



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:37 am BST

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](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.

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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

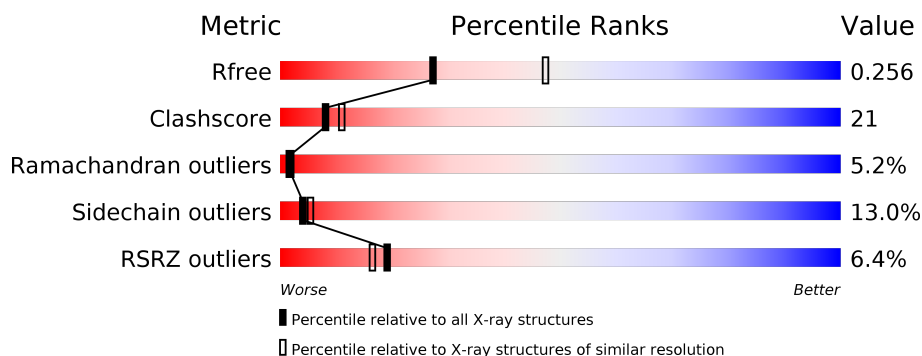
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on 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	393	<div> <div>7%</div> <div>53%</div> <div>19%</div> <div>7%</div> <div>18%</div> </div>
1	B	393	<div> <div>4%</div> <div>52%</div> <div>21%</div> <div>7%</div> <div>18%</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
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.

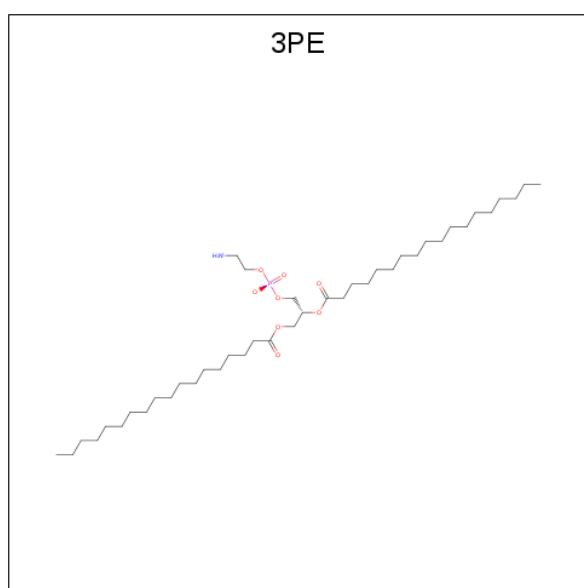
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

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

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

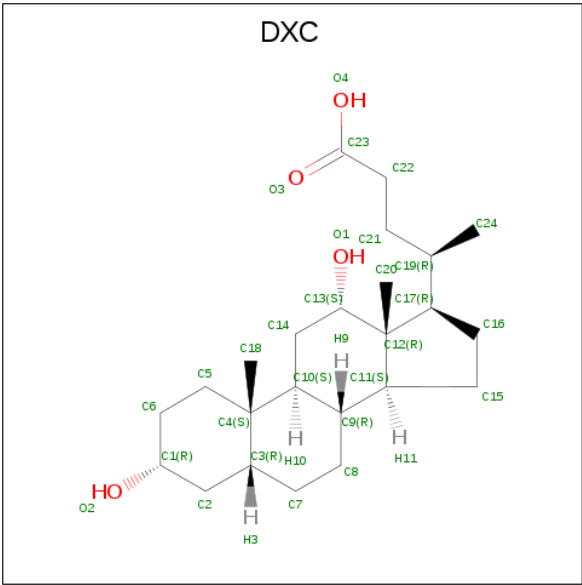
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



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: C<sub>24</sub>H<sub>40</sub>O<sub>4</sub>).



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		
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: O<sub>4</sub>S).



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		

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.

- Chain A:
- 
- 7% 53% 19% 7% 18%
- Met  
ASP  
GLU  
ASN  
GLU  
SER  
ASN  
GLN  
SER  
LEU  
MET  
THR  
SER  
GLN  
GLM  
GLN  
VAL  
ARG  
LYS  
ARG  
GLN  
ASN  
LYS  
SER  
ASP  
ALA  
ASP  
HIS  
SER  
GLY  
ALA  
ASP  
SER  
L100  
L107  
PHE  
SER  
ARG  
F110  
F111  
I112  
SER  
PHE  
LEU  
ASP  
THR  
ARG  
LEU  
GLU  
GLU  
ASP  
VAL  
THR  
LYS
- D62  
G63  
R64  
F65  
W66  
M67  
P68  
W69  
T70  
W71  
W72  
K73  
W74  
S75  
S76  
I77  
P78  
H79  
VAL  
LEU  
LEU  
GLU  
L180  
L185  
SER  
ASP  
ALA  
HIS  
SER  
P94  
S95  
S96  
L100  
L107  
F110  
F111  
I112  
E116  
E117  
A118  
G119  
V120  
R121  
E122  
A123  
G124  
L125  
R126  
V127  
L130  
E138  
E141  
L142  
I143  
F144  
L145  
T146  
D147  
S152  
P156  
M160  
R167  
T171  
I172  
S173  
E174  
L175  
P176  
I177  
I178  
D179  
G180  
V181  
M186  
H187  
L199  
R208  
W209  
F210  
L213  
G214  
L215  
L216  
D217  
W218  
W219  
V227  
I228  
E229  
W232  
W241  
D242  
V243  
V244  
F246  
P250  
S254
- E356  
P357  
P358  
L361  
L365  
E366  
F375  
R384  
Y385  
L386  
N387  
N388  
ASP  
ASP  
GLU  
ASN  
PHE  
D284  
T285  
G286  
Y287  
C288  
P289  
A290  
F291  
I294  
G295  
K296  
R297  
F298  
G299  
P300  
F301  
A304  
P307  
I308  
F316  
V322  
E325  
R329  
V334  
I342  
H343  
W344
- L273  
G274  
P275  
W276  
N277  
R278  
F279  
F280  
D284  
T285  
G286  
Y287  
C288  
P289  
A290  
F291  
I294  
G295  
K296  
R297  
F298  
G299  
P300  
F301  
A304  
P307  
I308  
F316  
V322  
E325  
R329  
V334  
I342  
H343  
W344

- Chain B:
- 
- | Category | Value |
|----------|-------|
| T258     | L142  |
| D262     | I143  |
| V265     | P156  |
| L266     | M160  |
| W267     | R167  |
| G268     | P177  |
| S269     | T171  |
| W270     | I172  |
| L273     | S173  |
| R278     | L175  |
| D284     | P177  |
| G285     | I178  |
| G286     | D179  |
| Y287     | A180  |
| C288     | V181  |
| P289     | H185  |
| A290     | N186  |
| F291     | H187  |
| G299     | L199  |
| P300     | N200  |
| V322     | F203  |
| D323     | E206  |
| P324     | L207  |
| E325     | A327  |
| G326     | W208  |
| A327     | F210  |
| V328     | L213  |
| R329     | G214  |
| V334     | L215  |
| M340     | Y110  |
| A341     | I111  |
| I342     | I112  |
| H343     | E116  |
| W344     | L117  |
| L349     | A118  |
| L355     | G119  |
| E356     | W120  |
| P357     | R121  |
| P358     | A122  |
| L365     | D242  |
| E366     | K243  |
| R367     | P250  |
| F375     | S251  |
| F376     | H253  |
| V377     | W254  |
| L378     | C255  |

N384	N387	N388	D389	ASP	GLU	ASN	PHE
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.10 Å 95.10 Å 444.17 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.65 Å)	Xtriage
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 <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage'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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DXC, SO4, 3PE

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 ⓘ

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:H203	4:B:610:DXC:H242	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	A	344	TRP
1	B	58	LYS
1	B	367	ARG
1	A	361	LEU
1	A	384	ARG

Some 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 carbohydrates 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$
4	DXC	A	504	-	28,31,31	0.87	2 (7%)	46,49,49	1.40	8 (17%)
4	DXC	B	610	-	28,31,31	0.94	2 (7%)	46,49,49	2.45	16 (34%)
5	SO4	A	509	-	4,4,4	0.40	0	6,6,6	0.31	0
5	SO4	B	611	-	4,4,4	0.60	0	6,6,6	0.66	0
4	DXC	A	505	-	28,31,31	0.91	1 (3%)	46,49,49	1.39	7 (15%)
4	DXC	A	506	-	28,31,31	0.90	1 (3%)	46,49,49	1.37	7 (15%)
4	DXC	B	601	-	28,31,31	0.94	1 (3%)	46,49,49	1.37	7 (15%)
4	DXC	B	608	-	28,31,31	1.12	2 (7%)	46,49,49	1.67	10 (21%)
5	SO4	A	508	-	4,4,4	0.44	0	6,6,6	0.44	0
4	DXC	B	602	-	28,31,31	0.90	1 (3%)	46,49,49	1.24	6 (13%)
3	3PE	B	606	2	43,43,50	1.03	2 (4%)	46,48,55	1.41	5 (10%)
3	3PE	A	503	2	43,43,50	0.97	2 (4%)	46,48,55	1.37	4 (8%)
4	DXC	B	607	-	28,31,31	1.09	4 (14%)	46,49,49	1.55	10 (21%)
4	DXC	A	507	-	28,31,31	1.24	3 (10%)	46,49,49	3.61	22 (47%)
4	DXC	B	609	-	28,31,31	1.15	3 (10%)	46,49,49	2.16	14 (30%)
4	DXC	B	603	-	28,31,31	1.31	3 (10%)	46,49,49	3.94	22 (47%)

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	A	504	-	-	0/7/71/71	0/4/4/4
4	DXC	B	610	-	-	7/7/71/71	1/4/4/4
4	DXC	A	505	-	-	0/7/71/71	0/4/4/4
4	DXC	A	506	-	-	1/7/71/71	0/4/4/4
4	DXC	B	601	-	-	0/7/71/71	0/4/4/4
4	DXC	B	608	-	-	1/7/71/71	0/4/4/4
4	DXC	B	602	-	-	1/7/71/71	0/4/4/4
3	3PE	B	606	2	-	18/47/47/54	-
3	3PE	A	503	2	-	18/47/47/54	-
4	DXC	B	607	-	-	0/7/71/71	0/4/4/4
4	DXC	A	507	-	-	4/7/71/71	0/4/4/4
4	DXC	B	609	-	-	1/7/71/71	0/4/4/4
4	DXC	B	603	-	-	3/7/71/71	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 138 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 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	610	DXC	C12-C17-C19-C24
4	B	610	DXC	C16-C17-C19-C21
3	B	606	3PE	C1-O11-P-O12
3	A	503	3PE	C1-O11-P-O12
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	A	504	DXC	3	0
4	B	610	DXC	8	0
5	B	611	SO4	2	0
4	A	505	DXC	3	0
4	B	601	DXC	2	0
4	B	608	DXC	2	0
5	A	508	SO4	1	0
4	B	602	DXC	2	0

