



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2024 – 08:48 PM EST

PDB ID : 4QN9
Title : Structure of human NAPE-PLD
Authors : Garau, G.
Deposited on : 2014-06-17
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

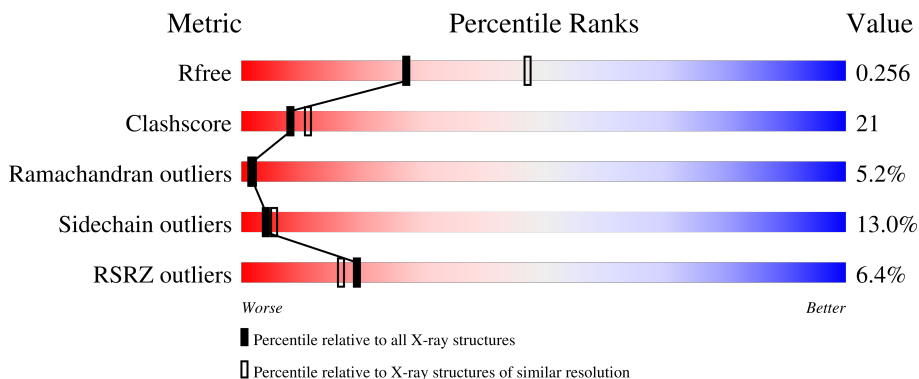
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 $\leq 5\%$. 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	393	 7% 53% 19% 7% 18%
1	B	393	 4% 52% 21% 7% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DXC	B	610	-	-	-	X
5	SO4	B	611	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5875 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.

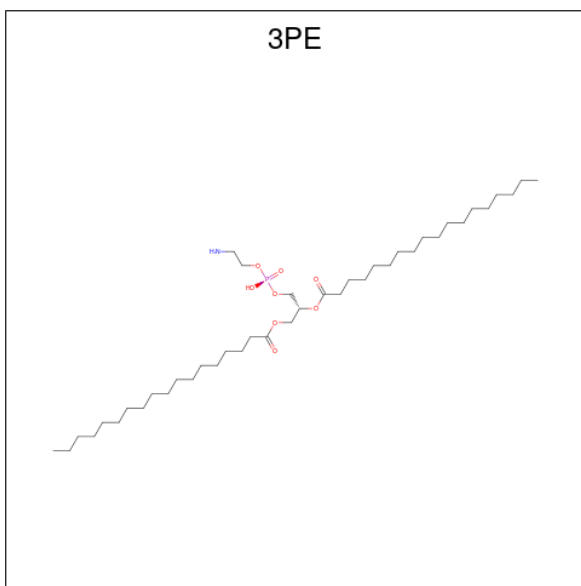
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	Total 2679	C 1732	N 452	O 482	S 13	0	8	0
1	B	322	Total 2682	C 1732	N 452	O 485	S 13	0	7	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

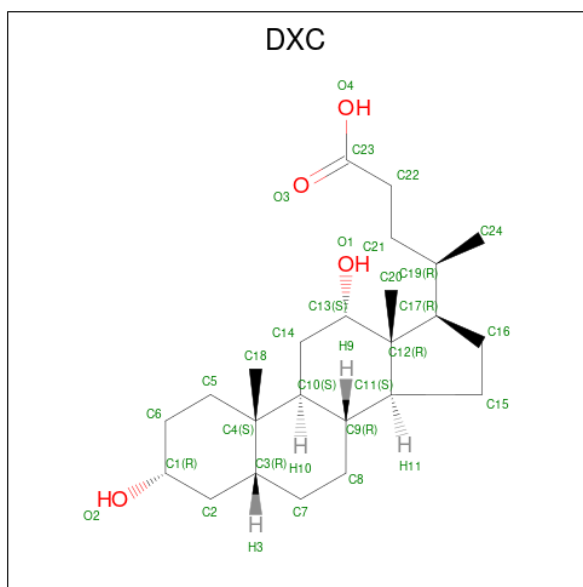
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: C₂₄H₄₀O₄).



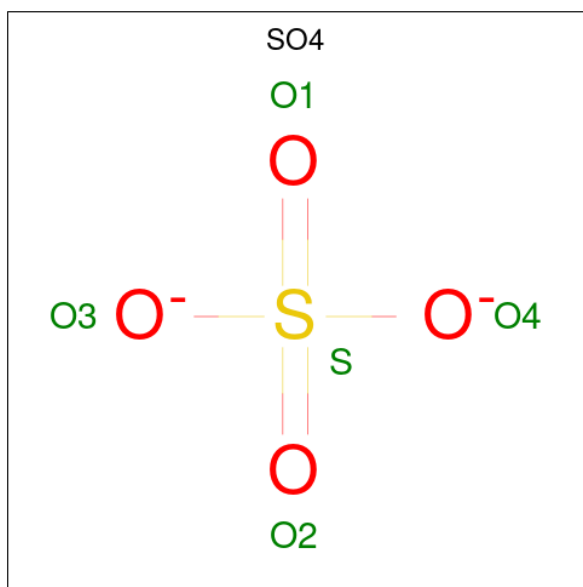
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	62	Total	O	0	1
			63	63		

3354		
N357		
N358		
D359		
ASP		
GLU		
ASN		
PHE		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.10Å 95.10Å 444.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.36 – 2.65 82.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.36-2.65) 100.0 (82.36-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.65Å)	Xtrriage
Refinement program	CCP4, REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.253 0.217 , 0.256	Depositor DCC
R_{free} test set	1794 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: 3PE, SO4, DXC, ZN

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	0.66	1/2774 (0.0%)	1.12	25/3777 (0.7%)
1	B	0.83	2/2773 (0.1%)	1.13	25/3777 (0.7%)
All	All	0.75	3/5547 (0.1%)	1.13	50/7554 (0.7%)

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	A	0	9
1	B	0	8
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	TRP	CB-CG	8.52	1.65	1.50
1	A	72	TRP	CB-CG	6.10	1.61	1.50
1	B	69	TRP	CB-CG	-5.59	1.40	1.50

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-22.64	108.98	120.30
1	B	121	ARG	NE-CZ-NH1	-16.39	112.10	120.30
1	B	121	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	A	121	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	A	121	ARG	CD-NE-CZ	10.84	138.77	123.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	GLU	Peptide
1	A	117	GLU	Peptide
1	A	118	ALA	Peptide
1	A	121	ARG	Sidechain
1	A	175[A]	LEU	Peptide

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	2679	0	2572	94	0
1	B	2682	0	2567	108	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	1	0
3	B	44	0	62	1	0
4	A	112	0	156	18	0
4	B	196	0	273	34	0
5	A	10	0	0	1	0
5	B	5	0	0	2	0
6	A	36	0	0	0	0
6	B	63	0	0	3	0
All	All	5875	0	5692	244	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 21.

The worst 5 of 244 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:B:118:ALA:HB1	1:B:138:GLU:OE1	1.41	1.17
4:B:610:DXC:H242	4:B:610:DXC:H203	1.19	1.14
1:A:118:ALA:HB1	1:A:138:GLU:OE1	1.50	1.10
1:B:175[B]:LEU:HB2	1:B:176[B]:PRO:HD2	1.09	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TRP:HZ3	1:A:267:TRP:O	1.39	1.06

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	325/393 (83%)	284 (87%)	22 (7%)	19 (6%)	1	1
1	B	325/393 (83%)	281 (86%)	26 (8%)	18 (6%)	2	1
All	All	650/786 (83%)	565 (87%)	48 (7%)	37 (6%)	2	1

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	67	ASN
1	A	119	GLY
1	A	120	VAL
1	A	121	ARG

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	291/352 (83%)	250 (86%)	41 (14%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	291/352 (83%)	257 (88%)	34 (12%)	5	7
All	All	582/704 (83%)	507 (87%)	75 (13%)	4	5

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	243	LYS
1	B	377	VAL
1	B	262	ASP
1	B	344	TRP
1	A	242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	B	277	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
5	SO4	A	509	-	4,4,4	0.40	0	6,6,6	0.31	0
4	DXC	B	608	-	31,31,31	1.12	2 (6%)	49,49,49	1.59	10 (20%)
4	DXC	B	603	-	31,31,31	1.28	3 (9%)	49,49,49	3.81	23 (46%)
4	DXC	A	505	-	31,31,31	0.97	1 (3%)	49,49,49	1.32	6 (12%)
4	DXC	B	601	-	31,31,31	0.96	1 (3%)	49,49,49	1.36	7 (14%)
4	DXC	A	504	-	31,31,31	0.93	2 (6%)	49,49,49	1.34	7 (14%)
4	DXC	B	609	-	31,31,31	1.15	3 (9%)	49,49,49	2.11	13 (26%)
3	3PE	B	606	2	43,43,50	1.03	2 (4%)	46,48,55	1.41	5 (10%)
4	DXC	A	506	-	31,31,31	0.95	1 (3%)	49,49,49	1.32	6 (12%)
5	SO4	B	611	-	4,4,4	0.60	0	6,6,6	0.66	0
4	DXC	B	610	-	31,31,31	1.00	2 (6%)	49,49,49	2.37	16 (32%)
5	SO4	A	508	-	4,4,4	0.44	0	6,6,6	0.44	0
4	DXC	B	602	-	31,31,31	0.94	1 (3%)	49,49,49	1.19	6 (12%)
3	3PE	A	503	2	43,43,50	0.97	2 (4%)	46,48,55	1.37	4 (8%)
4	DXC	A	507	-	31,31,31	1.23	3 (9%)	49,49,49	3.49	20 (40%)
4	DXC	B	607	-	31,31,31	1.08	4 (12%)	49,49,49	1.51	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DXC	B	608	-	-	3/9/71/71	0/4/4/4
4	DXC	B	603	-	-	3/9/71/71	0/4/4/4
4	DXC	A	505	-	-	2/9/71/71	0/4/4/4
4	DXC	B	601	-	-	0/9/71/71	0/4/4/4
4	DXC	A	504	-	-	2/9/71/71	0/4/4/4
4	DXC	B	609	-	-	1/9/71/71	0/4/4/4
3	3PE	B	606	2	-	18/47/47/54	-
4	DXC	A	506	-	-	3/9/71/71	0/4/4/4
4	DXC	B	610	-	-	9/9/71/71	1/4/4/4
4	DXC	B	602	-	-	3/9/71/71	0/4/4/4
3	3PE	A	503	2	-	18/47/47/54	-
4	DXC	A	507	-	-	4/9/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DXC	B	607	-	-	0/9/71/71	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	606	3PE	O21-C21	4.82	1.47	1.34
4	B	603	DXC	C12-C11	-4.80	1.47	1.55
3	A	503	3PE	O21-C21	4.27	1.46	1.34
4	A	507	DXC	C12-C11	-3.10	1.50	1.55
4	A	507	DXC	C12-C17	-3.02	1.50	1.55

