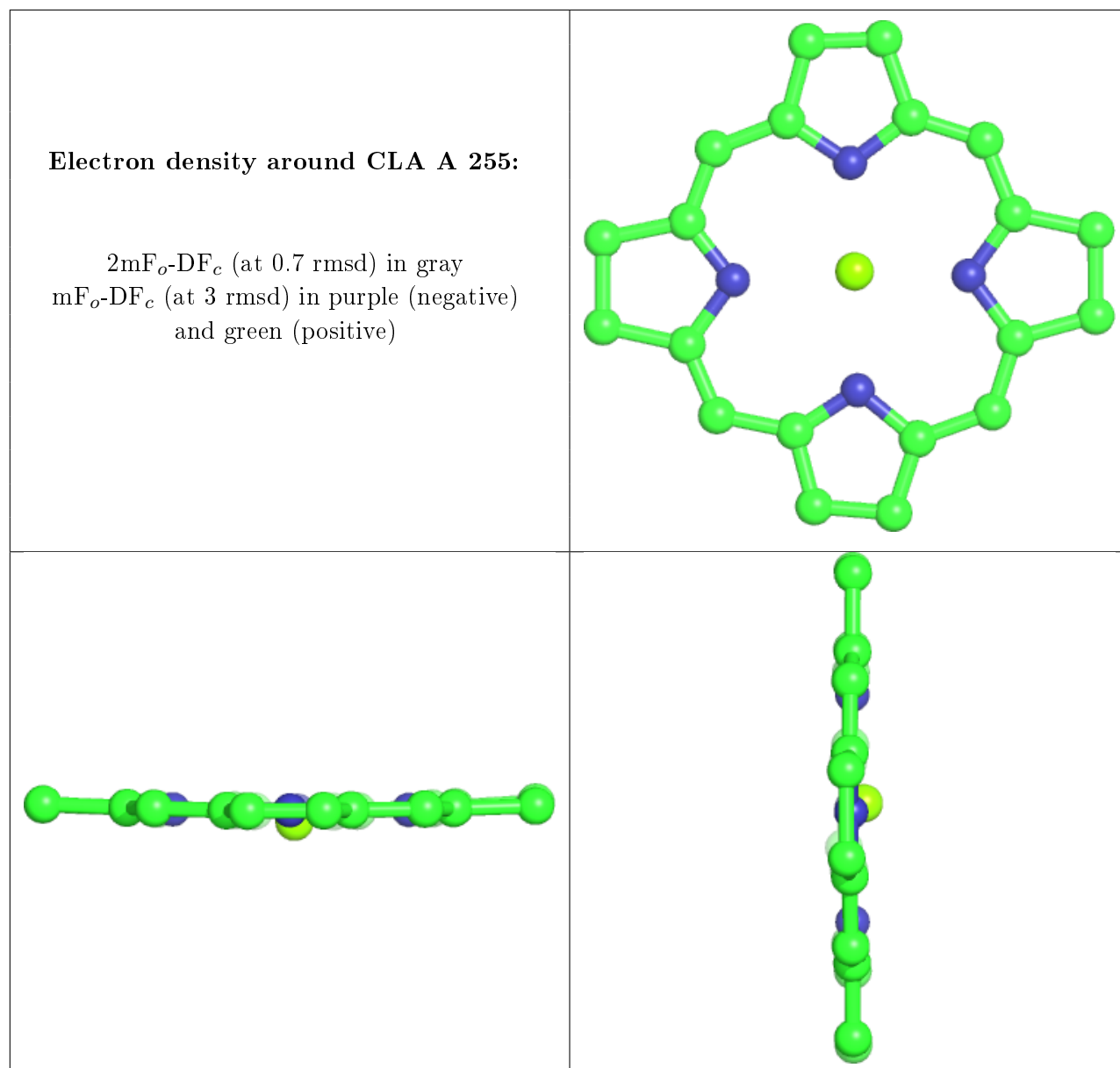
There are no carbohydrates in this entry.

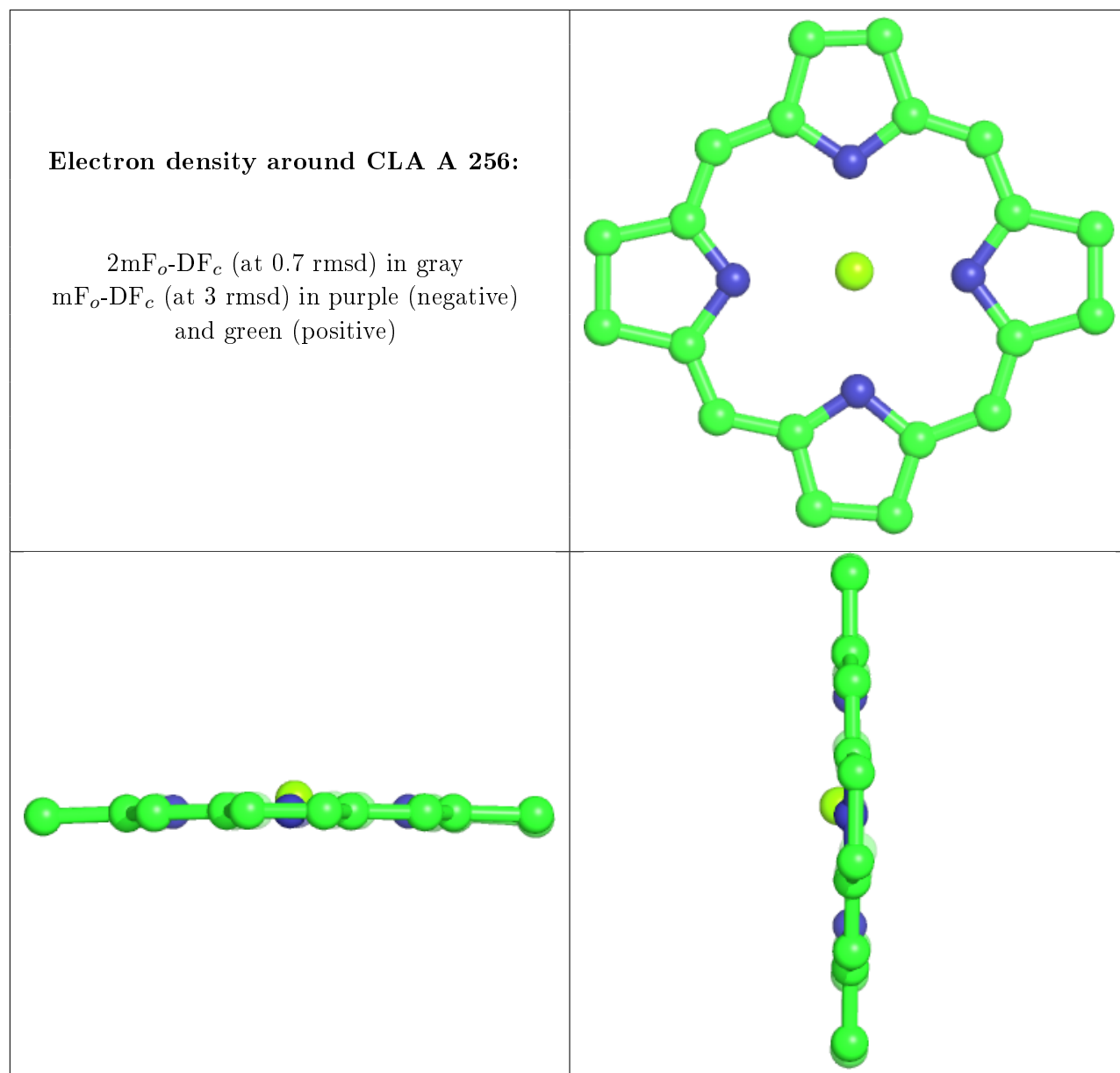
6.4 Ligands ⓘ

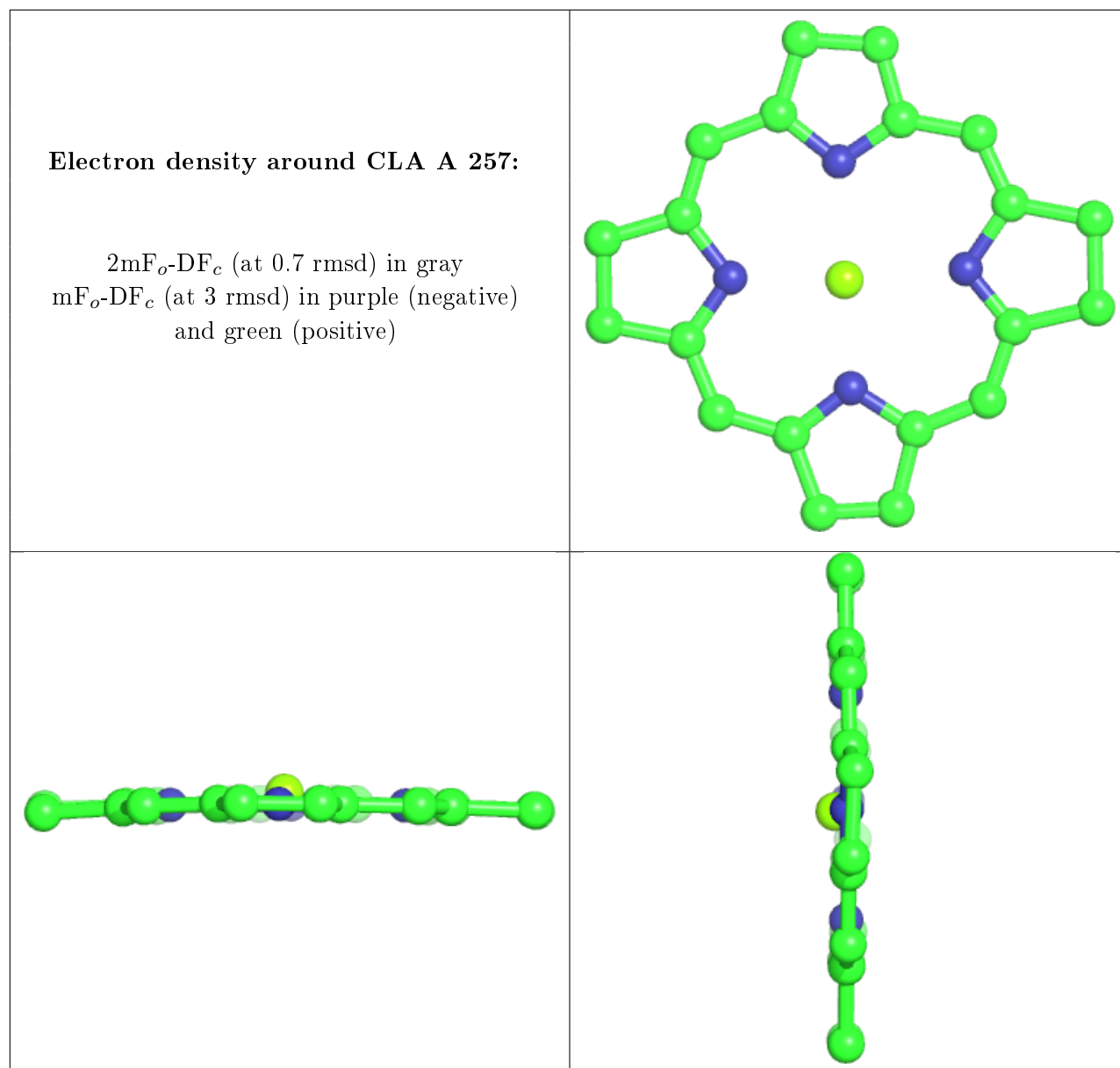