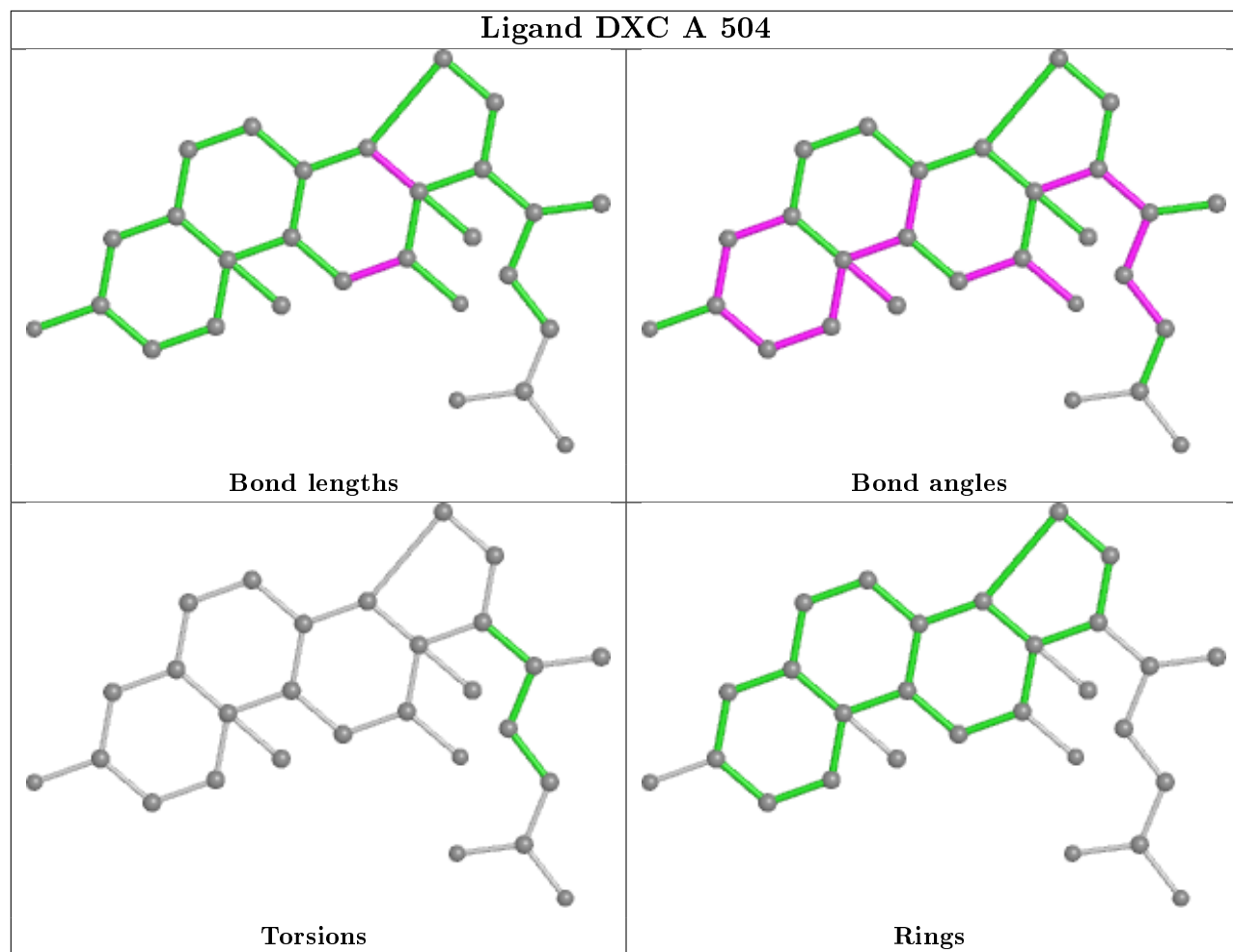
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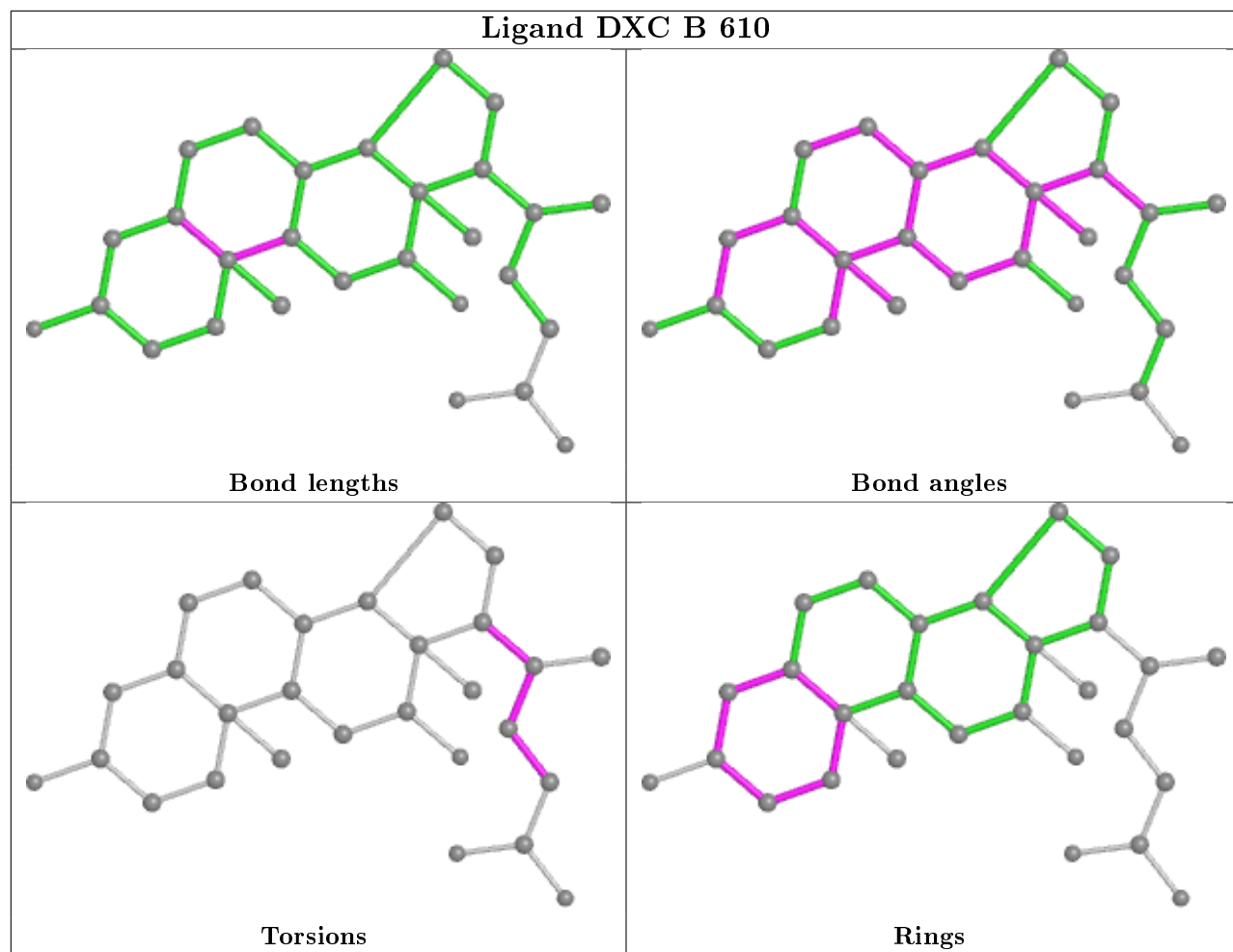
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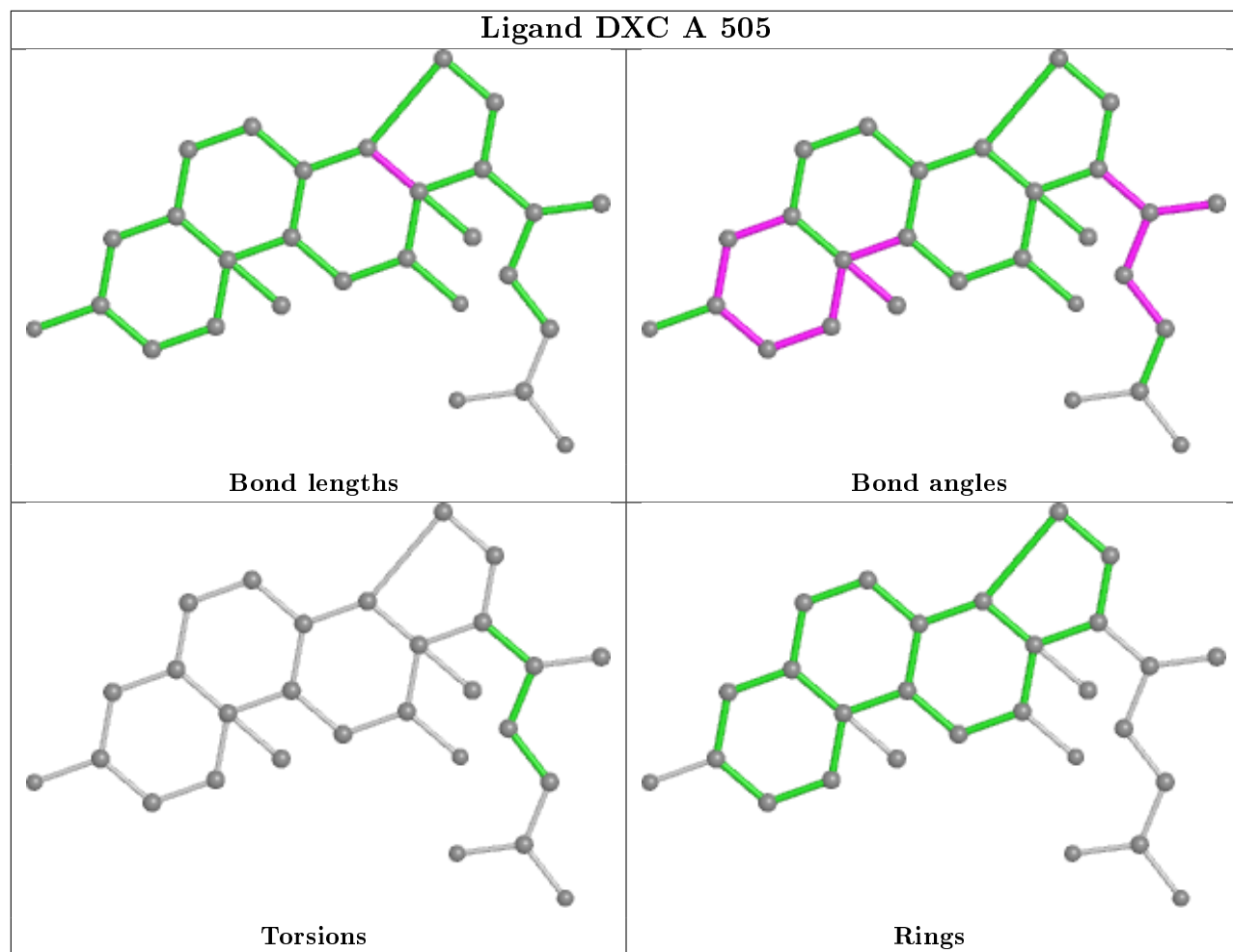
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	3PE	1	0
3	A	503	3PE	1	0
4	B	607	DXC	3	0
4	A	507	DXC	12	0
4	B	609	DXC	8	0
4	B	603	DXC	11	0