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	DXC	C12-C11-C9	-14.48	98.73	114.71
4	A	507	DXC	C12-C11-C9	-13.45	99.87	114.71
4	B	603	DXC	C11-C9-C10	-11.35	93.89	109.09
4	A	507	DXC	C11-C9-C10	-10.81	94.61	109.09
4	B	603	DXC	C11-C12-C13	7.72	114.59	107.40

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	3PE	C1-O11-P-O12
3	B	606	3PE	C1-O11-P-O12
4	B	610	DXC	C12-C17-C19-C24
4	B	610	DXC	C16-C17-C19-C21
3	A	503	3PE	O32-C31-O31-C3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	610	DXC	C1-C2-C3-C4-C5-C6

14 monomers are involved in 54 short contacts:

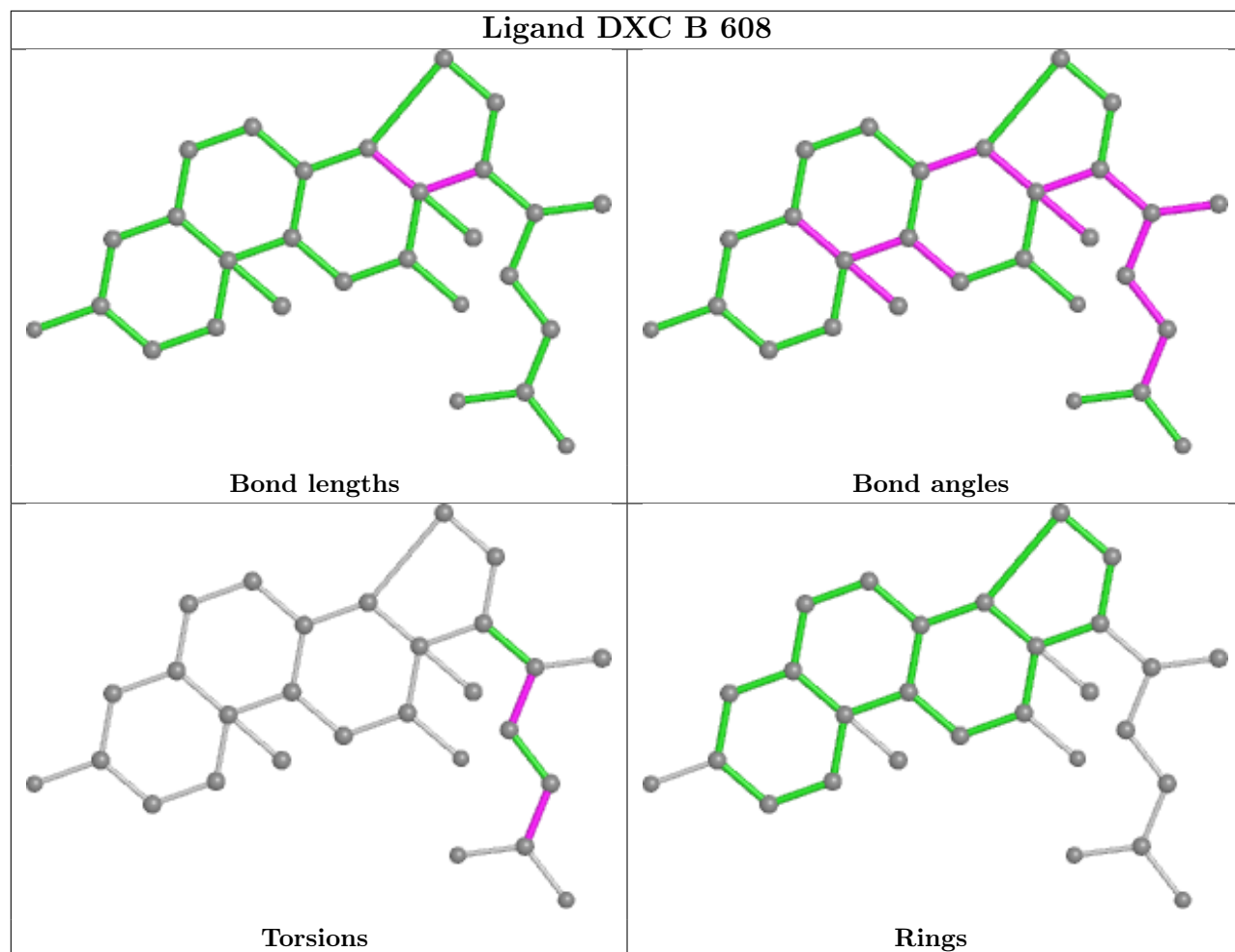
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	608	DXC	2	0
4	B	603	DXC	11	0
4	A	505	DXC	3	0