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

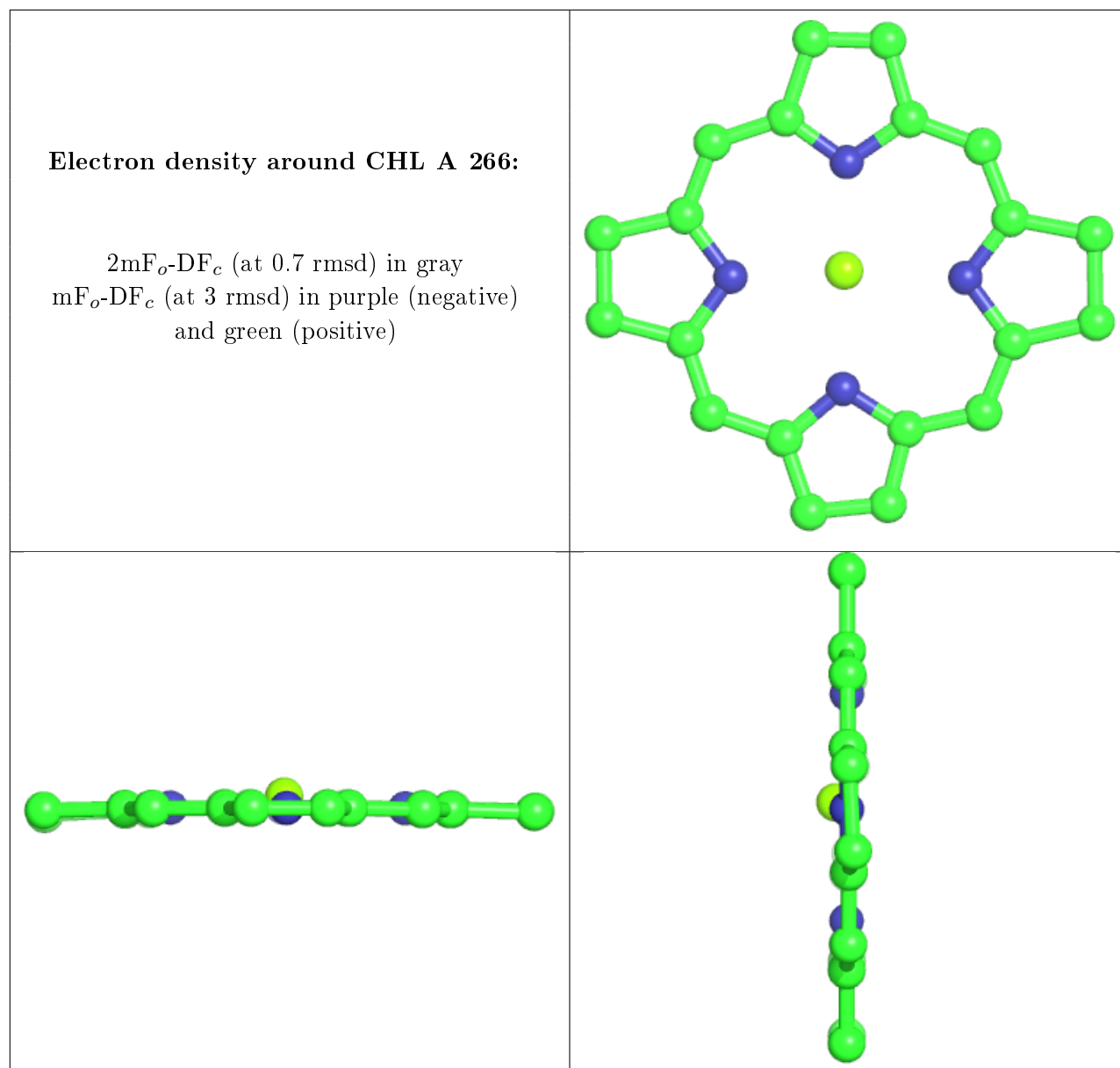
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CLA	A	255	