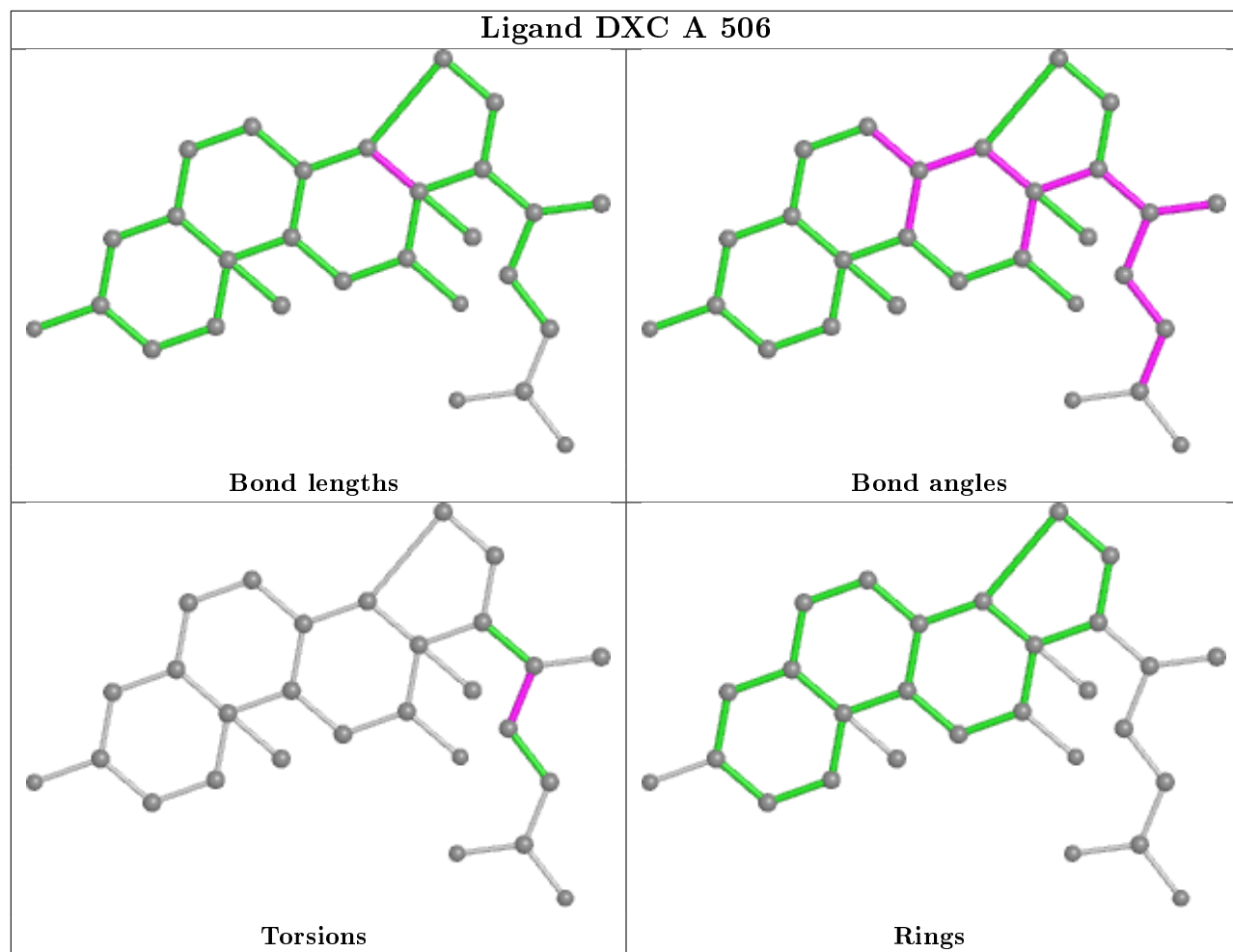
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