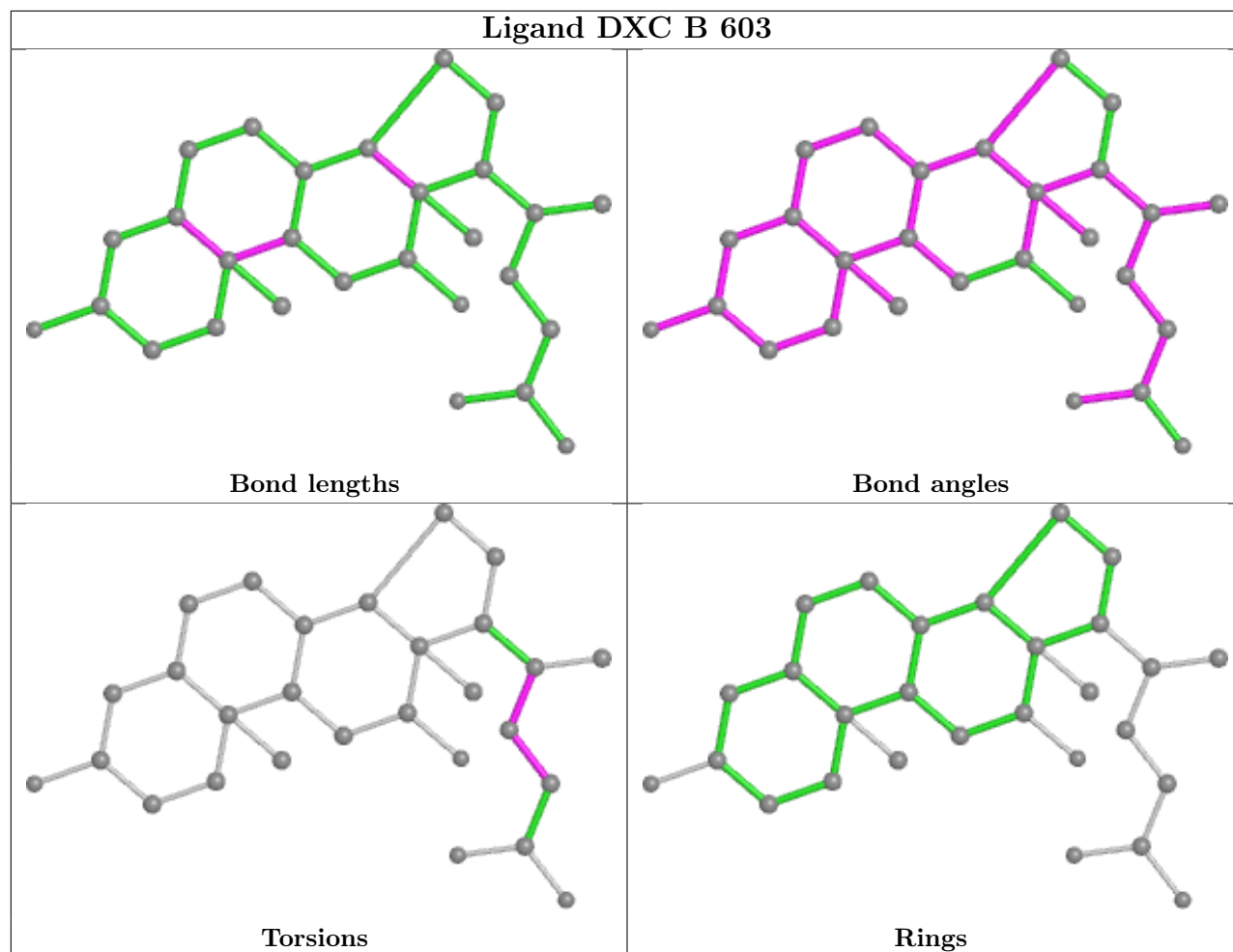
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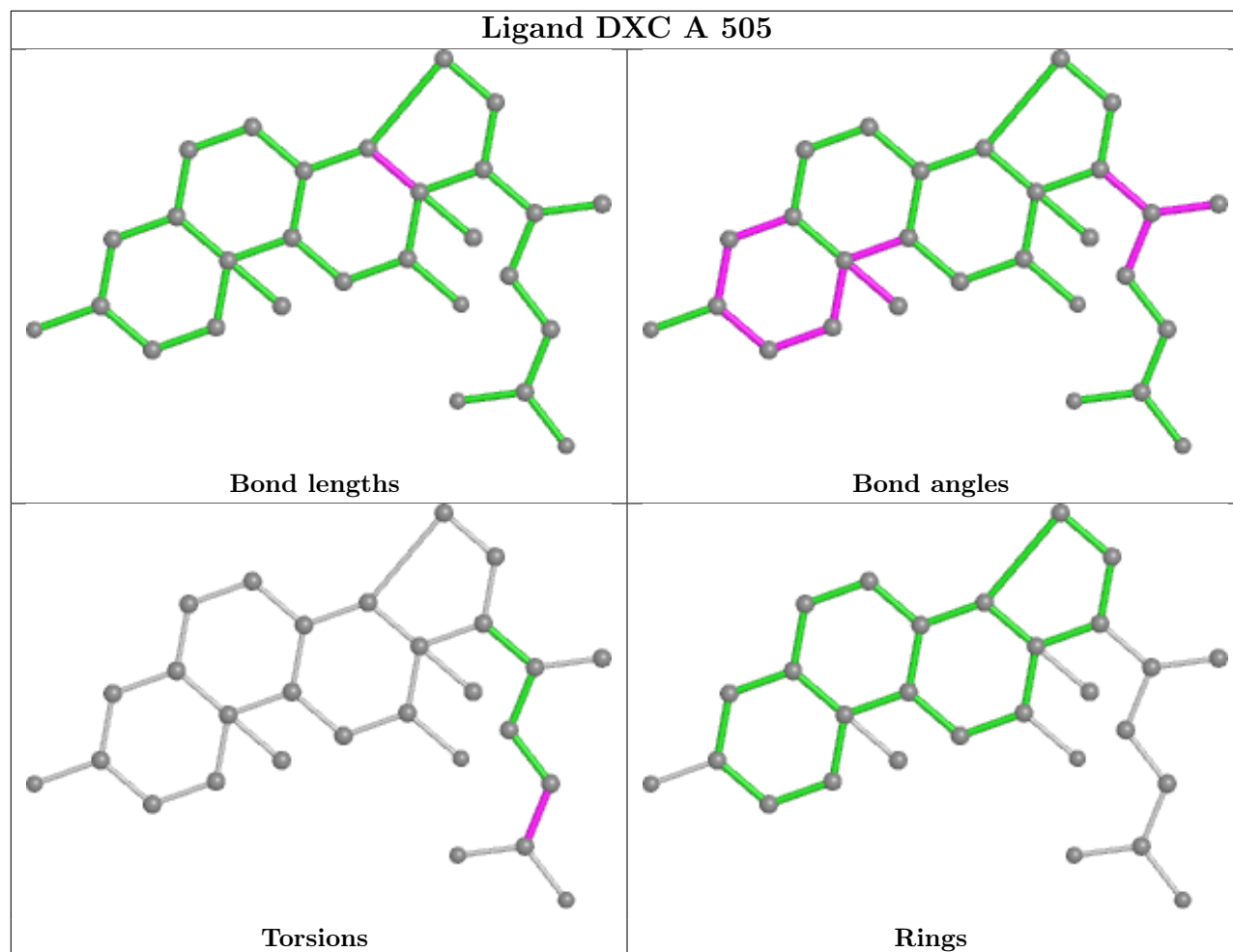
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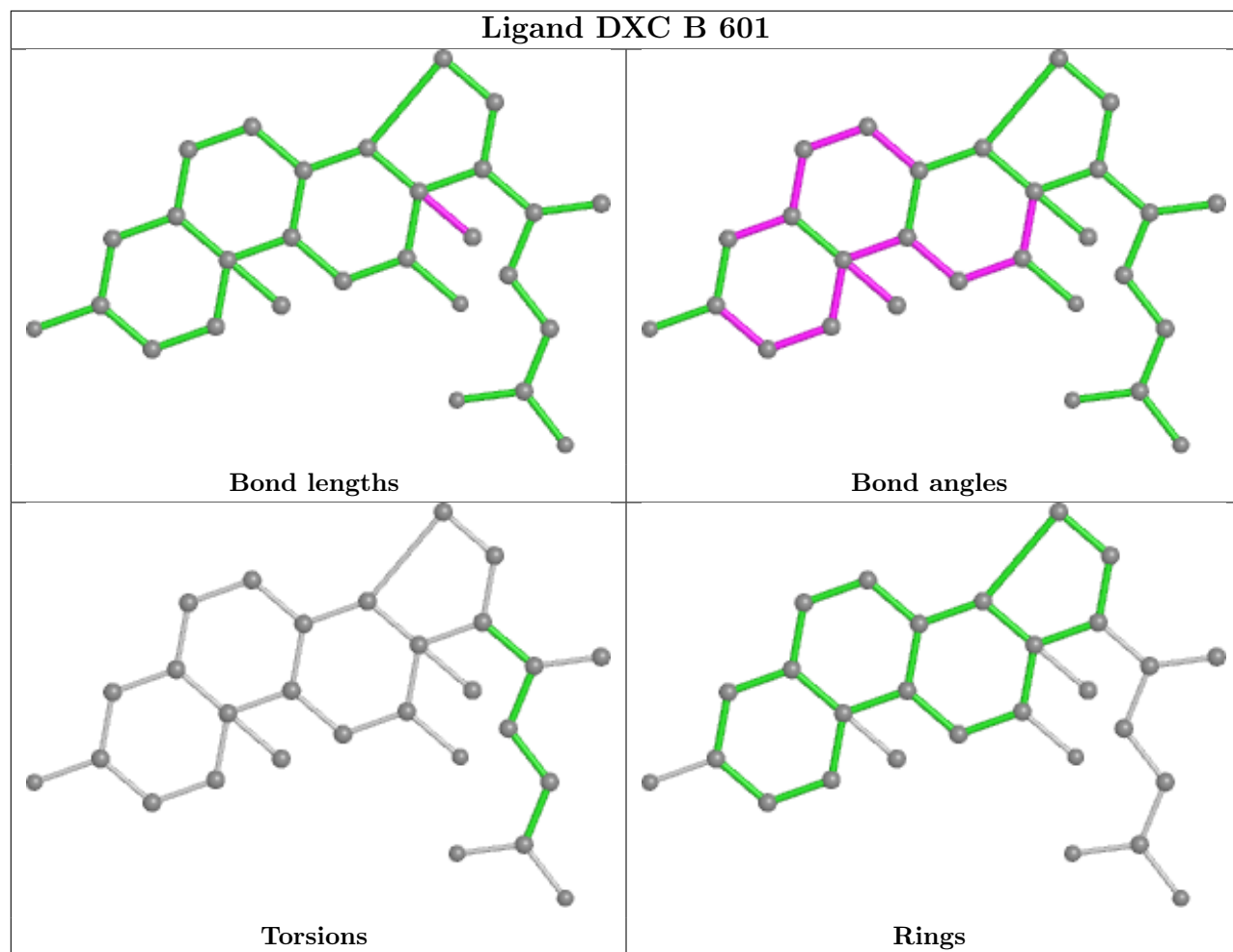
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	DXC	2	0
4	A	504	DXC	3	0
4	B	609	DXC	8	0
3	B	606	3PE	1	0
5	B	611	SO4	2	0
4	B	610	DXC	8	0
5	A	508	SO4	1	0
4	B	602	DXC	2	0
3	A	503	3PE	1	0
4	A	507	DXC	12	0
4	B	607	DXC	3	0

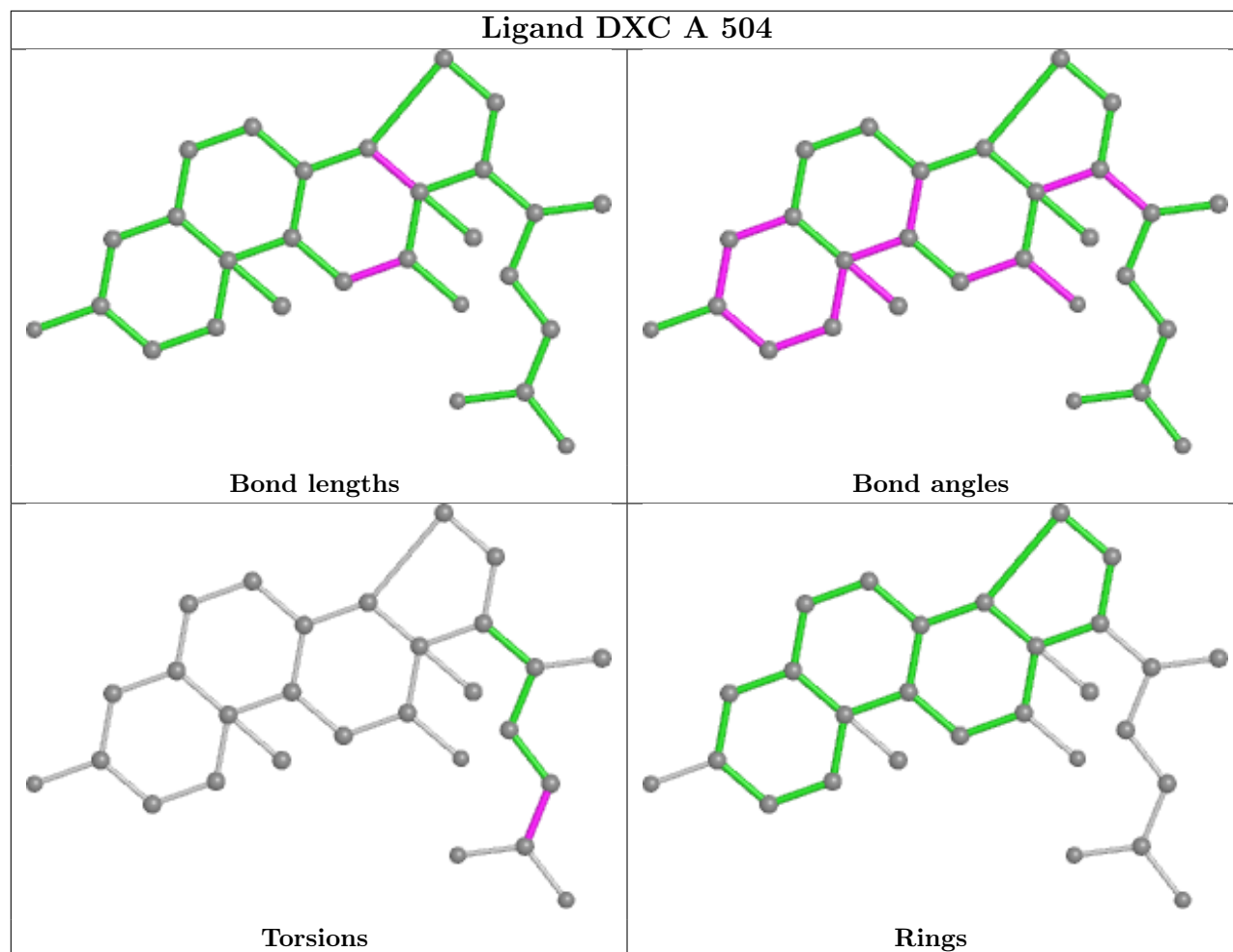
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

