



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:34 pm BST

PDB ID : 5MVM  
Title : X-ray structure of the F14'A -N15'A double mutant of GLIC in complex with propofol  
Authors : Fourati, Z.; Delarue, M.  
Deposited on : 2017-01-16  
Resolution : 3.10 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](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

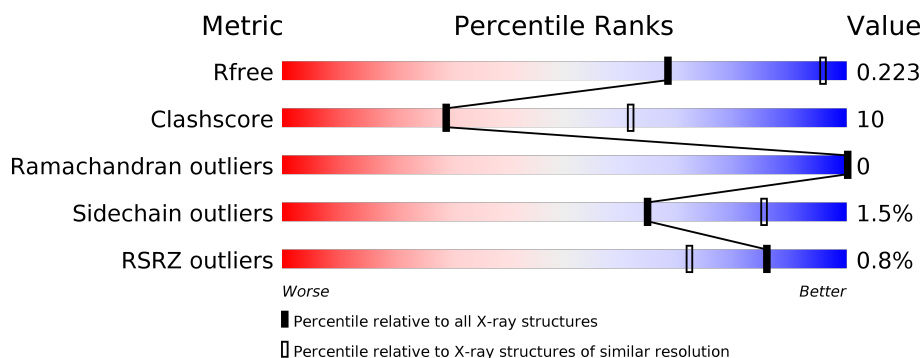
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	317	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>
1	B	317	<div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	C	317	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	D	317	<div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	E	317	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </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	LMT	E	402	-	-	-	X
4	CL	B	503	-	-	-	X
5	NA	E	405	-	-	-	X
6	PLC	A	507	-	-	-	X
6	PLC	A	508	-	-	-	X
6	PLC	B	506	-	-	-	X
6	PLC	B	507	-	-	-	X
6	PLC	B	508	-	-	-	X
6	PLC	C	406	-	-	-	X
6	PLC	D	407	-	-	-	X
6	PLC	E	407	-	-	-	X
7	PFL	A	510	-	-	X	-
7	PFL	A	511	-	-	X	-
7	PFL	B	510	-	-	X	-
7	PFL	C	408	-	-	X	-
7	PFL	E	409	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13400 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.

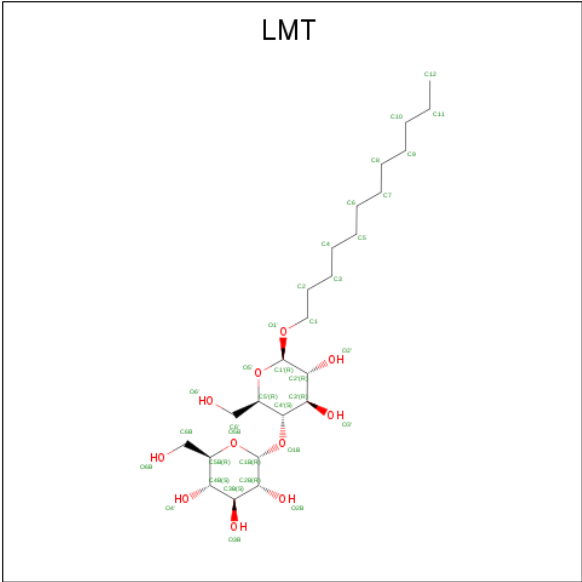
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	2	0
			2534	1668	406	456	4			
1	B	311	Total	C	N	O	S	0	1	0
			2525	1662	404	455	4			
1	C	311	Total	C	N	O	S	0	1	0
			2525	1662	404	455	4			
1	D	311	Total	C	N	O	S	0	2	0
			2533	1666	406	457	4			
1	E	311	Total	C	N	O	S	0	2	0
			2536	1671	405	456	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ALA	PHE	engineered mutation	UNP Q7NDN8
A	239	ALA	ASN	engineered mutation	UNP Q7NDN8
B	238	ALA	PHE	engineered mutation	UNP Q7NDN8
B	239	ALA	ASN	engineered mutation	UNP Q7NDN8
C	238	ALA	PHE	engineered mutation	UNP Q7NDN8
C	239	ALA	ASN	engineered mutation	UNP Q7NDN8
D	238	ALA	PHE	engineered mutation	UNP Q7NDN8
D	239	ALA	ASN	engineered mutation	UNP Q7NDN8
E	238	ALA	PHE	engineered mutation	UNP Q7NDN8
E	239	ALA	ASN	engineered mutation	UNP Q7NDN8