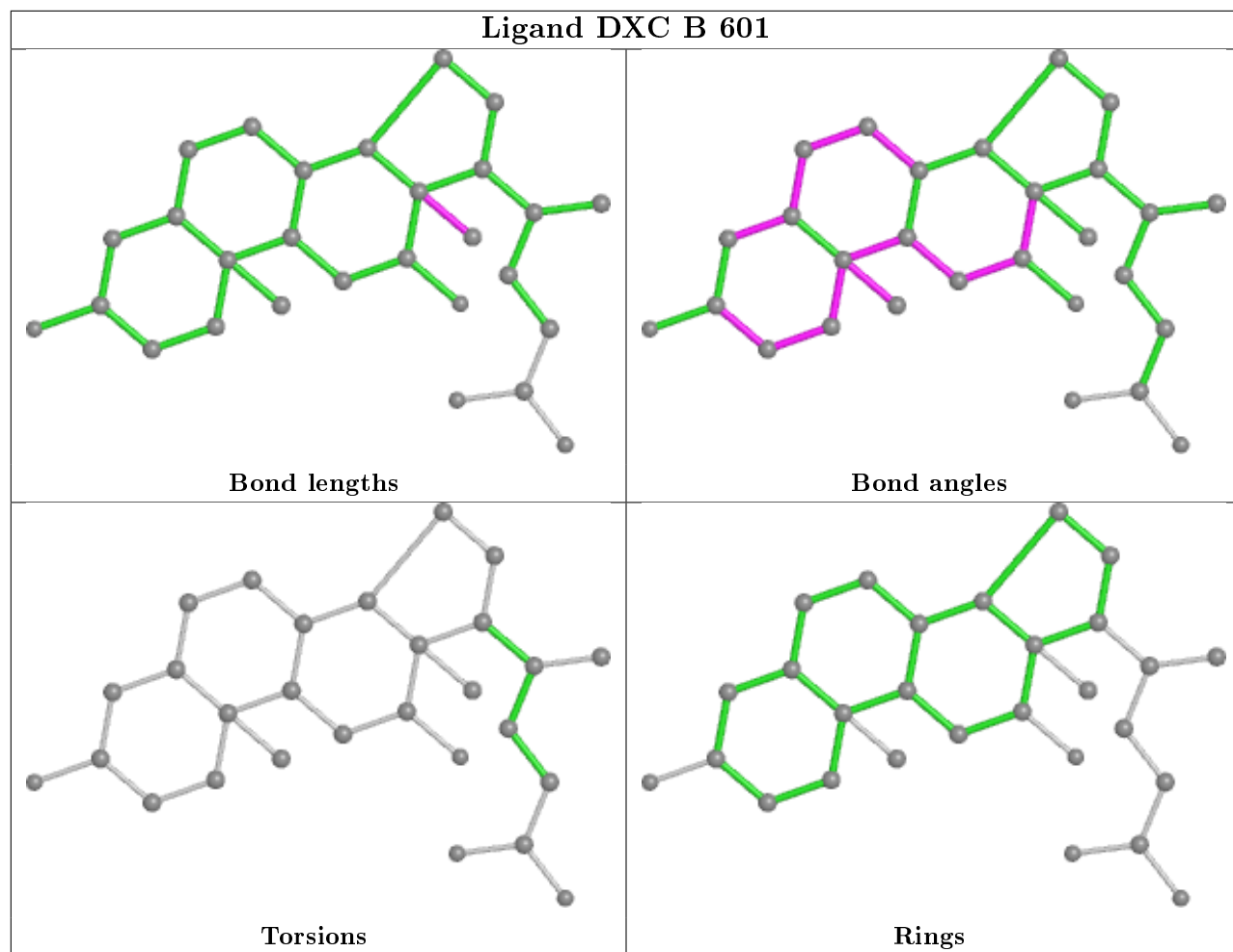


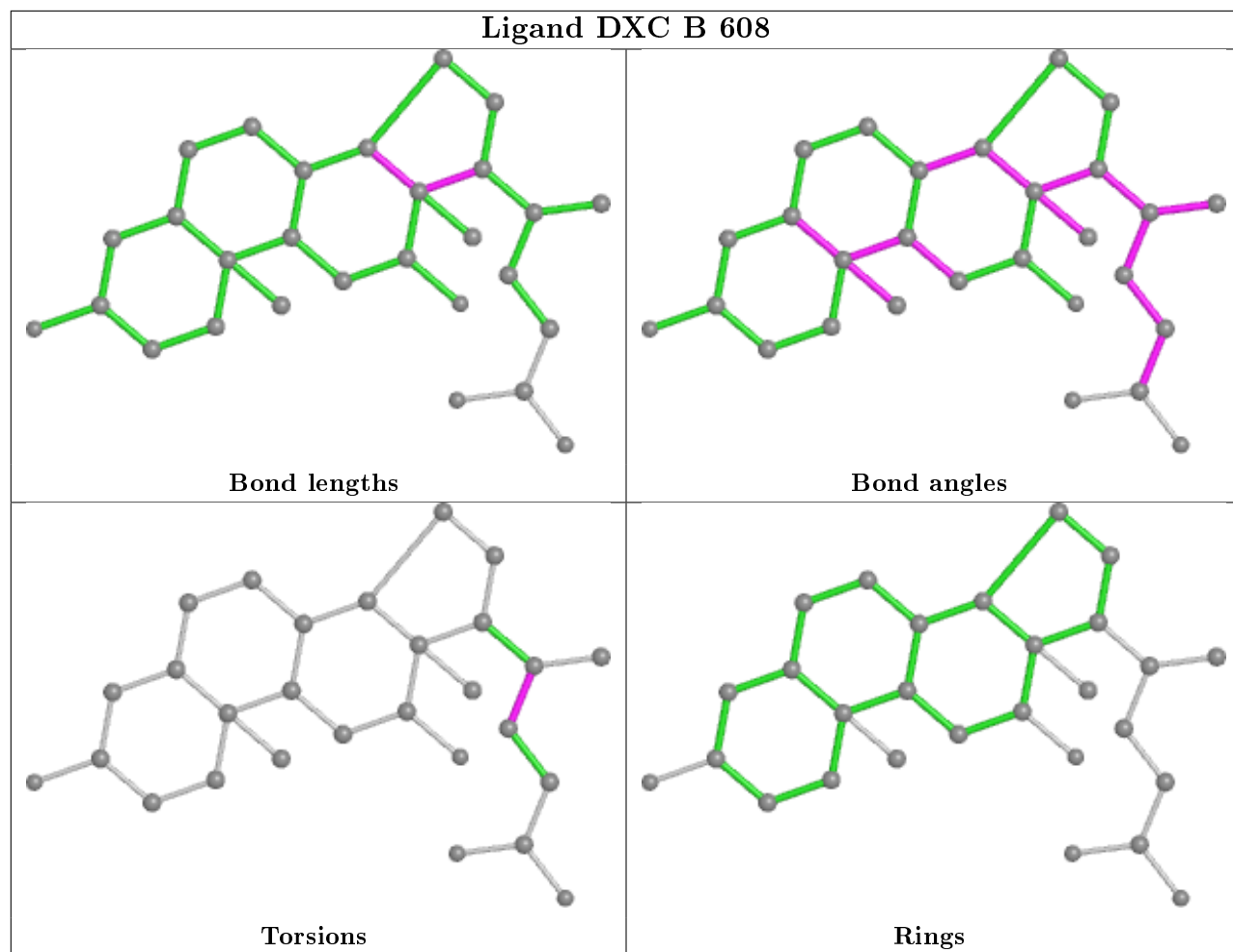


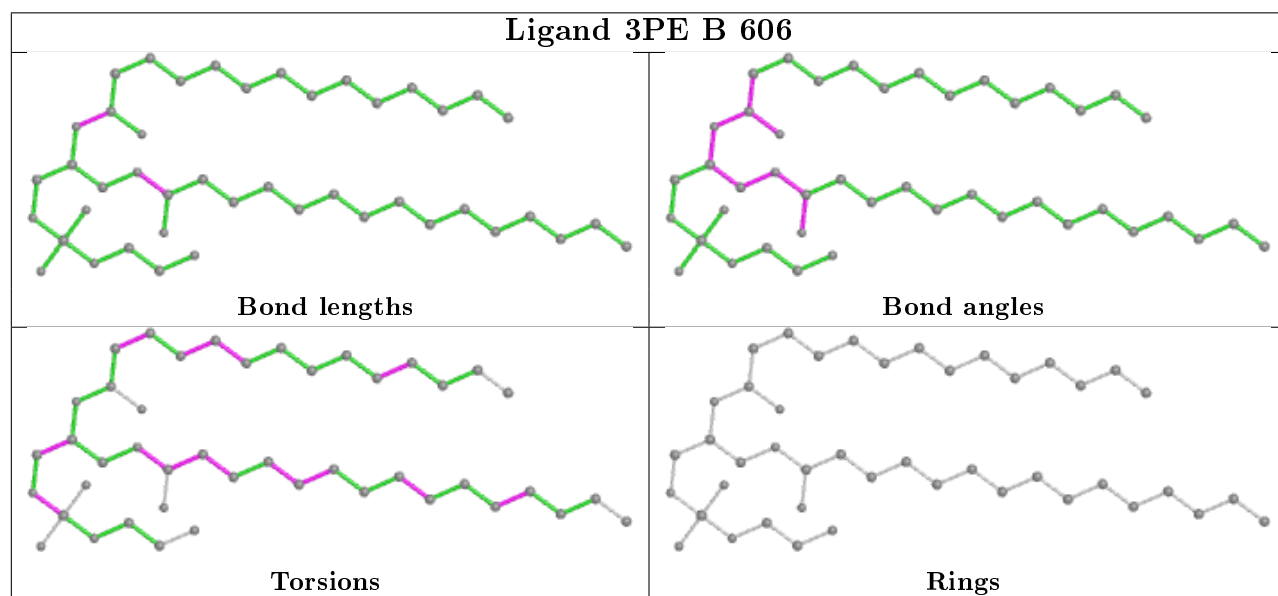
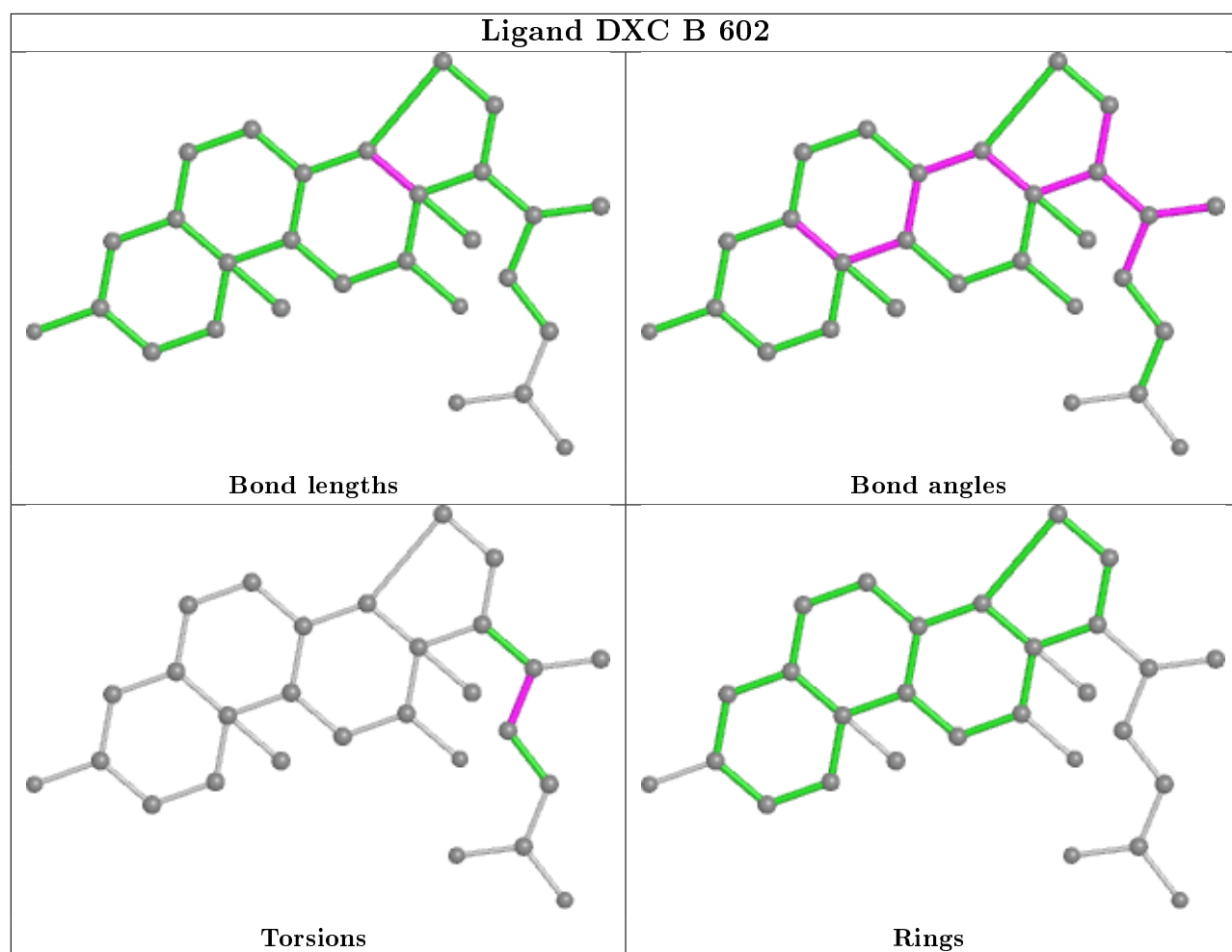