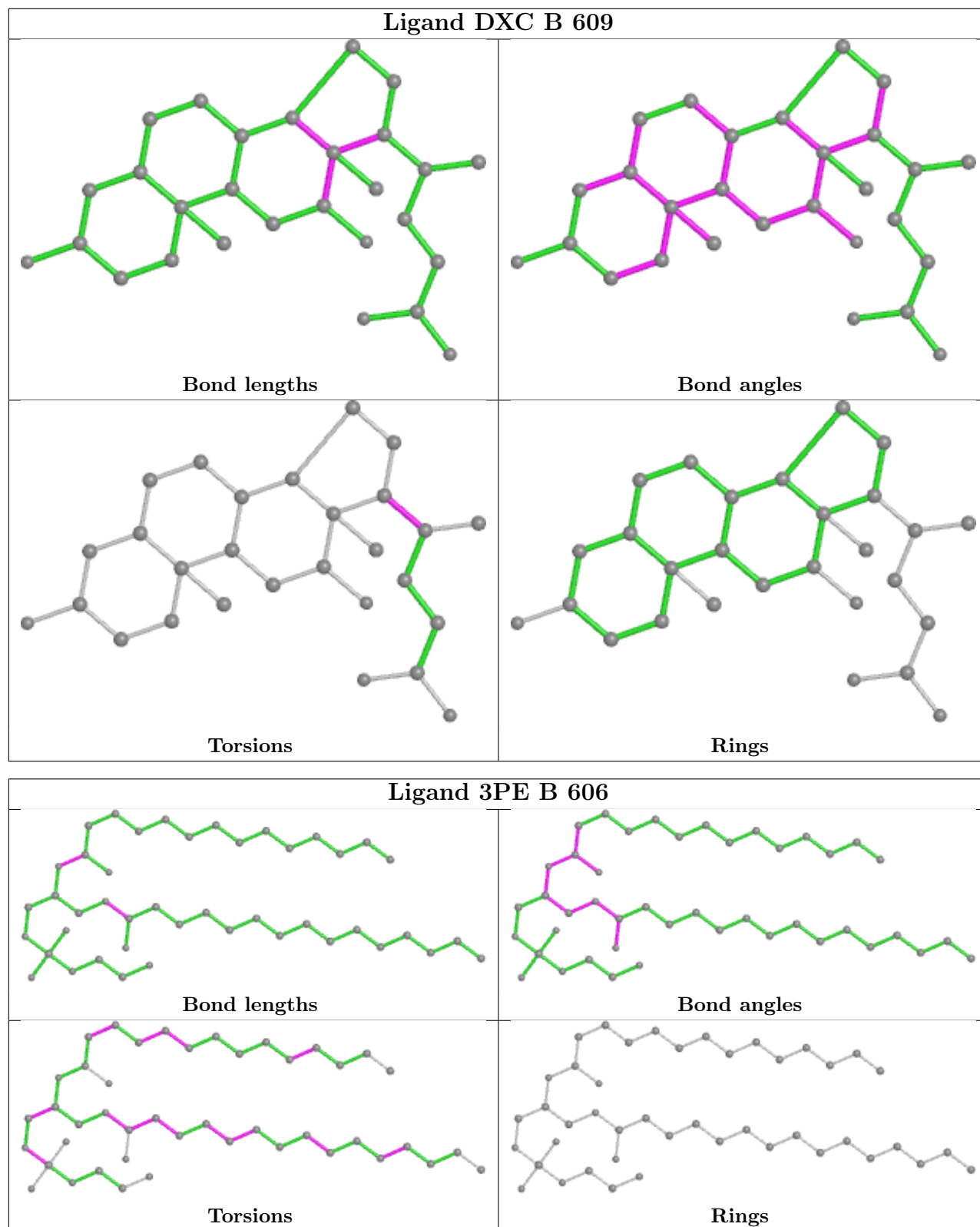


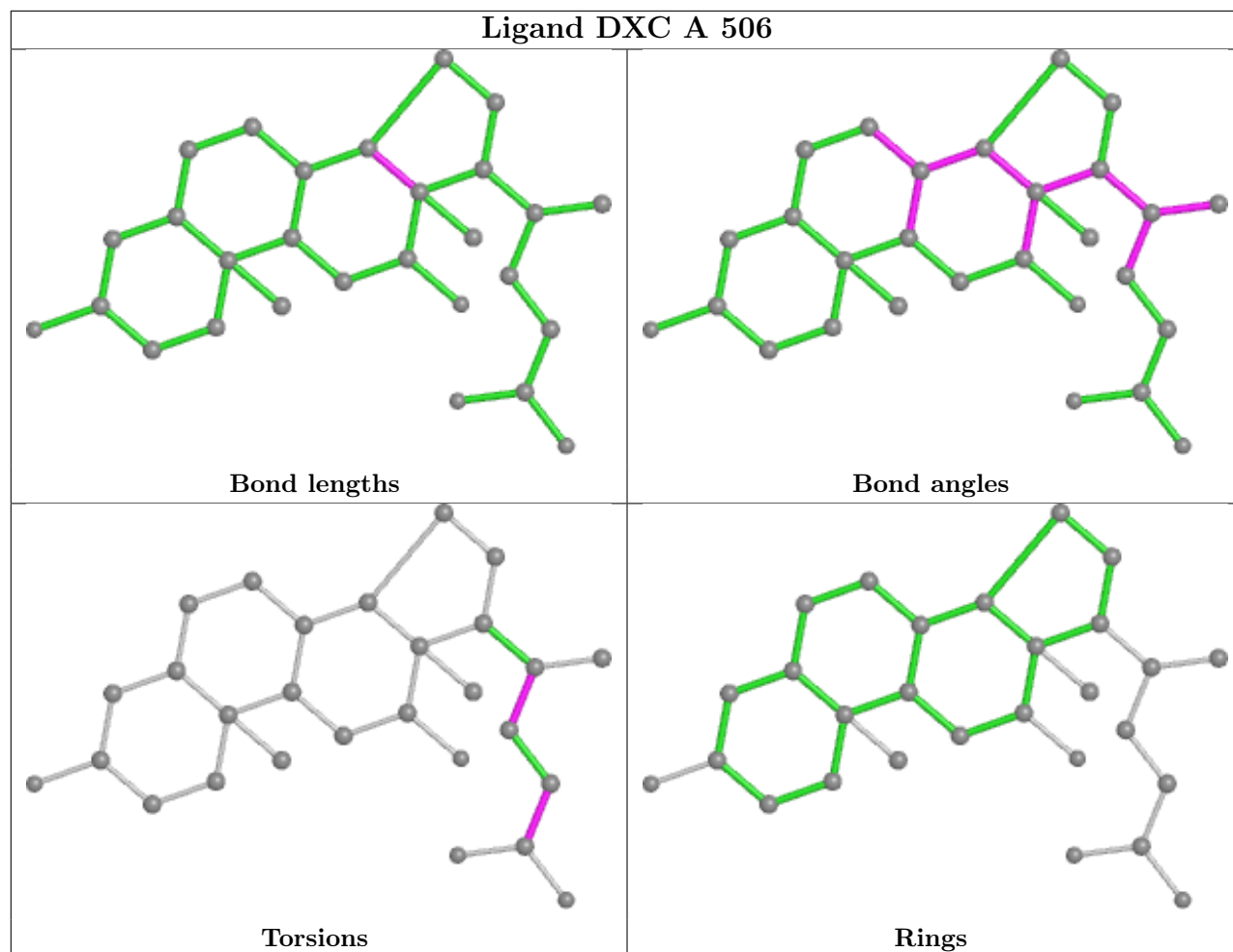


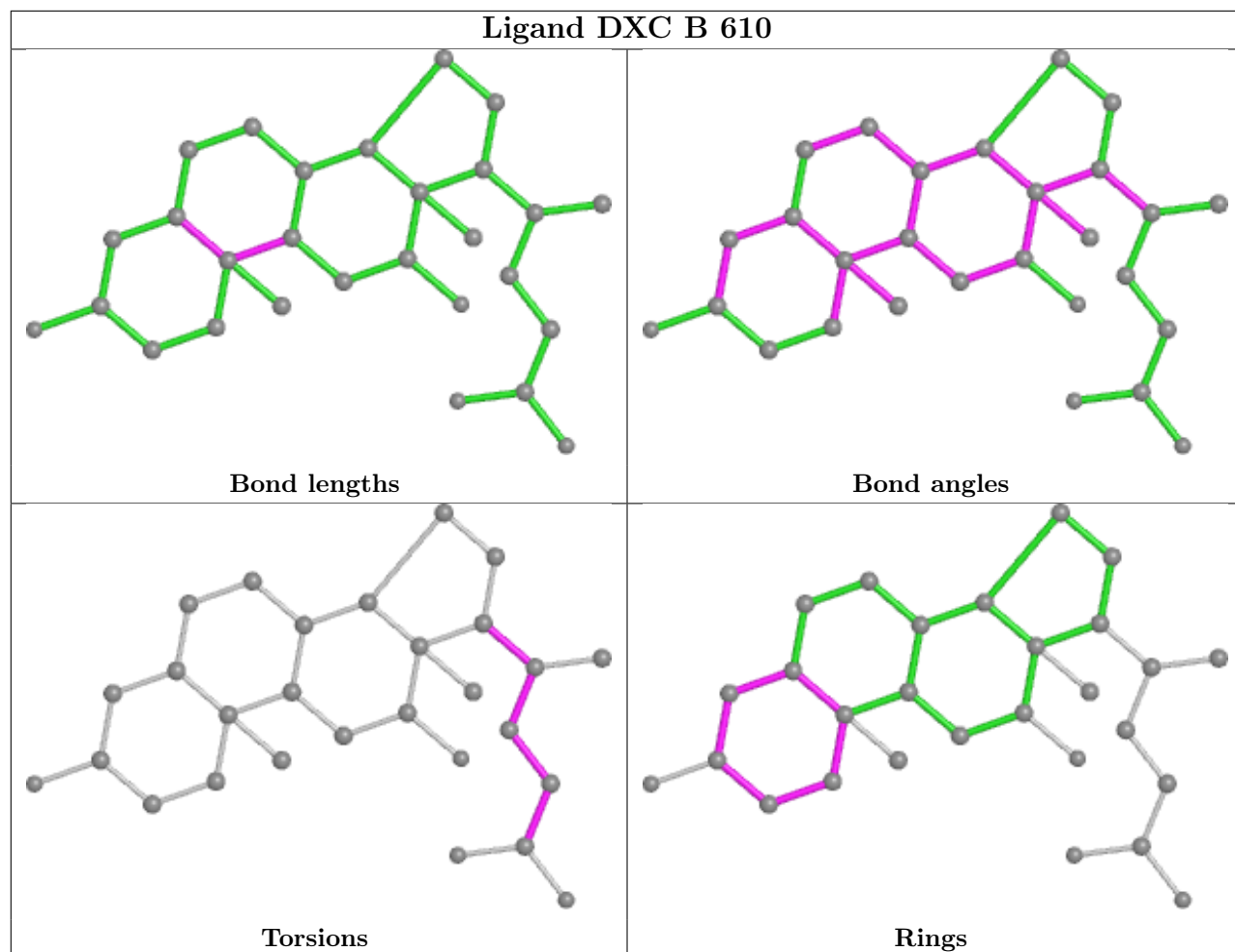


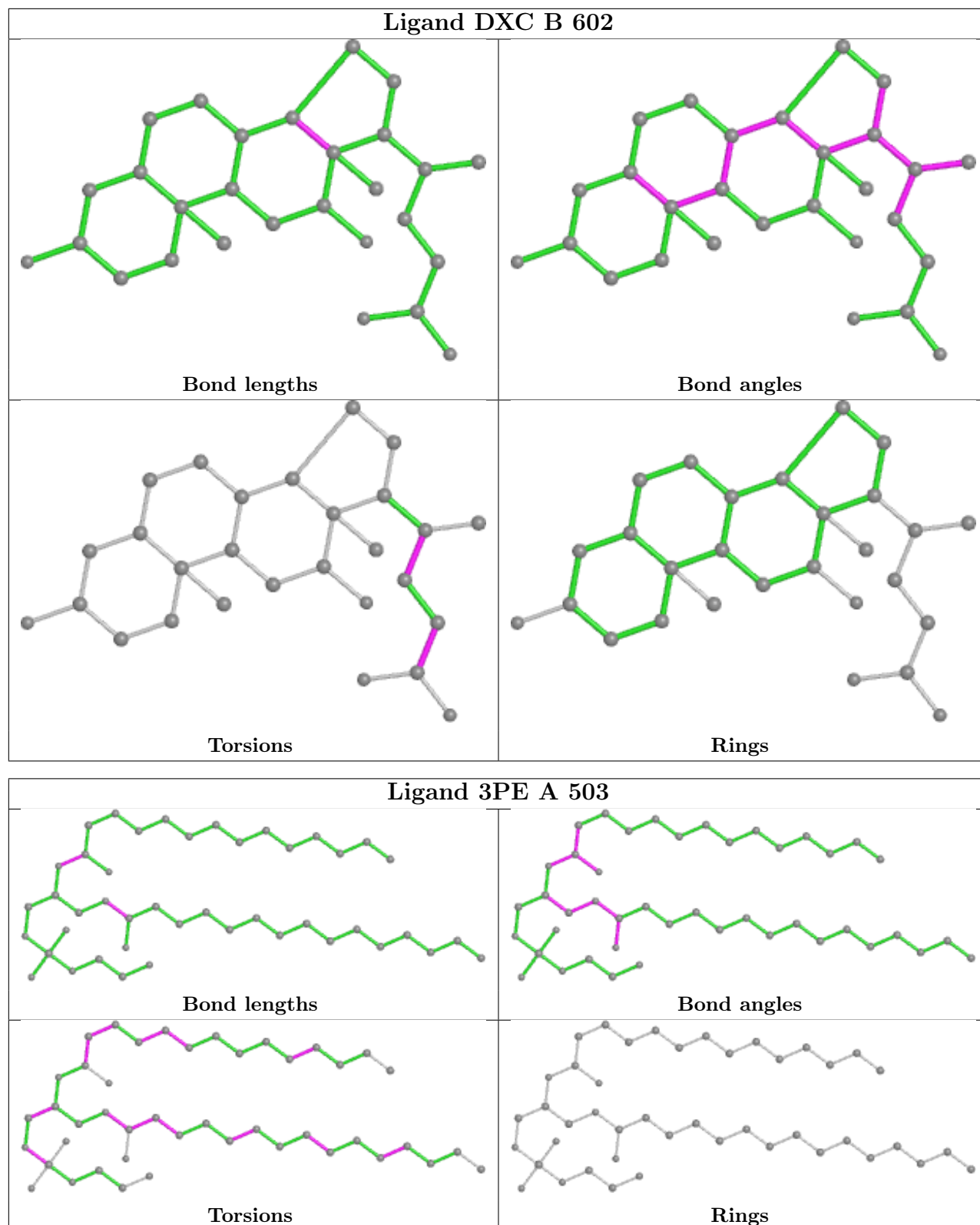


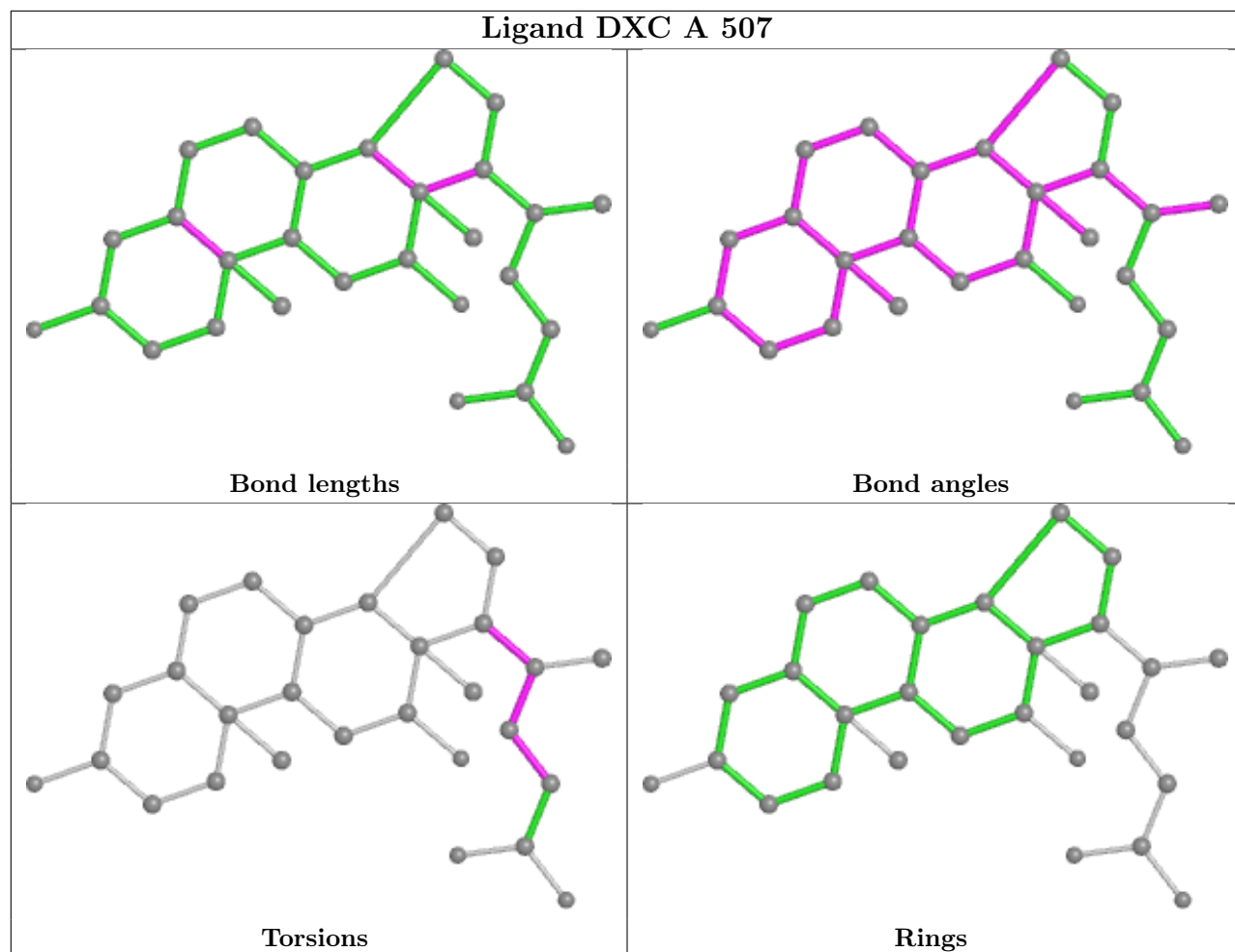


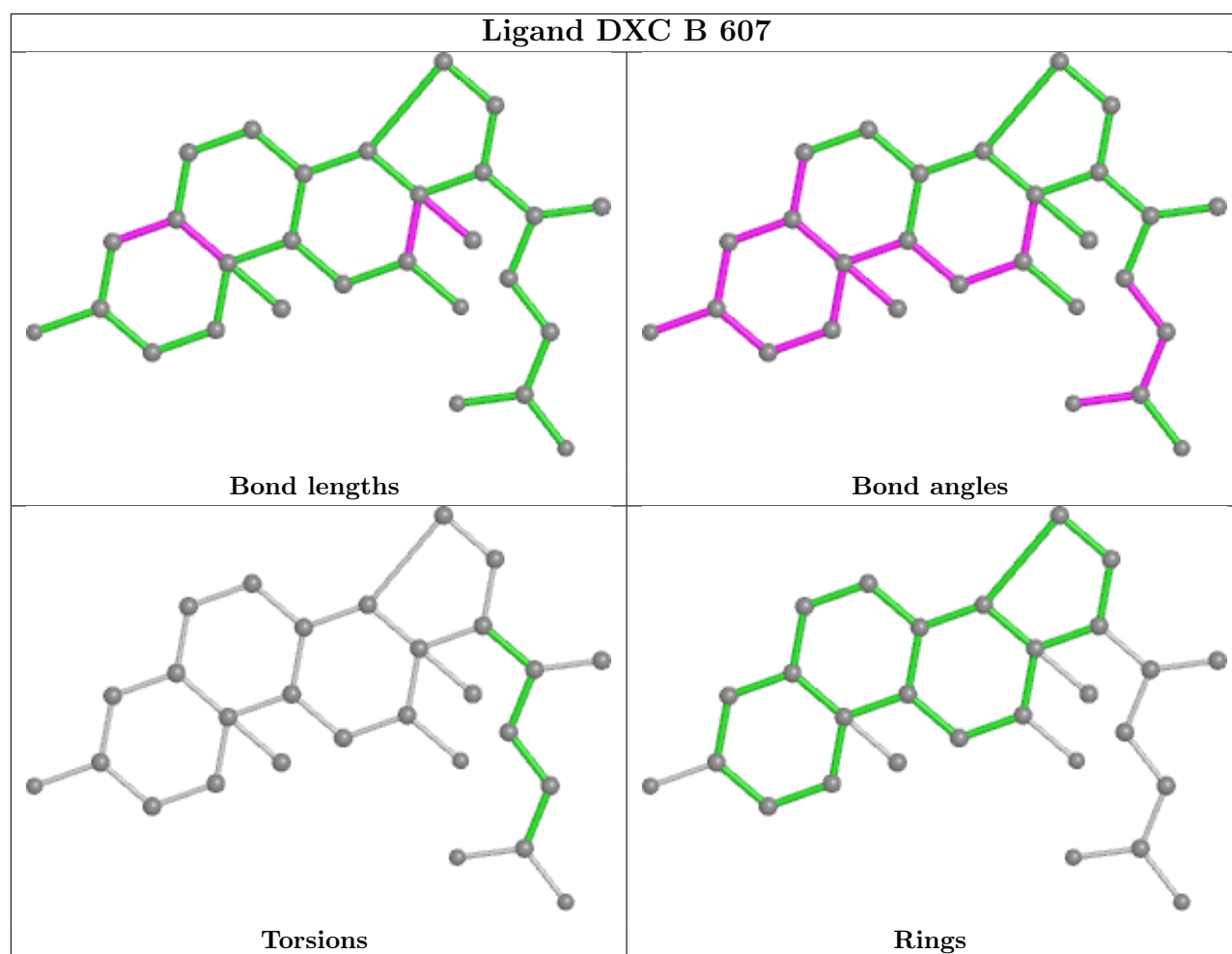












5.7 Other polymers [i](#)

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, 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	321/393 (81%)	0.62	26 (8%) 12 9	50, 82, 135, 166	0
1	B	322/393 (81%)	0.52	15 (4%) 31 28	42, 62, 110, 134	0
All	All	643/786 (81%)	0.57	41 (6%) 19 16	42, 72, 125, 166	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ASN	7.1