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	13	1		
2	B	1	Total	C	O	0	0
			14	13	1		
2	C	1	Total	C	O	0	0
			14	13	1		
2	D	1	Total	C	O	0	0
			14	13	1		
2	E	1	Total	C		0	0
			12	12			
2	E	1	Total	C	O	0	0
			14	13	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

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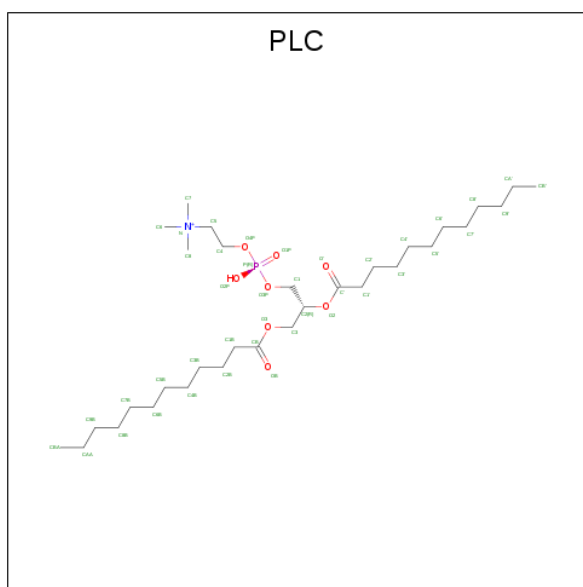
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	A	2	Total	Na	0	0
			2	2		
5	D	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	E	2	Total	Na	0	0
			2	2		

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C<sub>32</sub>H<sub>65</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			34	24	1	8	1		

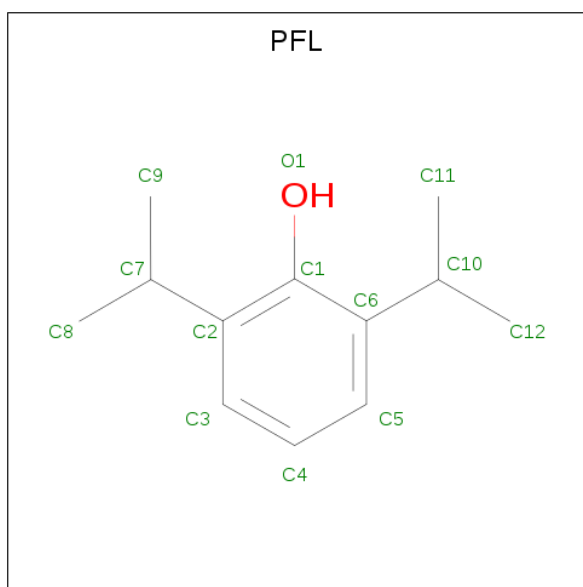
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 24 24	0	0
6	A	1	Total C 12 12	0	0
6	B	1	Total C N O P 34 24 1 8 1	0	0
6	B	1	Total C 24 24	0	0
6	B	1	Total C 12 12	0	0
6	C	1	Total C N O P 34 24 1 8 1	0	0
6	C	1	Total C 24 24	0	0
6	C	1	Total C 12 12	0	0
6	D	1	Total C N O P 34 24 1 8 1	0	0
6	D	1	Total C 24 24	0	0
6	D	1	Total C 12 12	0	0
6	E	1	Total C N O P 34 24 1 8 1	0	0
6	E	1	Total C 24 24	0	0
6	E	1	Total C 12 12	0	0

- Molecule 7 is 2,6-BIS(1-METHYLETHYL)PHENOL (three-letter code: PFL) (formula: C<sub>12</sub>H<sub>18</sub>O).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	12	1		
7	A	1	Total	C	O	0	0
			13	12	1		
7	B	1	Total	C	O	0	0
			13	12	1		
7	C	1	Total	C	O	0	0
			13	12	1		
7	E	1	Total	C	O	0	0
			13	12	1		