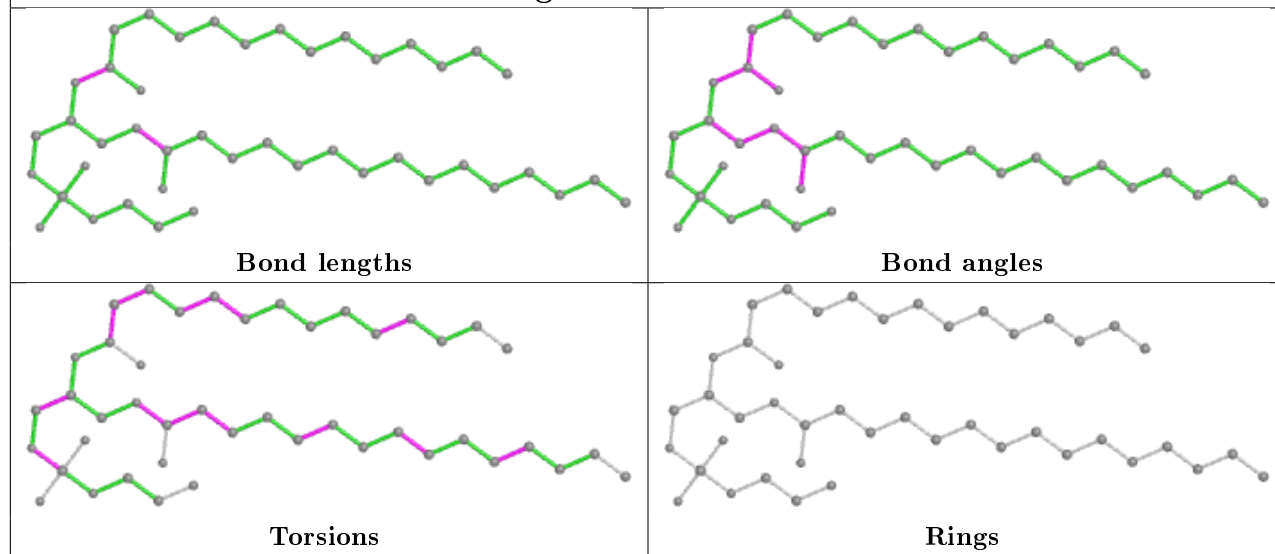




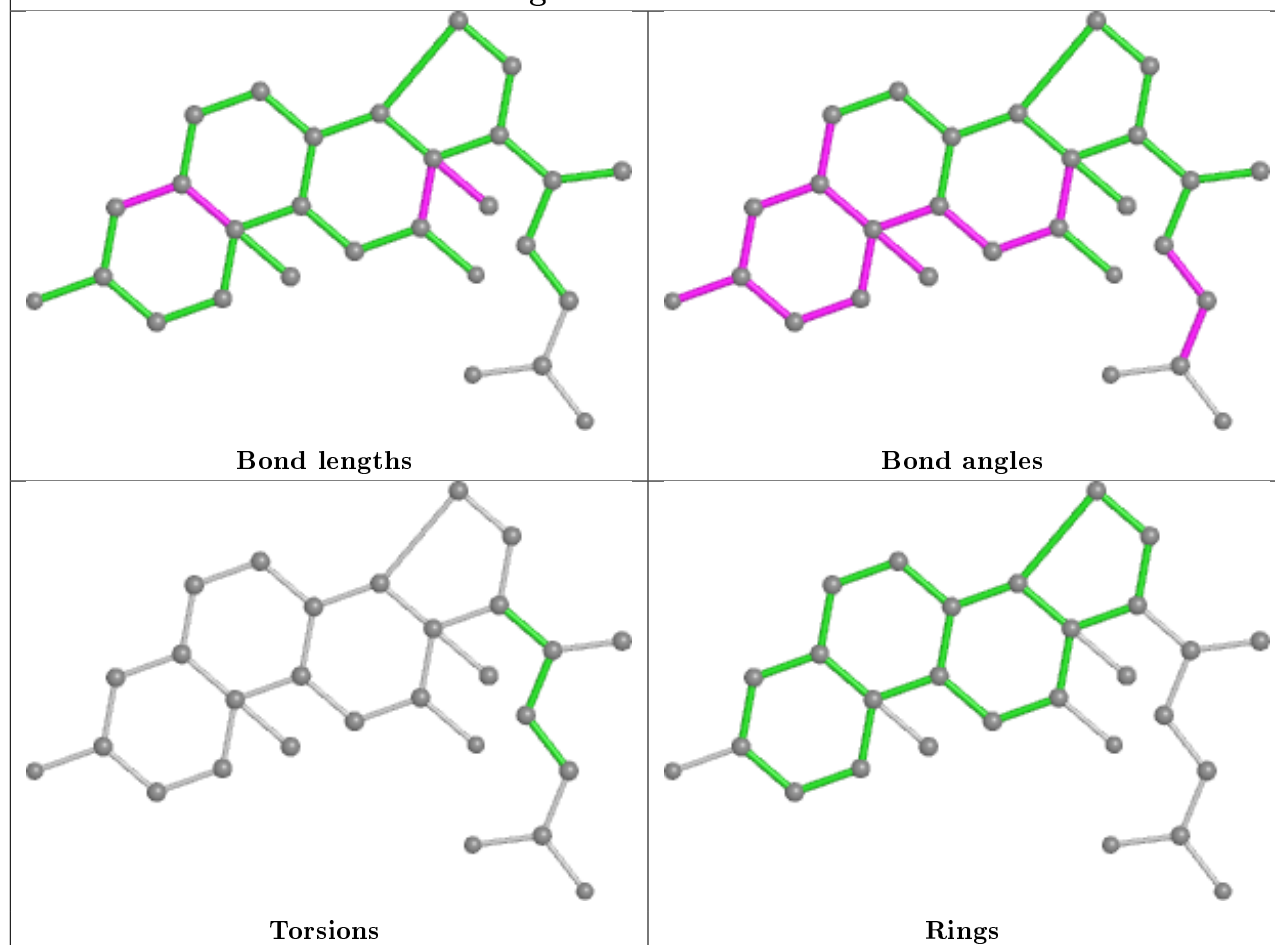




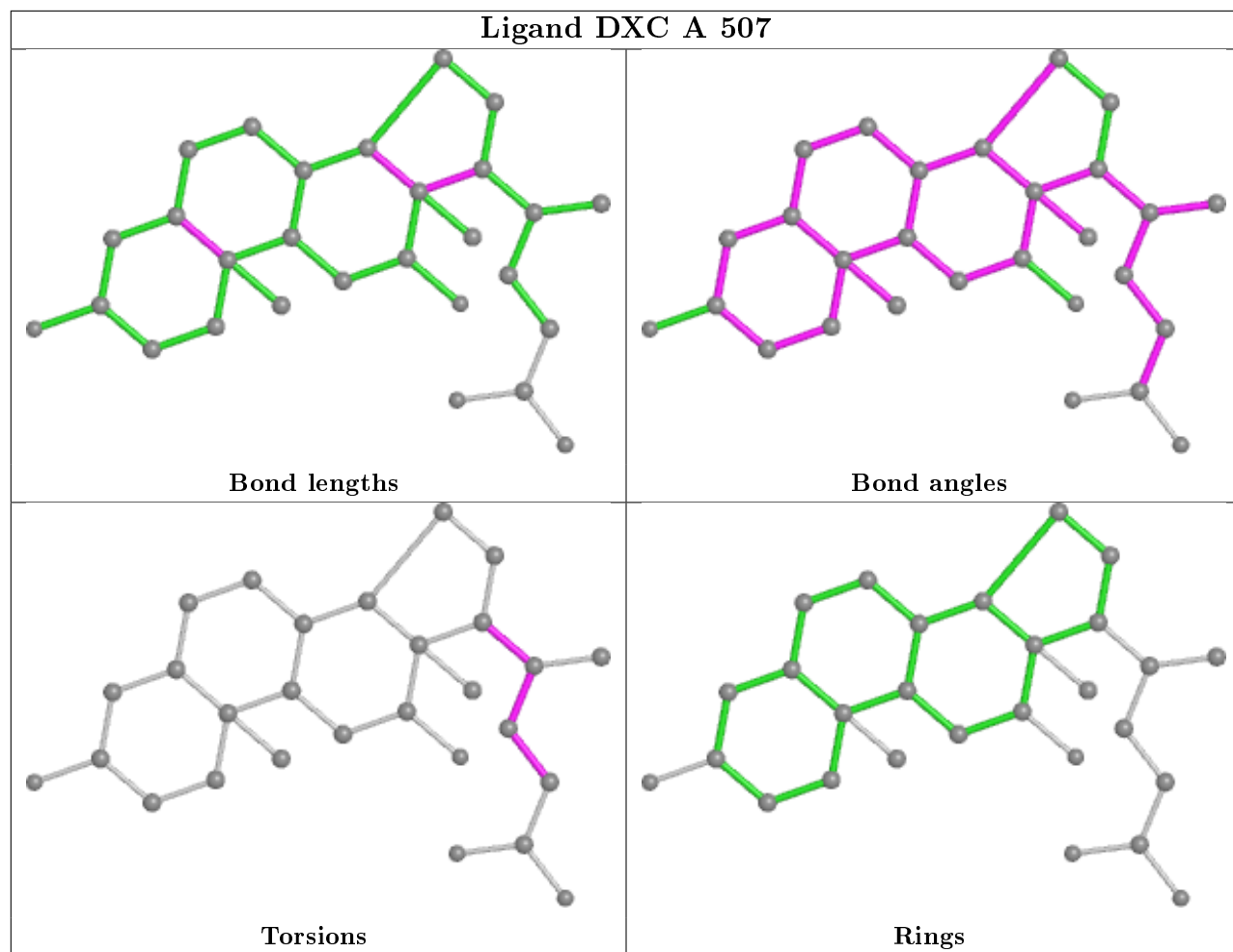
## Ligand 3PE A 503

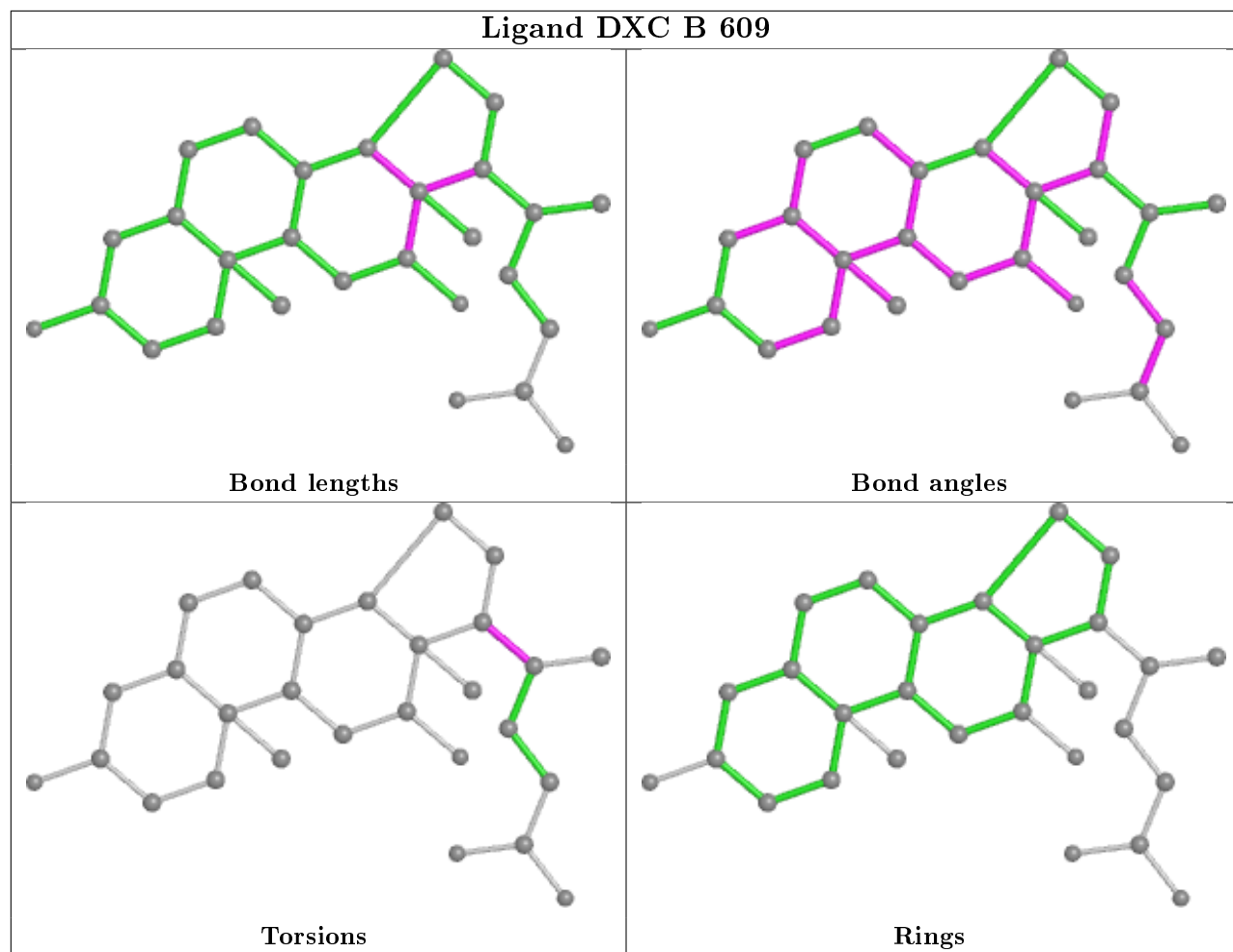


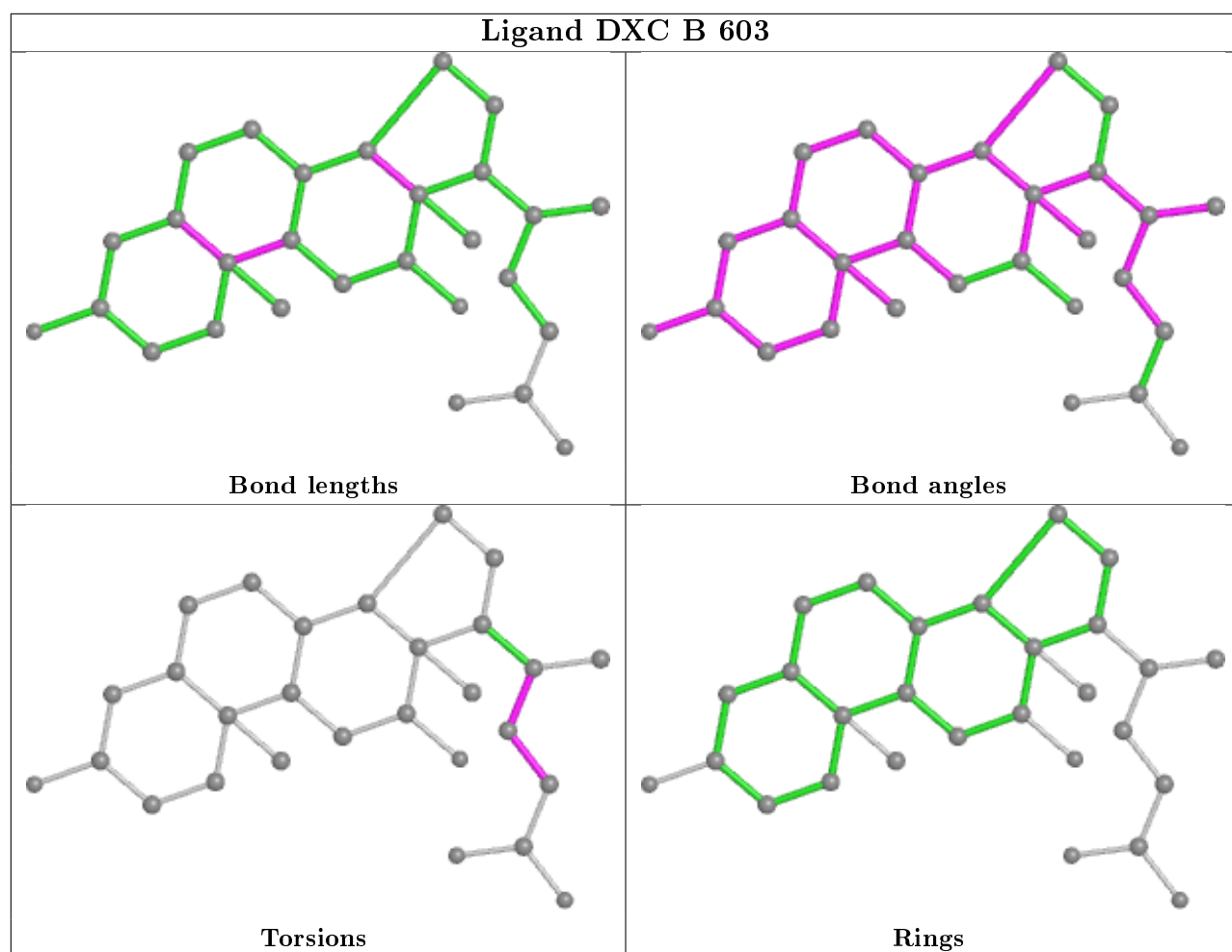
## Ligand DXC B 607











## 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	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

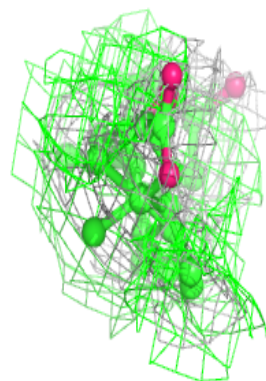
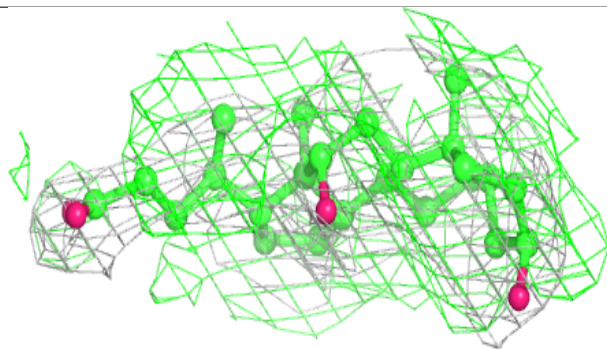
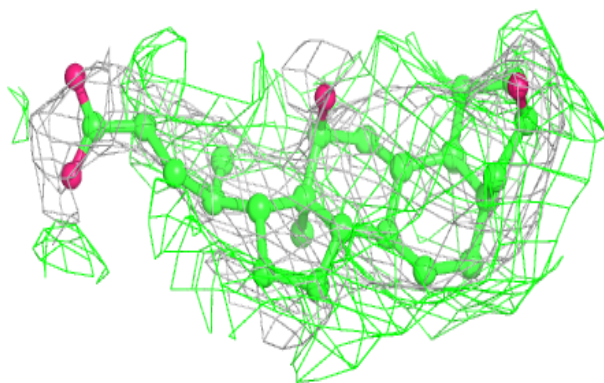
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	DXC	B	610	28/28	0.61	0.44	67,76,81,85	28