1	B	72	TRP	6.7
1	B	117	GLU	5.3
1	A	273	LEU	4.5
1	A	72	TRP	4.5

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

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

6.3 Carbohydrates [i](#)

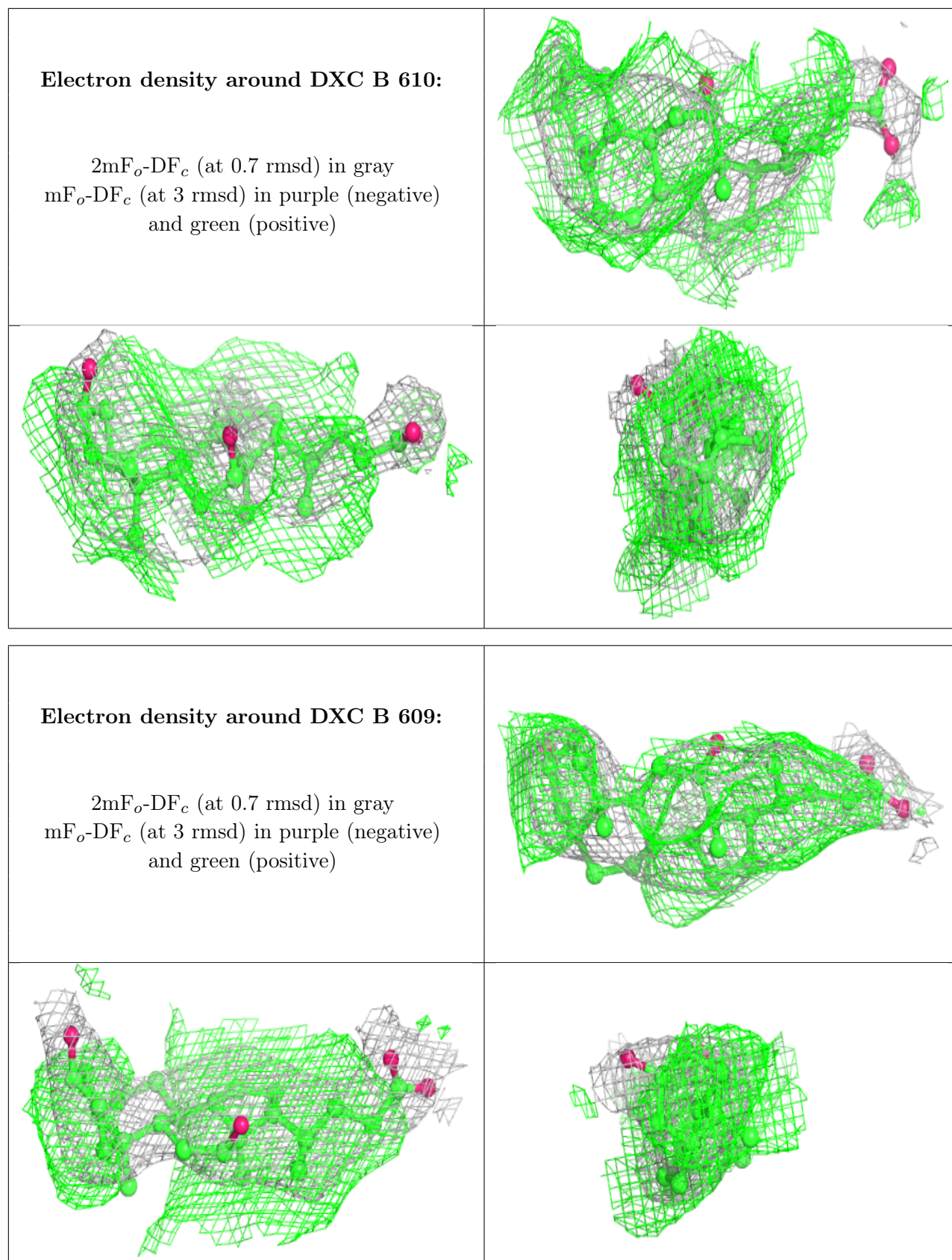
There are no monosaccharides in this entry.

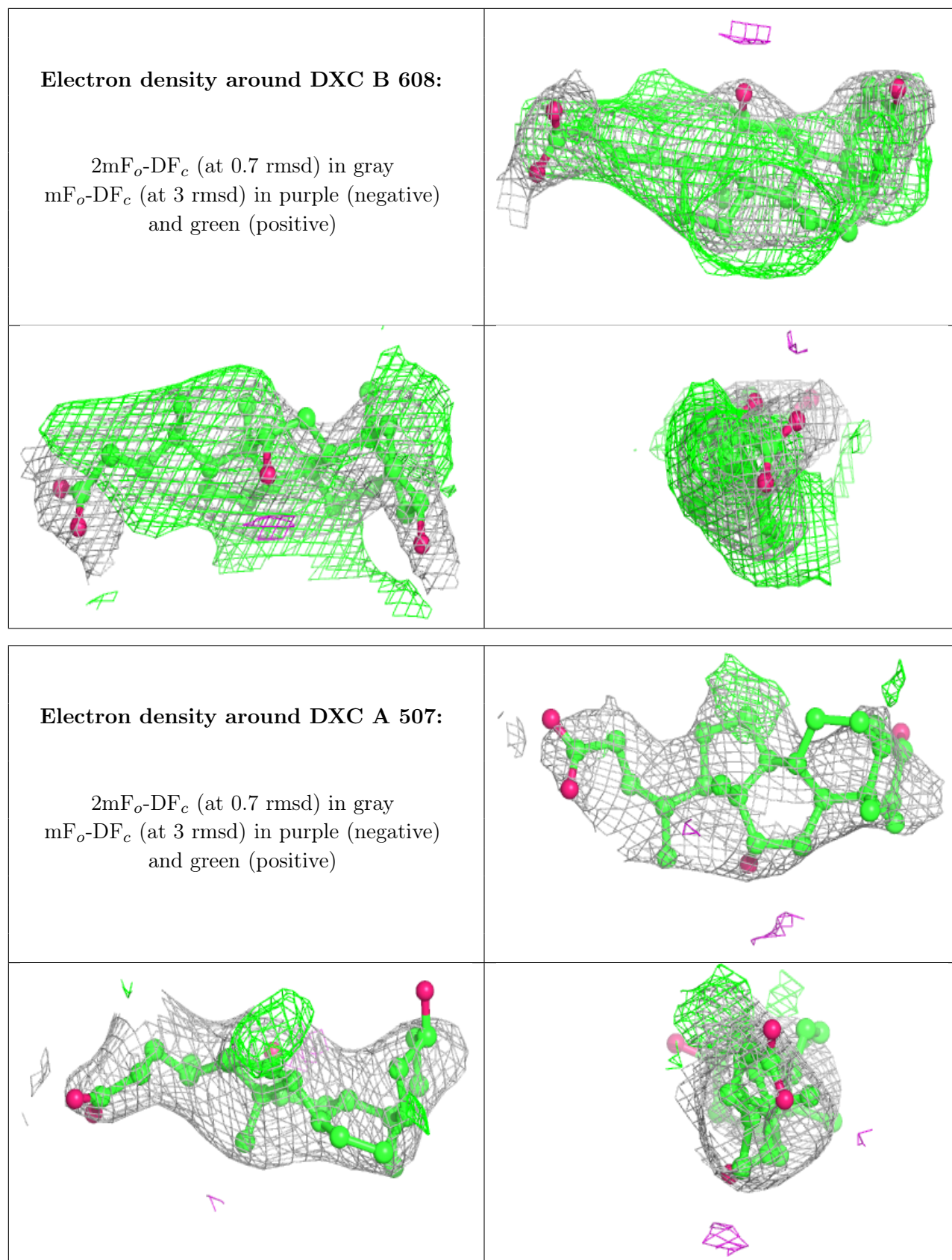
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	DXC	B	610	28/28	0.61	0.44	67,76,81,85	28
4	DXC	B	609	28/28	0.84	0.39	49,56,72,75	28
4	DXC	B	608	28/28	0.84	0.39	44,58,69,69	28
4	DXC	A	507	28/28	0.89	0.32	73,83,88,89	28
5	SO4	B	611	5/5	0.89	0.16	44,52,57,63	5
5	SO4	A	509	5/5	0.90	0.26	53,63,73,74	5
4	DXC	B	603	28/28	0.93	0.34	66,74,82,84	28
4	DXC	A	506	28/28	0.93	0.18	55,64,75,90	0
3	3PE	A	503	44/51	0.94	0.26	58,69,80,98	0
5	SO4	A	508	5/5	0.94	0.15	52,57,63,73	5
4	DXC	A	504	28/28	0.95	0.19	63,67,95,100	0
4	DXC	B	607	28/28	0.95	0.23	61,69,73,76	0
4	DXC	B	601	28/28	0.95	0.22	55,71,79,80	0
4	DXC	B	602	28/28	0.95	0.18	64,73,82,88	0
4	DXC	A	505	28/28	0.96	0.19	50,54,78,86	0
3	3PE	B	606	44/51	0.97	0.25	53,68,81,93	0
2	ZN	A	501	1/1	0.98	0.20	64,64,64,64	0
2	ZN	A	502	1/1	0.99	0.22	66,66,66,66	0
2	ZN	B	604	1/1	0.99	0.27	60,60,60,60	0
2	ZN	B	605	1/1	1.00	0.23	58,58,58,58	0