25/65	-0.69	2.07	296,296,296,296	0
2	CLA	A	256	25/65	-0.68	3.14	294,296,296,296	0
2	CLA	A	257	25/65	-0.64	2.57	296,296,296,296	0
3	CHL	A	266	25/66	-0.64	3.56	295,296,296,296	0
3	CHL	A	263	25/66	-0.59	2.96	294,296,296,296	0
2	CLA	A	252	25/65	-0.55	2.68	295,296,296,296	0
3	CHL	A	261	25/66	-0.53	3.75	295,296,296,296	0
2	CLA	A	253	25/65	-0.45	2.67	295,296,296,296	0
2	CLA	A	251	25/65	-0.32	2.67	293,296,296,296	0
3	CHL	A	265	25/66	-0.31	2.98	296,296,296,296	0
3	CHL	A	262	25/66	-0.23	2.43	295,296,296,296	0
2	CLA	A	254	25/65	-0.07	1.30	294,296,296,296	0

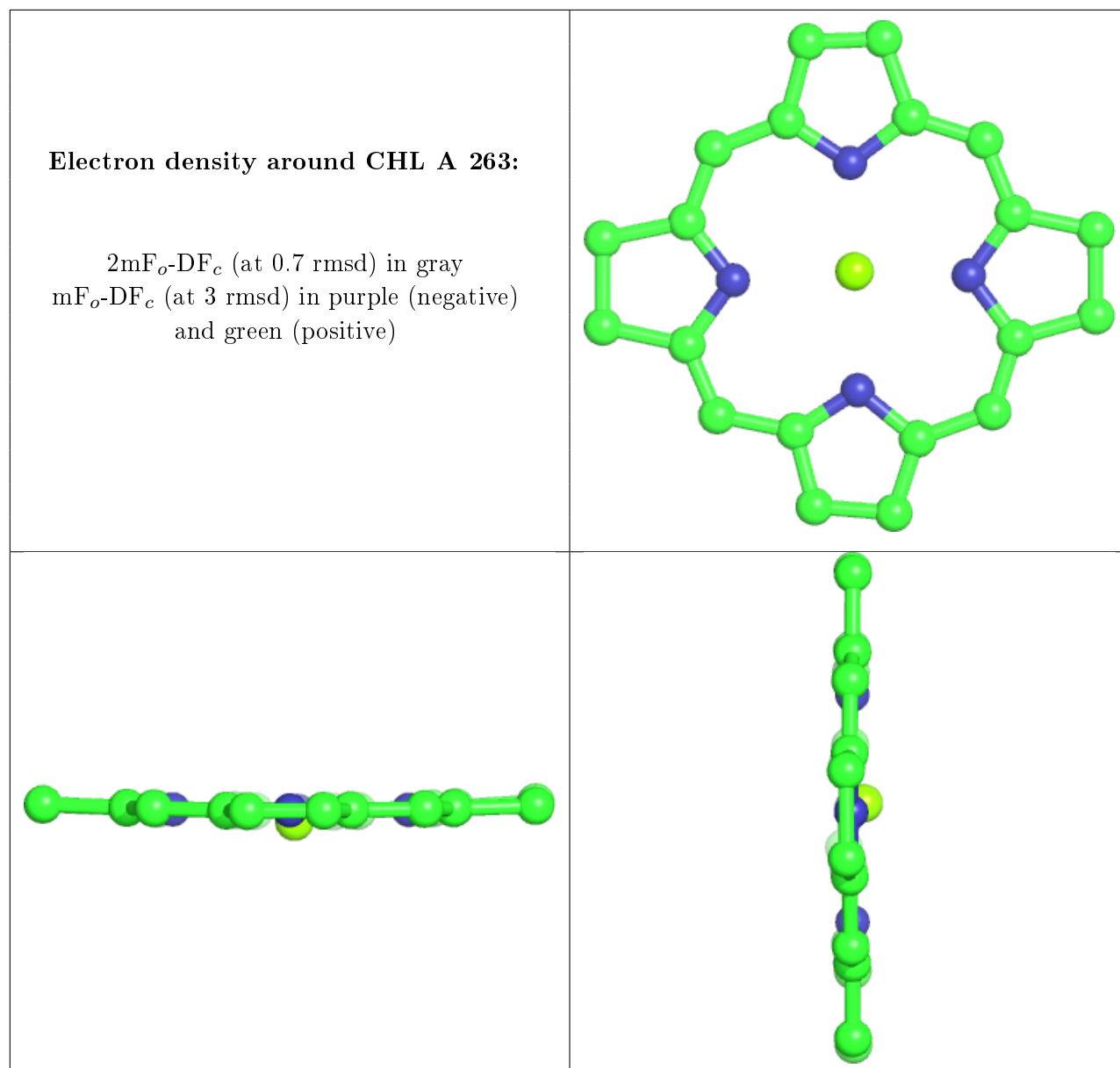
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

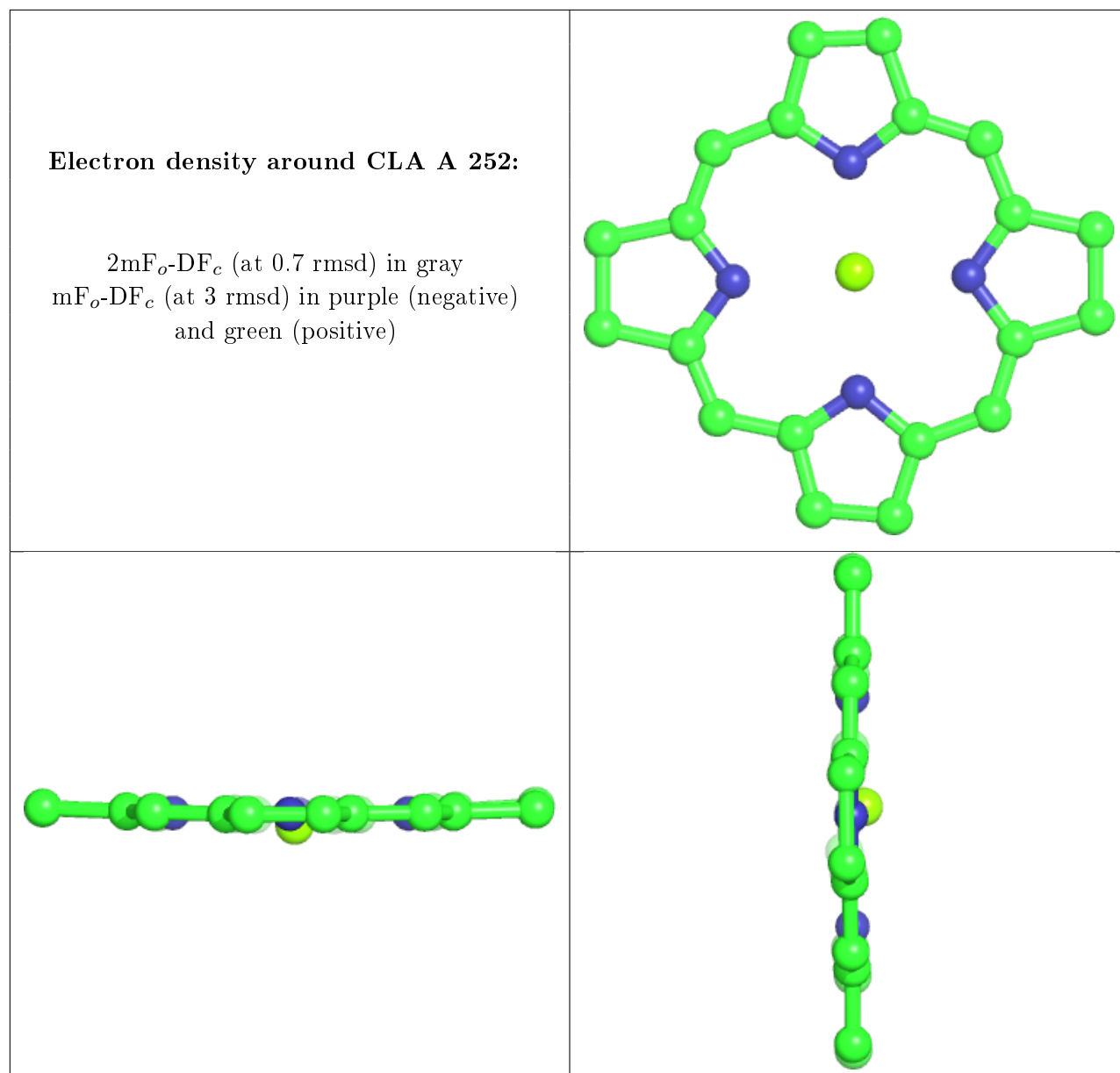