4	DXC	B	608	28/28	0.84	0.39	44,58,69,69	28
4	DXC	B	609	28/28	0.84	0.39	49,56,72,75	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	B	607	28/28	0.95	0.23	61,69,73,76	0
4	DXC	B	602	28/28	0.95	0.18	64,73,82,88	0
4	DXC	A	504	28/28	0.95	0.19	63,67,95,100	0
4	DXC	B	601	28/28	0.95	0.22	55,71,79,80	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

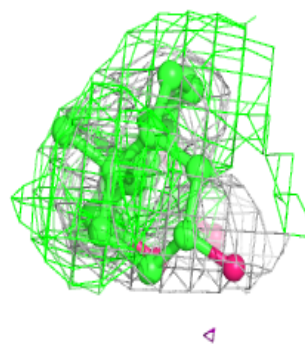
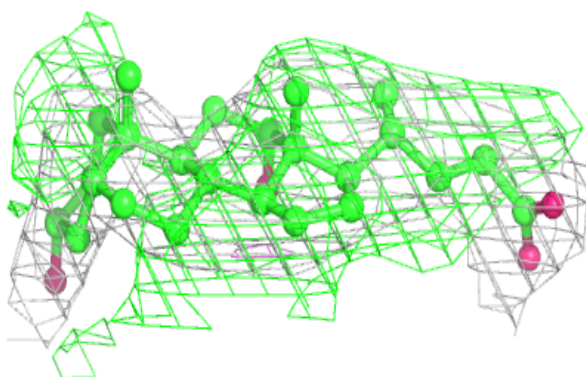
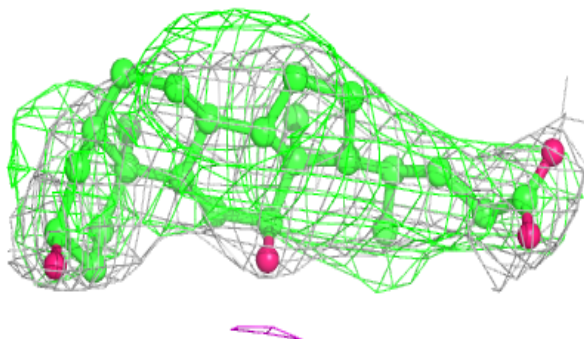
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DXC B 610:**