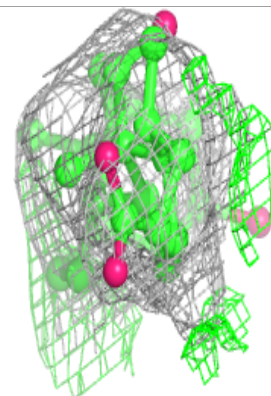
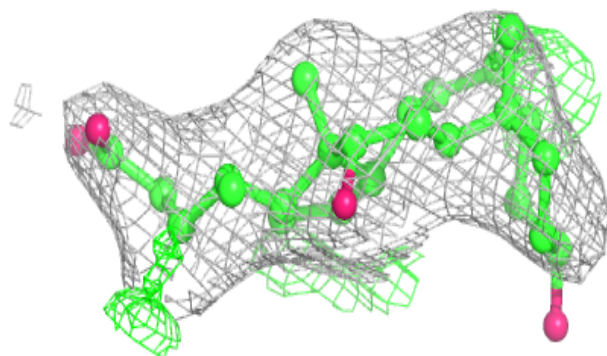
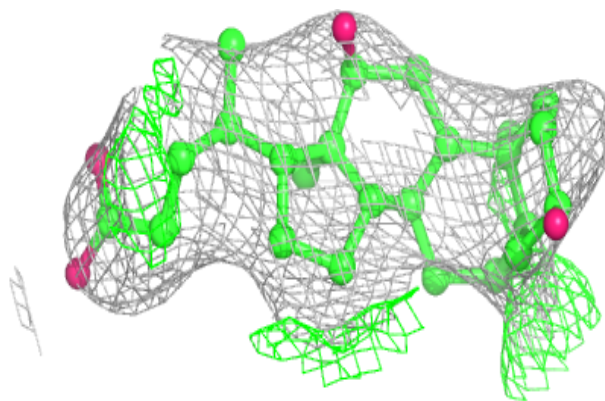
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



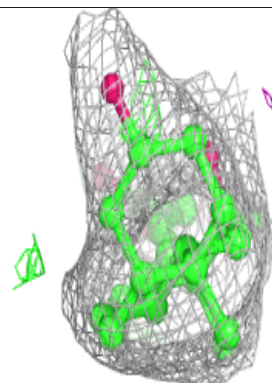
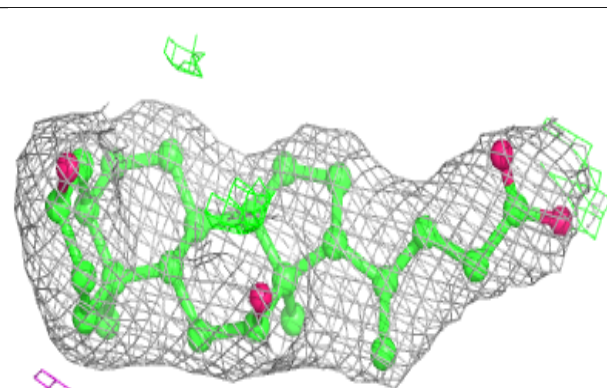
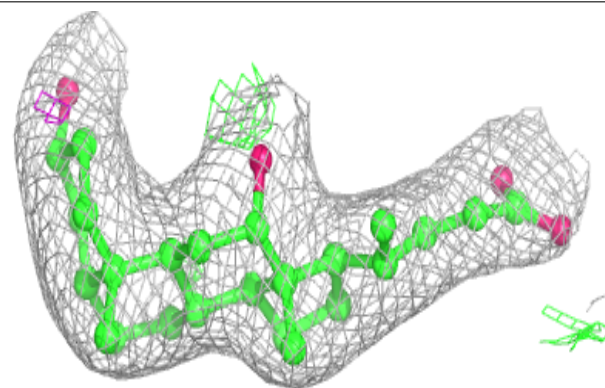


Electron density around DXC B 603:

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

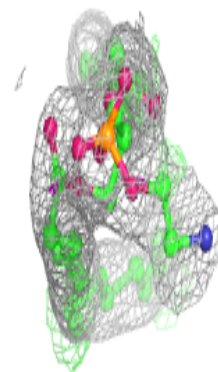
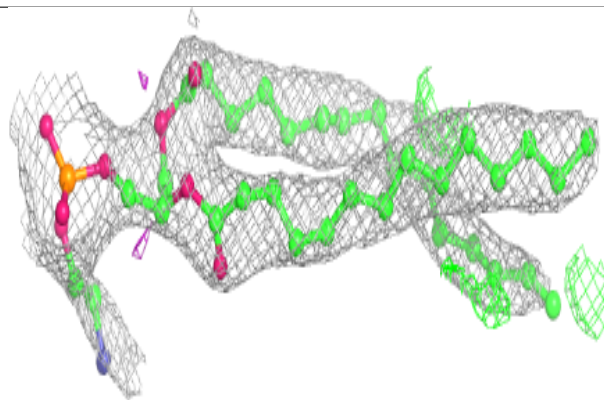
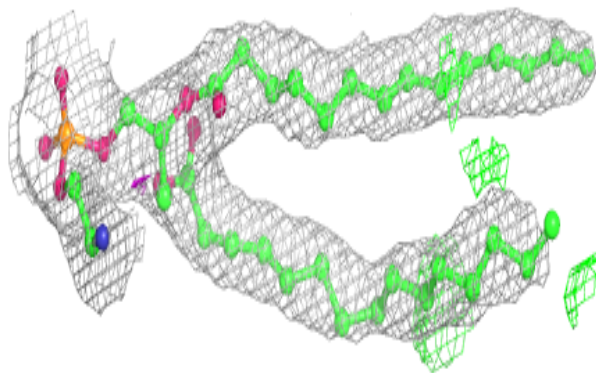
**Electron density around DXC A 506:**

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

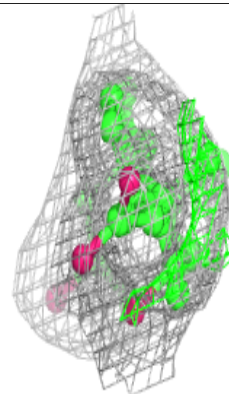
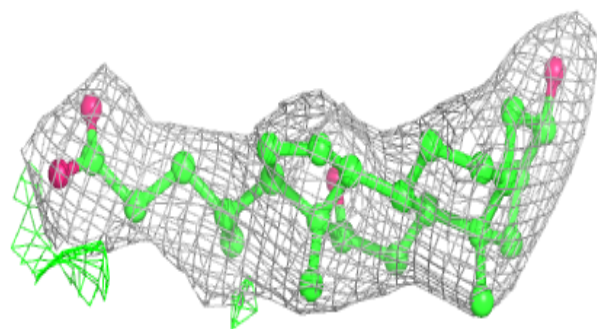
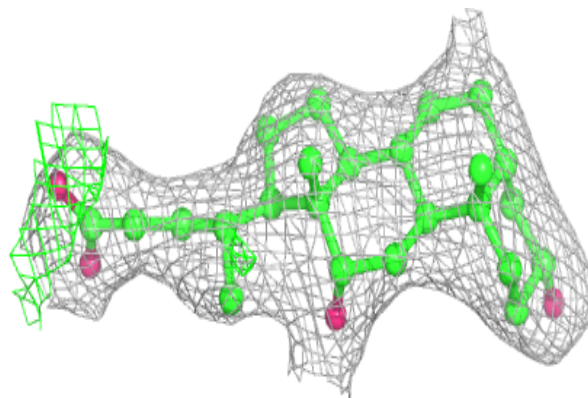