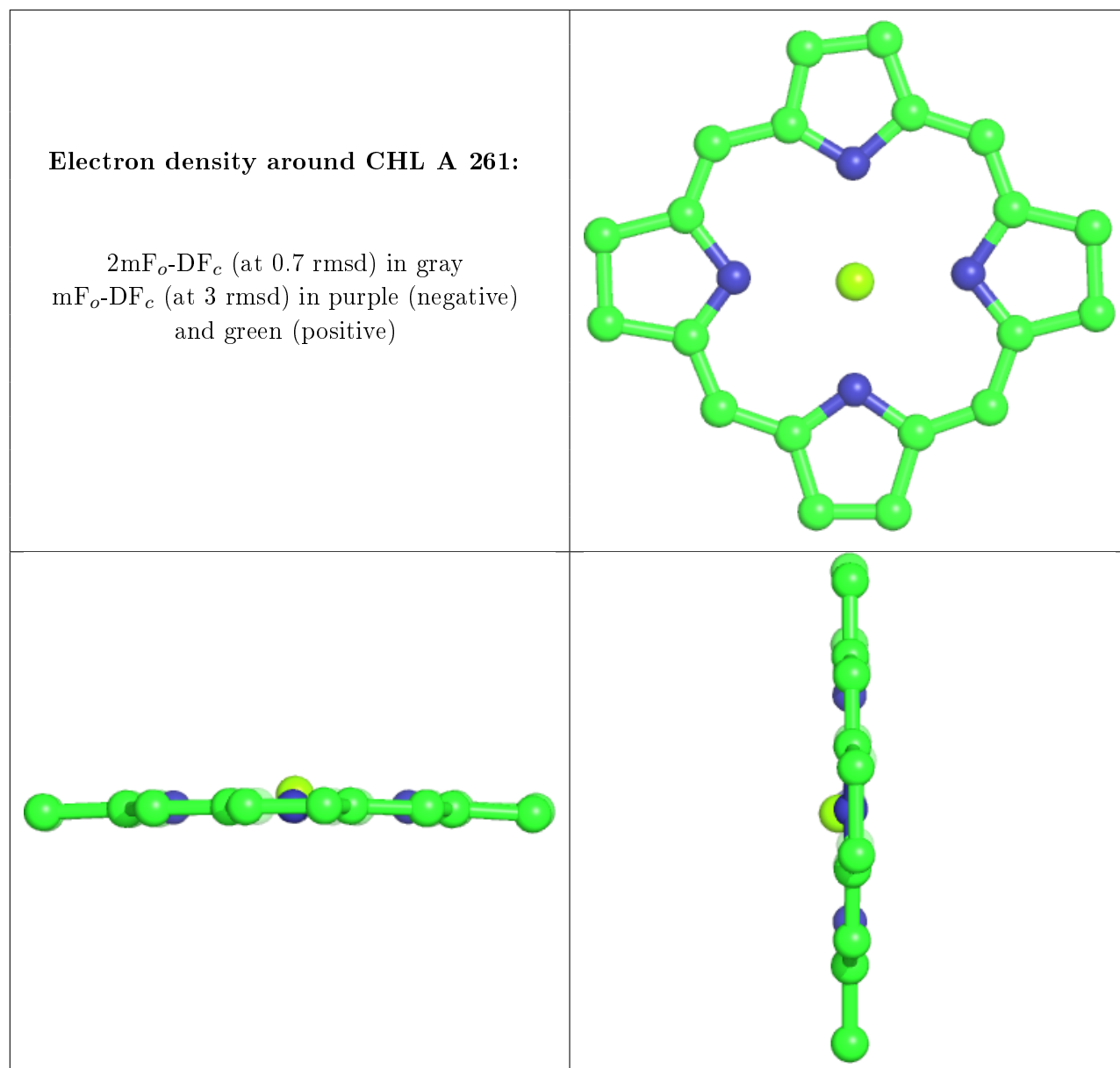


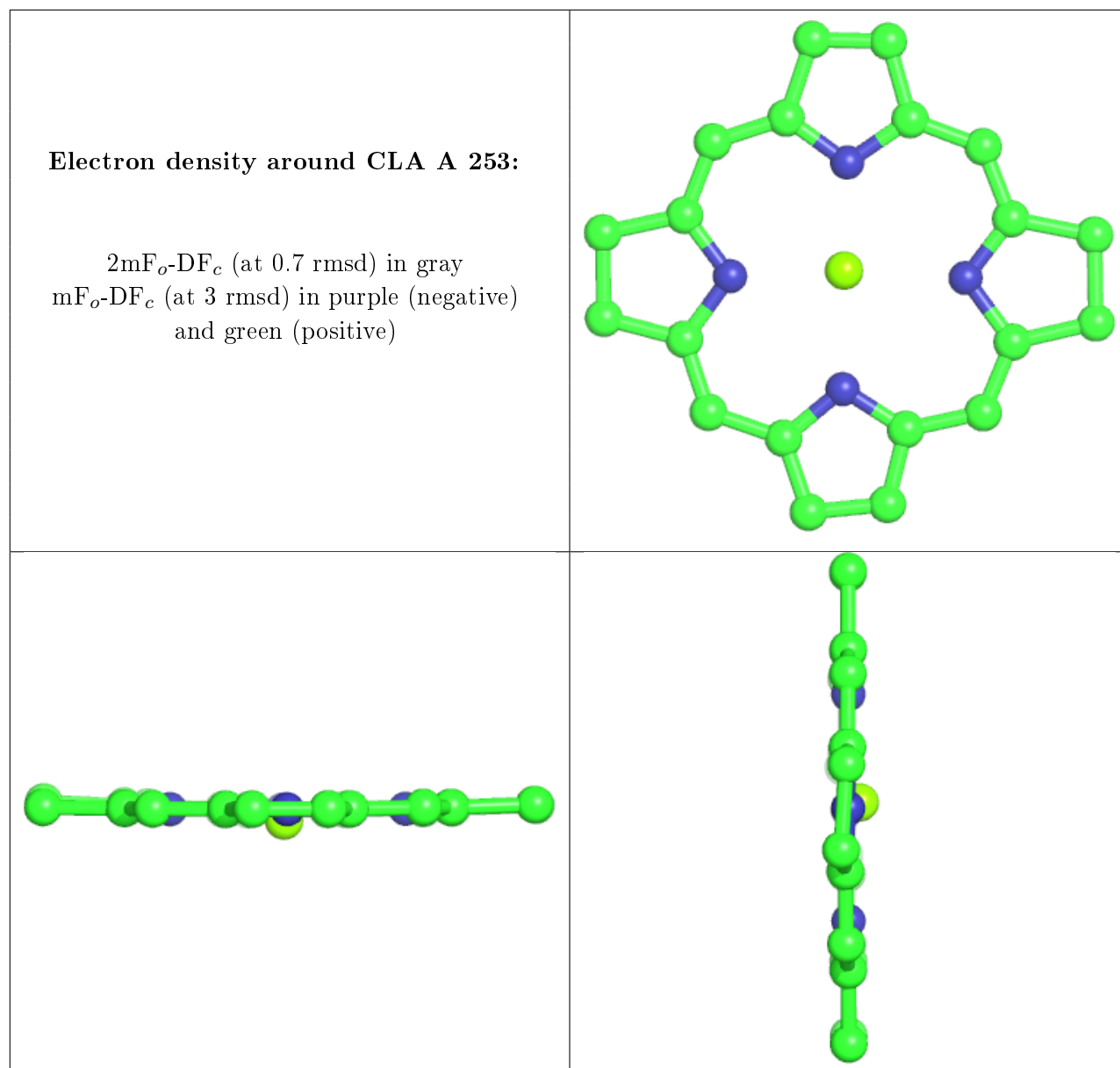


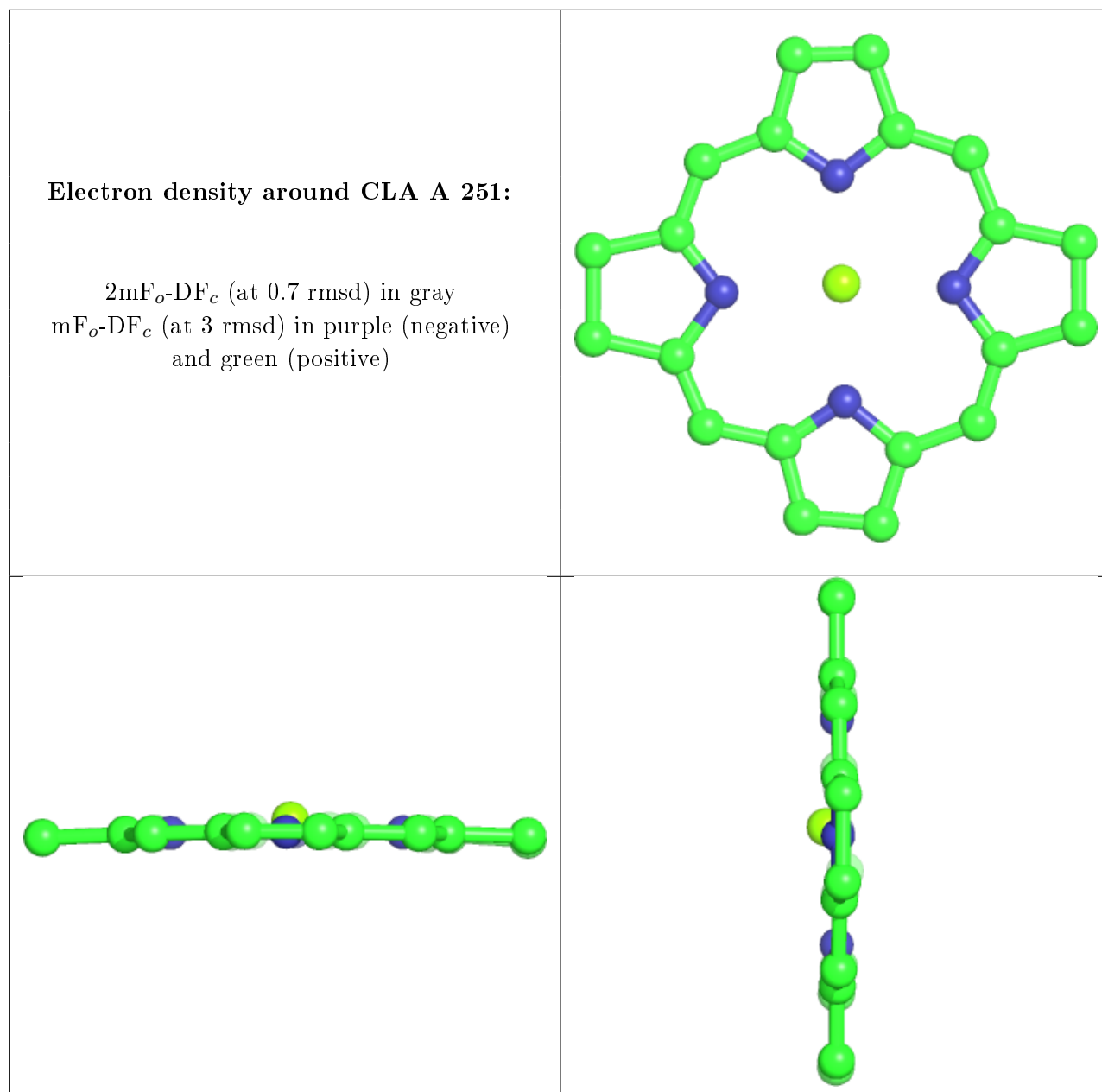


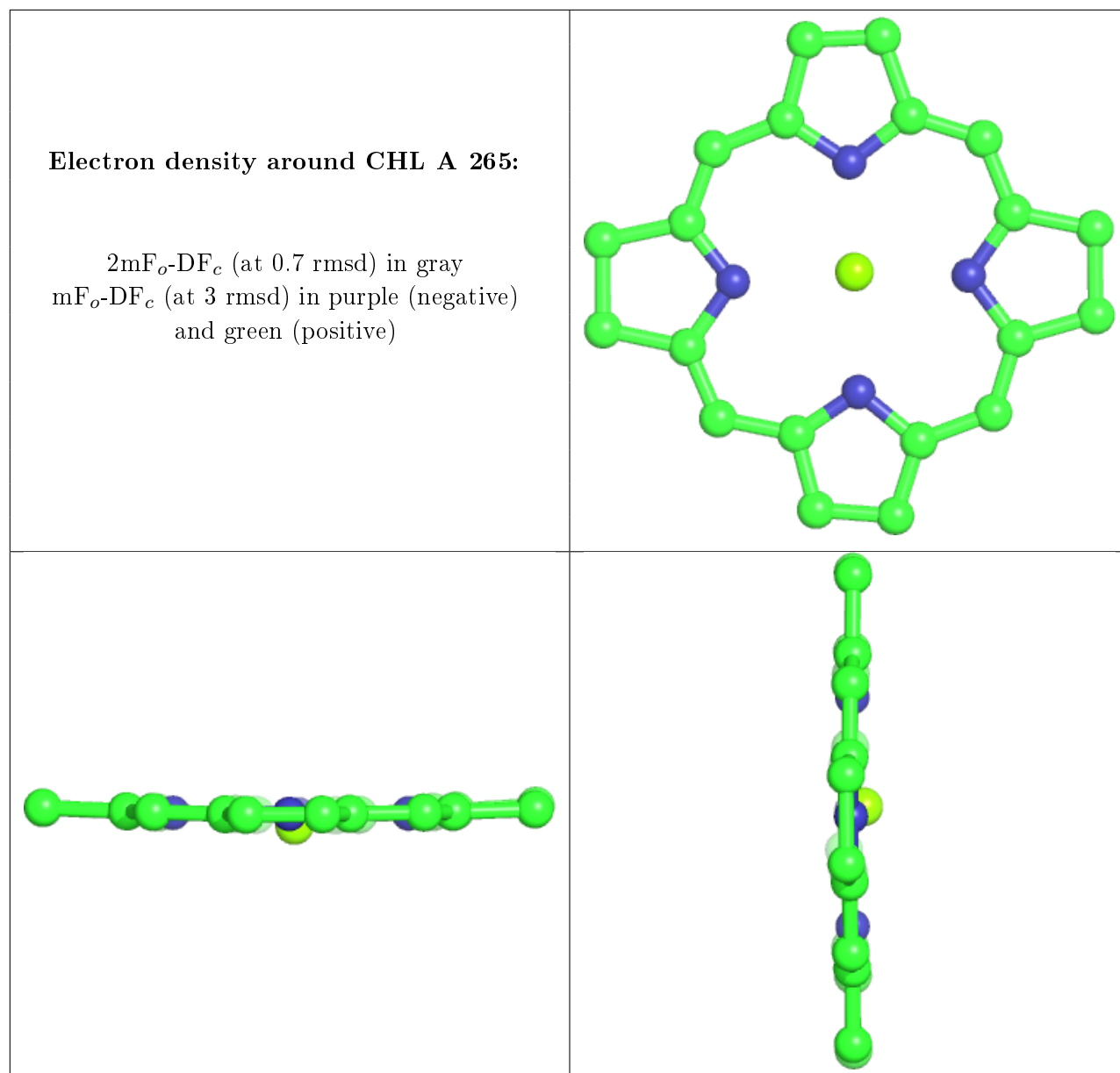