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

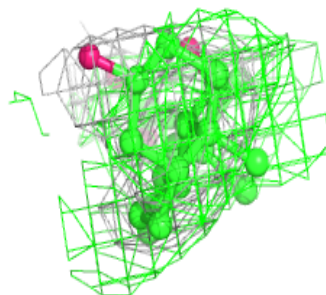
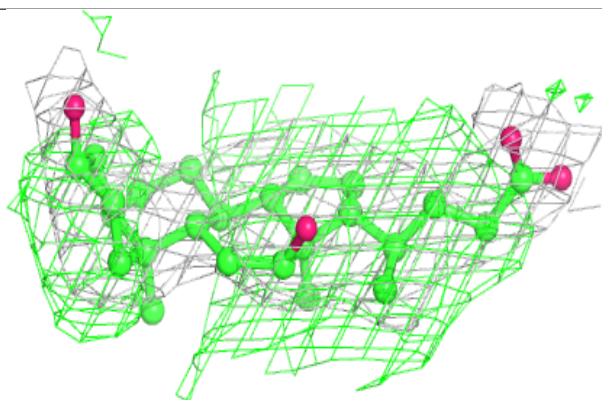
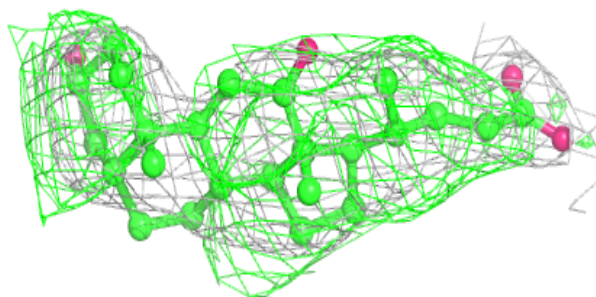
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

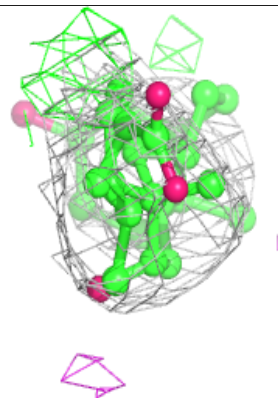
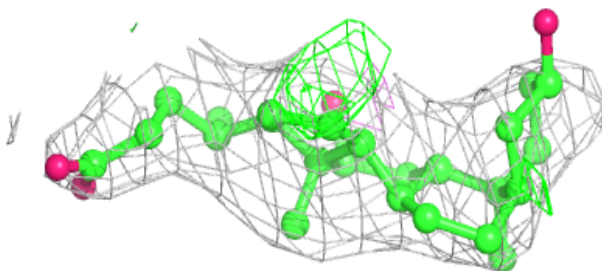
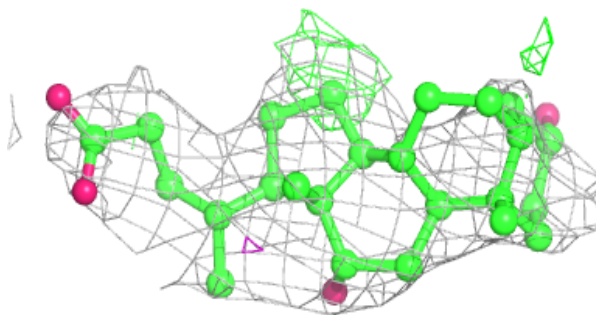


**Electron density around DXC B 609:**

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

**Electron density around DXC A 507:**

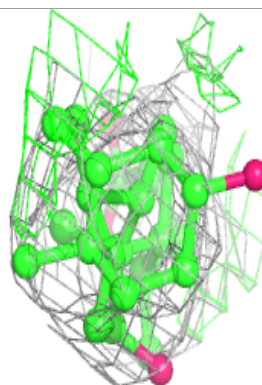
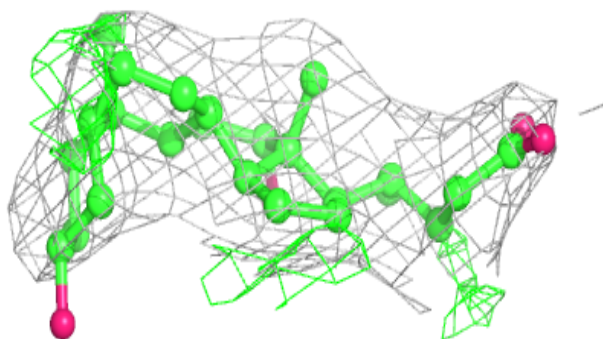
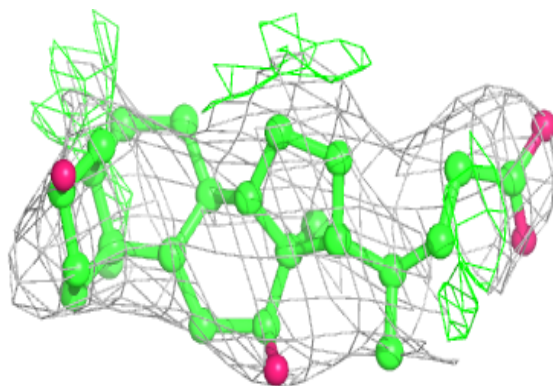
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



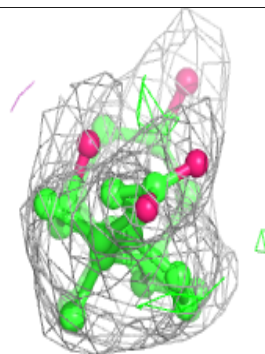
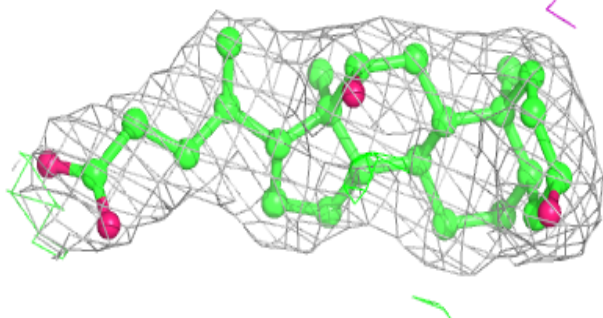
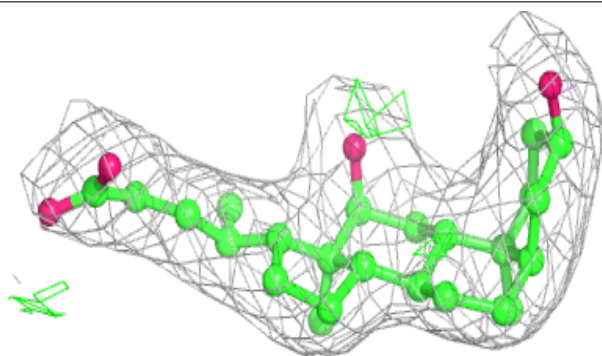


**Electron density around DXC B 603:**

$2mF_o-DF_c$  (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:**

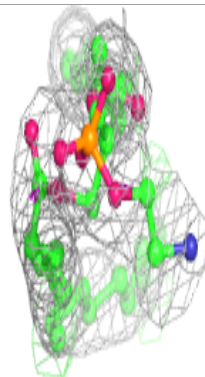
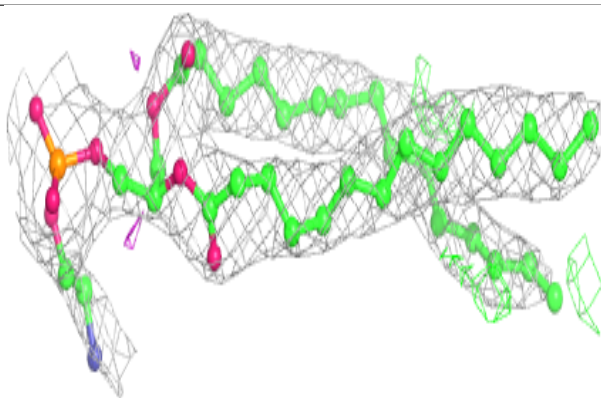
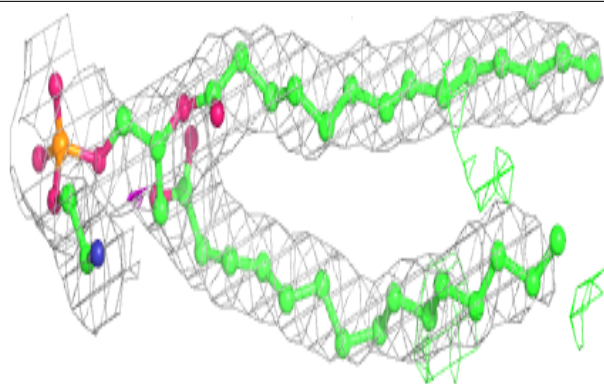
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



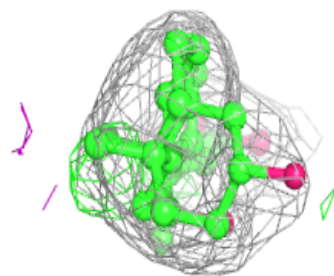
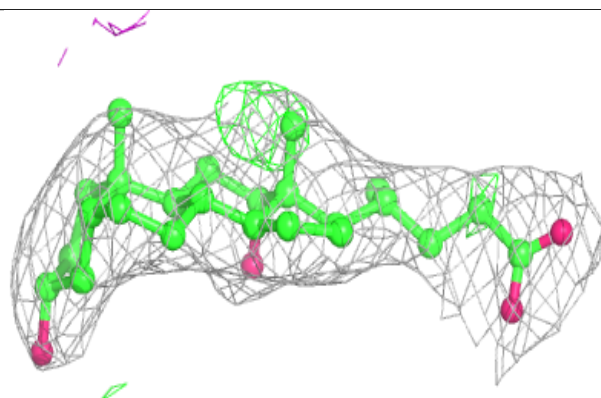
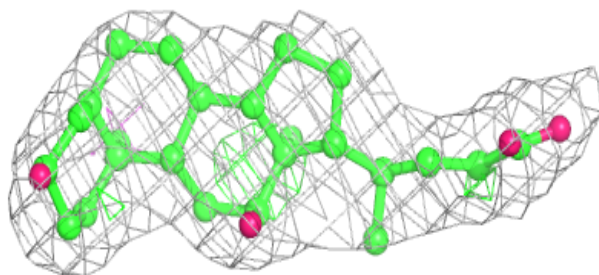