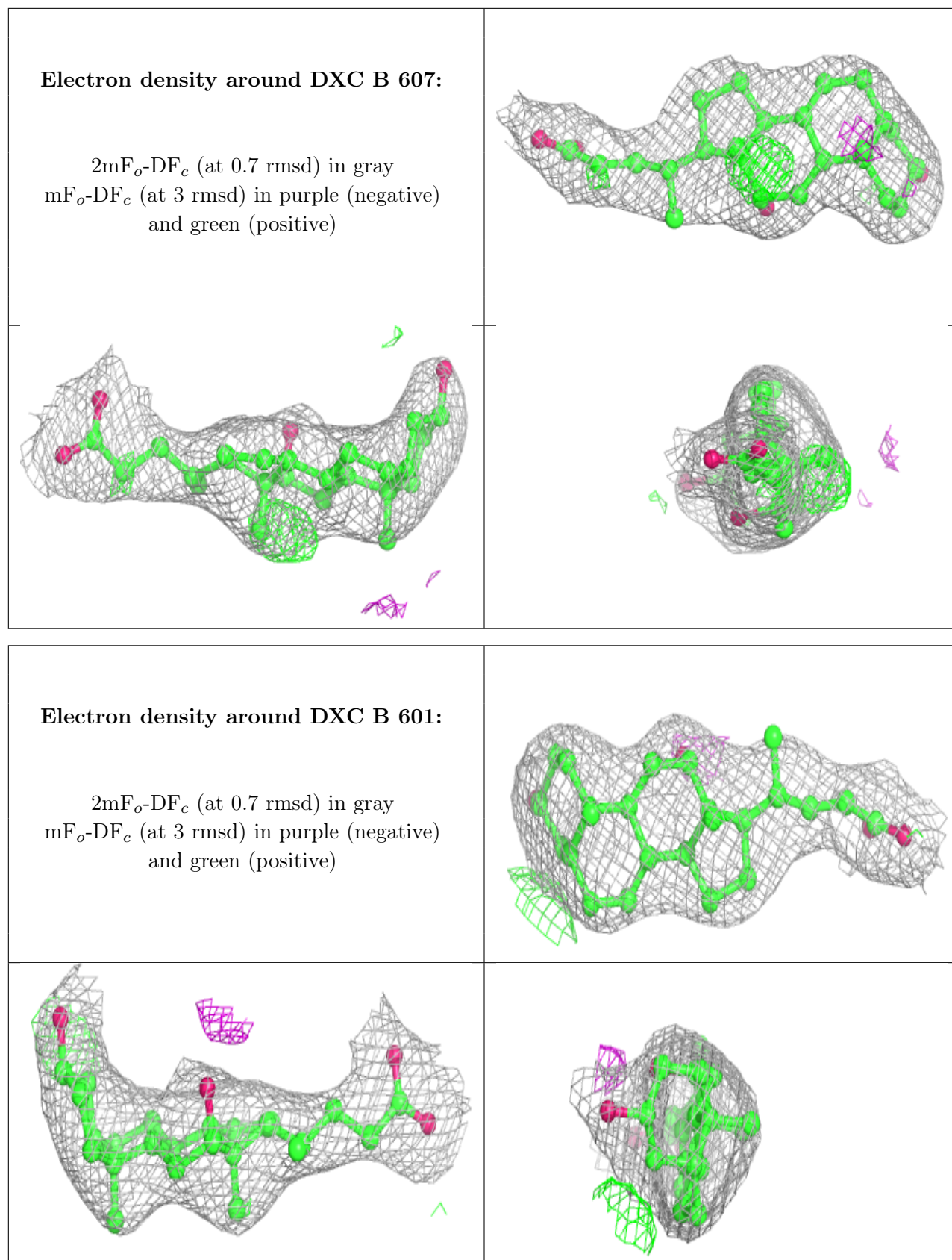
Electron density around 3PE A 503:

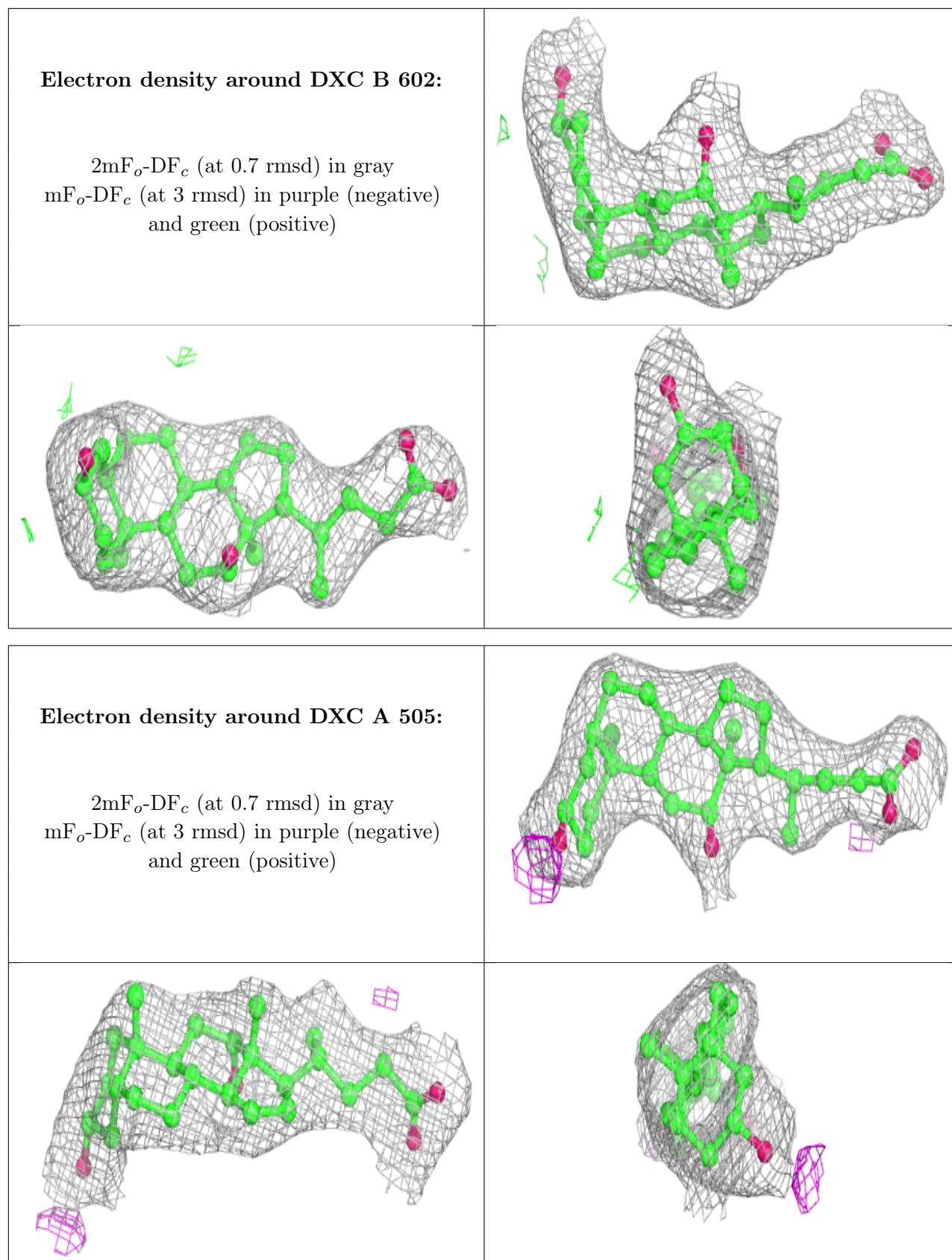
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

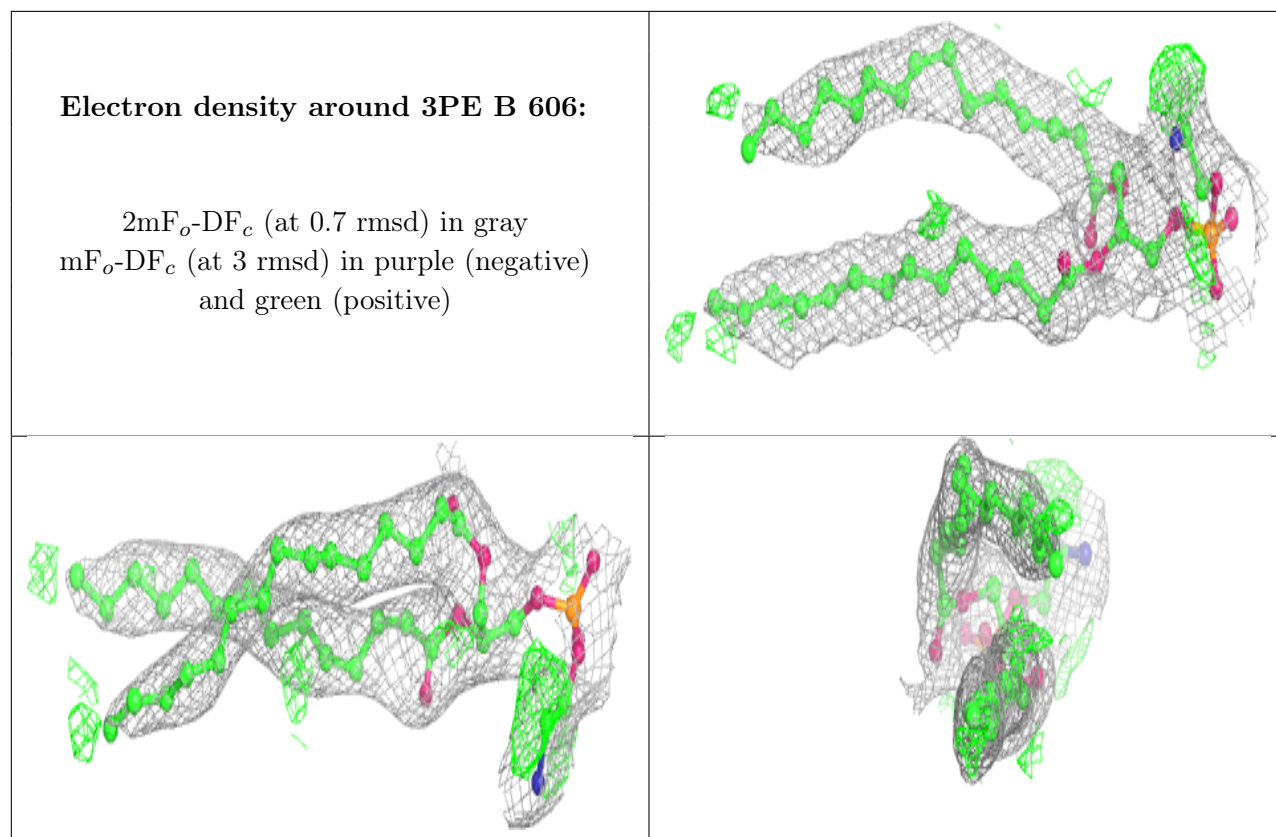
**Electron density around DXC A 504:**

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









6.5 Other polymers [i](#)

There are no such residues in this entry.