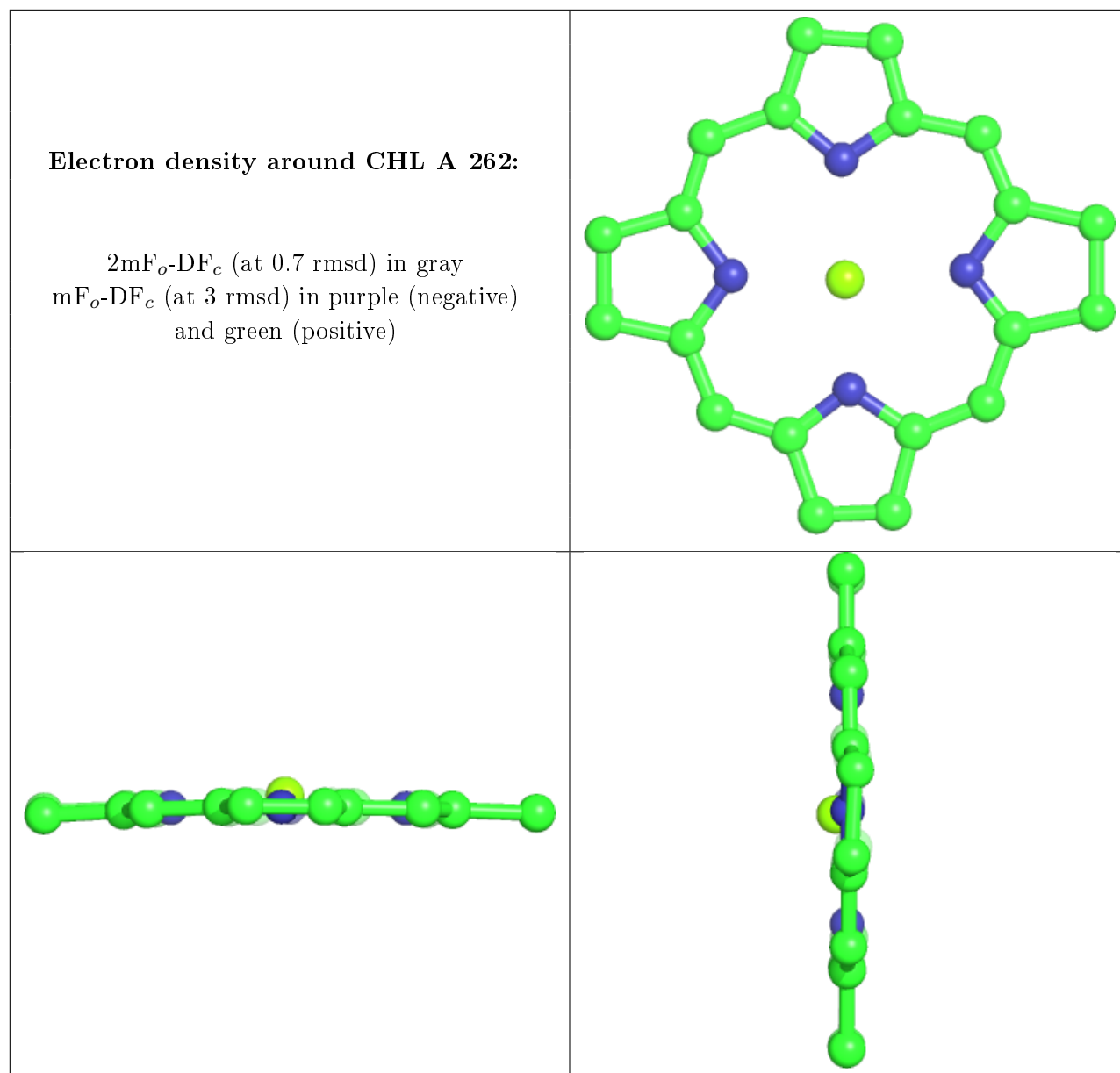


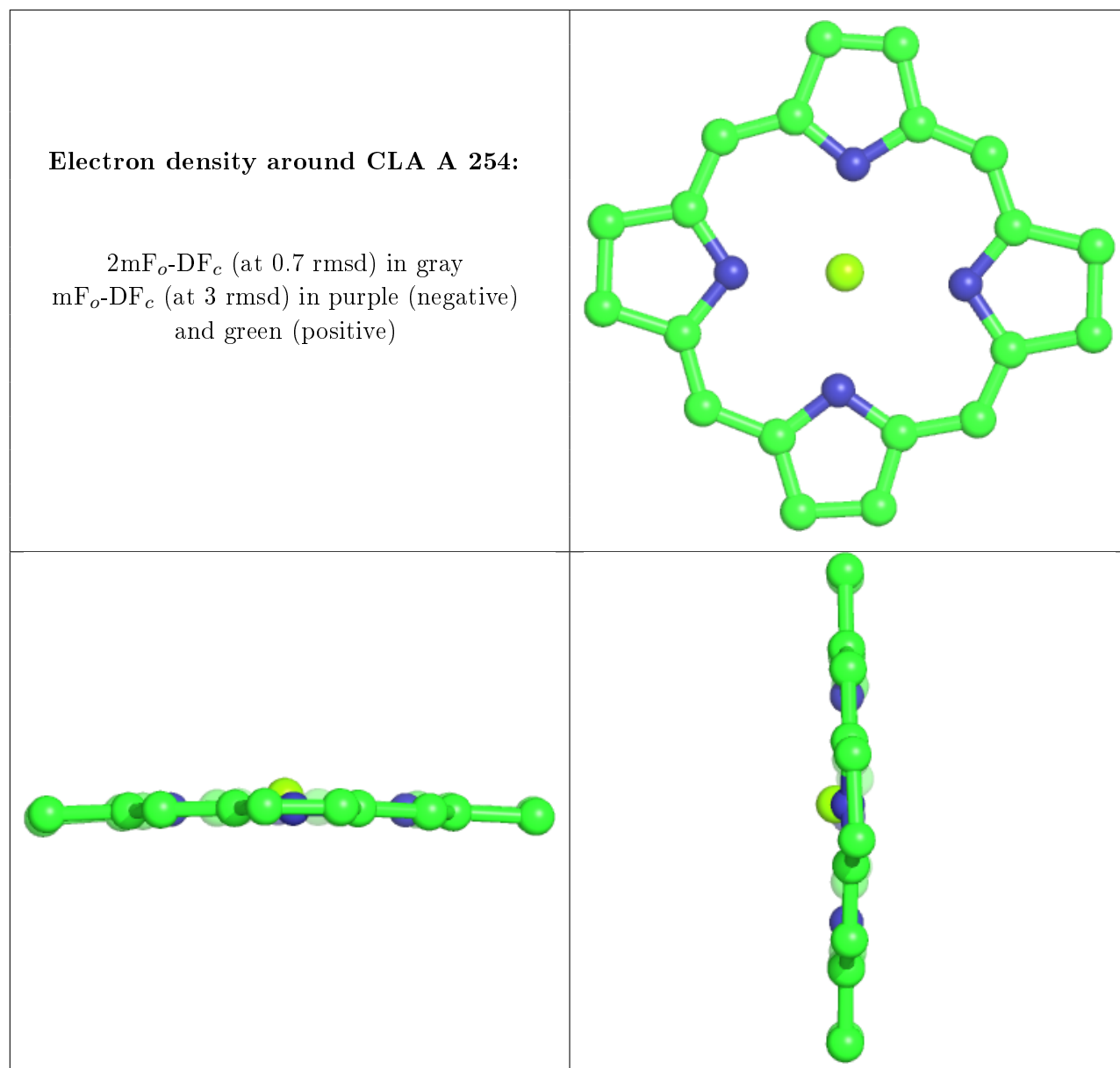












6.5 Other polymers [i](#)

There are no such residues in this entry.