**Electron density around 3PE A 503:**

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

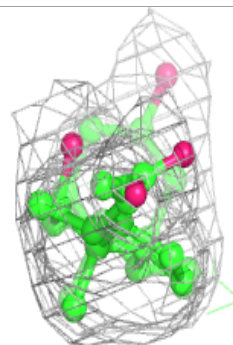
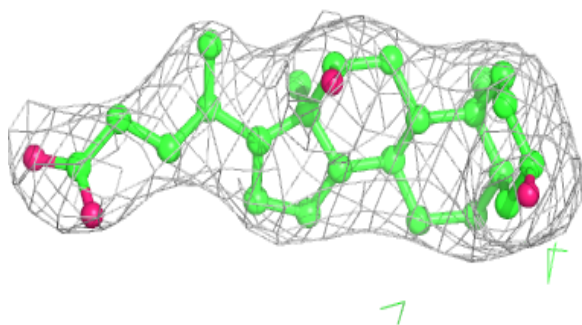
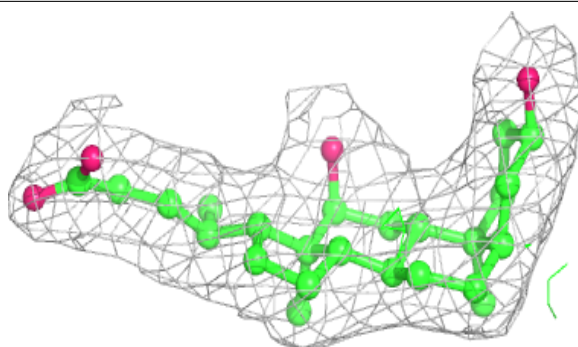
**Electron density around DXC B 607:**

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and green (positive)

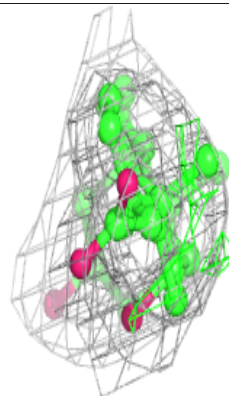
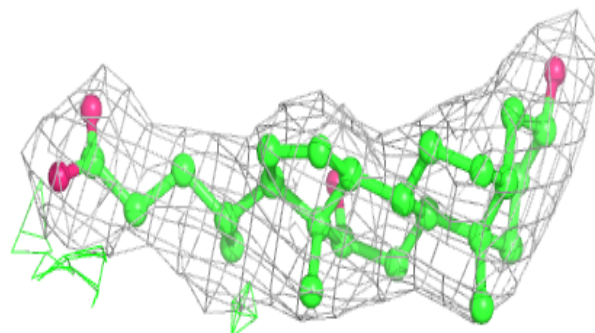
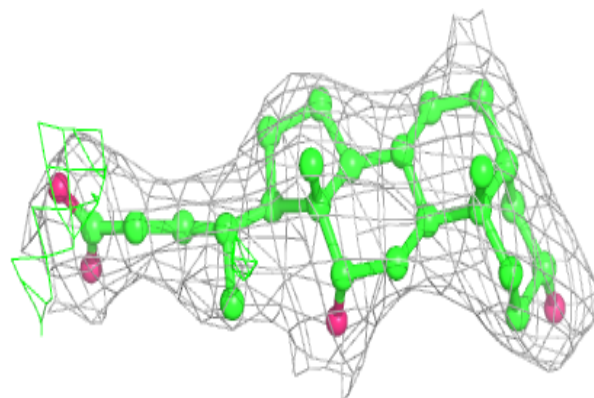


**Electron density around DXC B 602:**

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

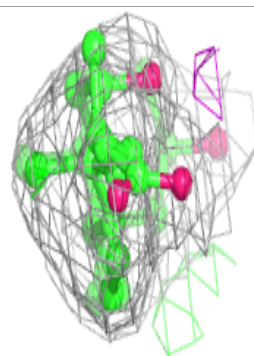
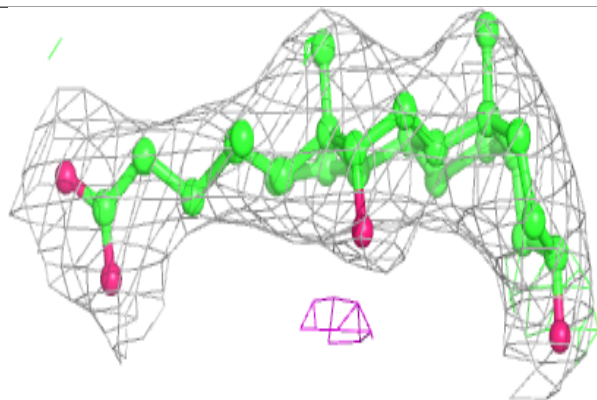
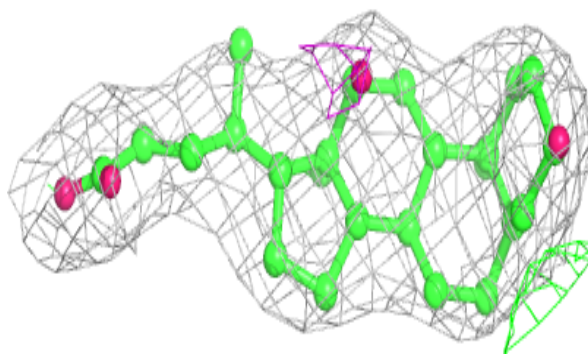
**Electron density around DXC A 504:**

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

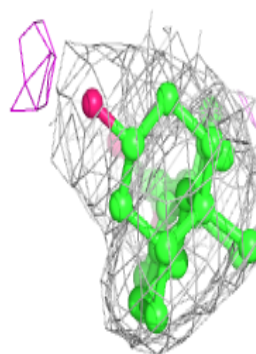
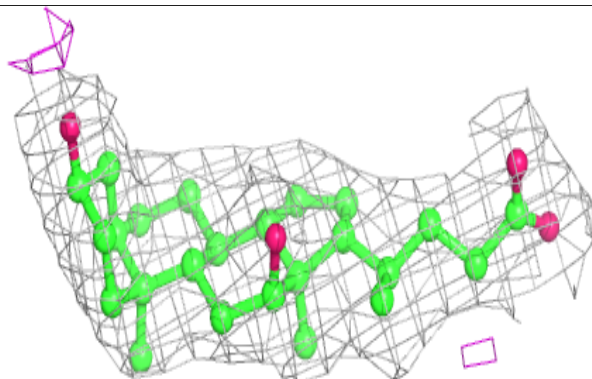
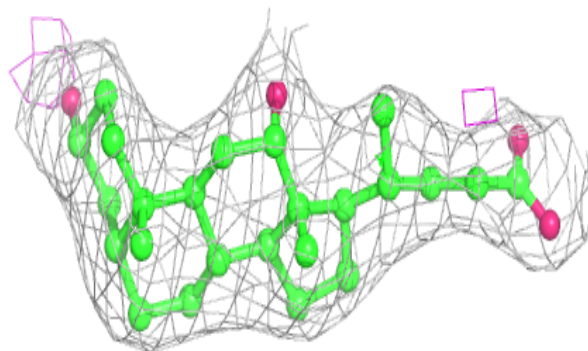


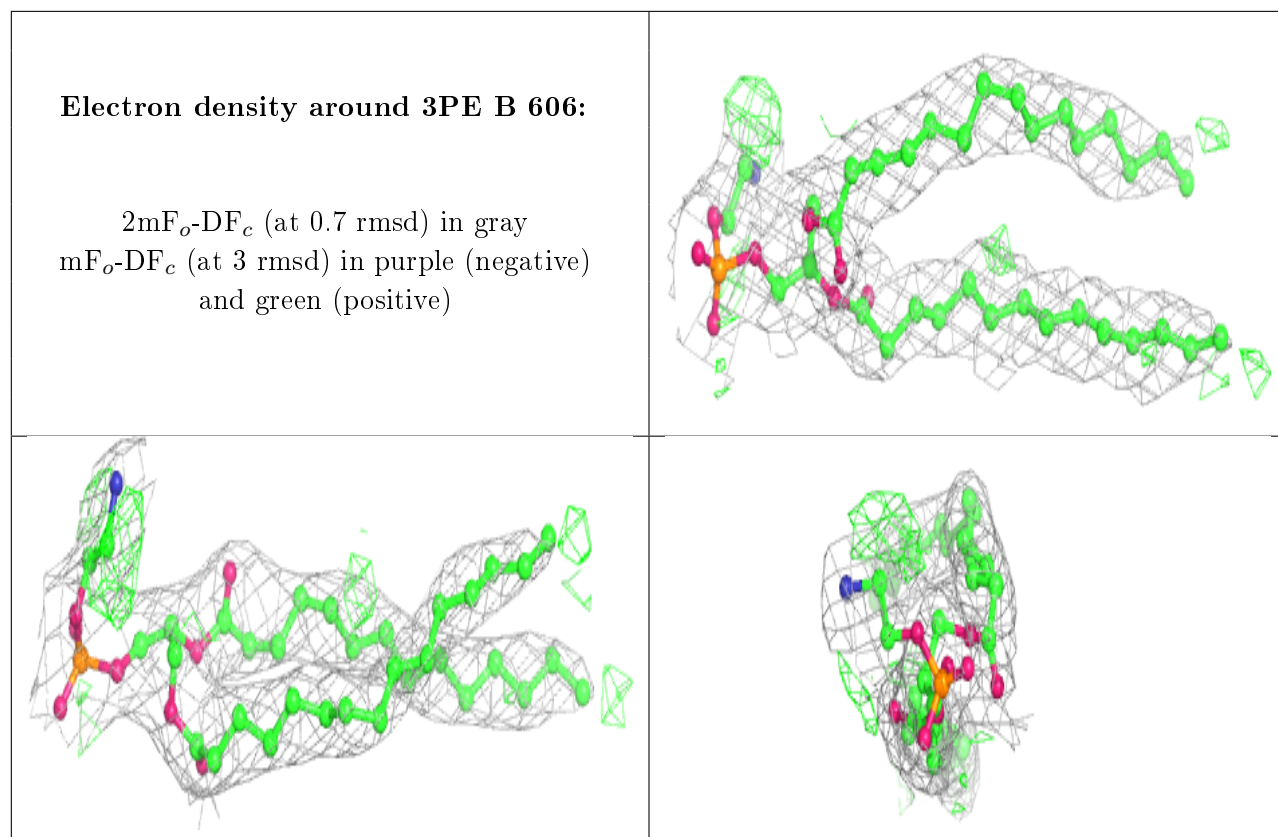
**Electron density around DXC B 601:**

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

**Electron density around DXC A 505:**

$2mF_o-DF_c$  (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.