- Molecule 8 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	45	Total	O	0	0
			45	45		
8	B	43	Total	O	0	0
			43	43		
8	C	34	Total	O	0	0
			34	34		
8	D	42	Total	O	0	0
			42	42		
8	E	34	Total	O	0	0
			34	34		

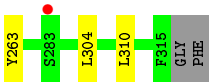
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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:
- 
- 82% 16%
- GLY GLN ASP MET V5 S6 P7 P10 P11 P12 P13 P14 P15 P16 P17 P18 P19 P20 P21 P22 P23 P24 P25 P26 P27 P28 P29 P30 P31 P32 P33 P34 P35 P36 P37 P38 P39 P40 P41 P42 P43 P44 P45 P46 P47 P48 P49 P50 P51 P52 P53 P54 P55 P56 P57 P58 P59 P60 P61 P62 P63 P64 P65 P66 P67 P68 P69 P70 P71 P72 P73 P74 P75 P76 P77 P78 P79 P80 P81 P82 P83 P84 P85 P86 P87 P88 P89 P90 P91 P92 P93 P94 P95 P96 P97 P98 P99 P100 P101 P102 P103 P104 P105 P106 P107 P108 P109 P110 P111 P112 P113 P114 P115 P116 P117 P118 P119 P120 P121 P122 P123 P124 P125 P126 P127 P128 P129 P130 P131 P132 P133 P134 P135 P136 P137 P138 P139 P140 P141 P142 P143 P144 P145 P146 P147 P148 P149 P150 P151 P152 P153 P154 P155 P156 P157 P158 P159 P160 P161 P162 P163 P164 P165 P166 P167 P168 P169 P170 P171 P172 P173 P174 P175 P176 P177 P178 P179 P180 P181 P182 P183 P184 P185 P186 P187 P188 P189 P190 P191 P192 P193 P194 P195 P196 P197 P198 P199 P200

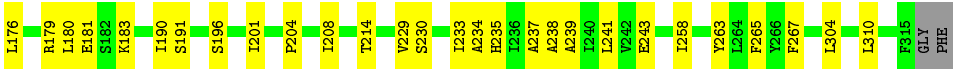
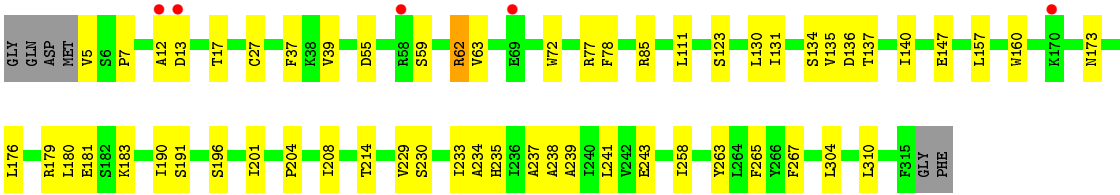
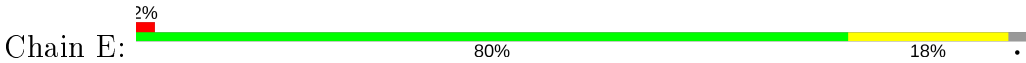
- Chain B:
- 
- 83% 15%
- GLY GLN ASP MET V5 S6 P7 P10 I11 A12 T17 Y28 F37 K38 V39 A53 V63 F78 R85 P96 S123 L126 I131 S134 V135 D136 T137 R138 H139 I140 K148 L157 W160 M173 L176 R179 L180 E181 S182 K183 I190 S191 R192 Q193 I201 M205 L208 T214 V229 V230 A234 E235 I236 A237 A238 A239 I240 L241 V242 E243 I258 L304 L310 F315 GLY PHE

- Chain C: 

- Chain D:  88% 10%
- | Residue | Category |
|---------|----------|
| GLY     | Green    |
| GLN     | Green    |
| ASP     | Green    |
| MET     | Green    |
| V5      | Green    |
| S6      | Green    |
| P7      | Green    |
| P10     | Green    |
| I11     | Green    |
| A12     | Green    |
| T17     | Green    |
| V39     | Green    |
| I72     | Green    |
| F78     | Green    |
| E82     | Green    |
| R85     | Green    |
| R109    | Green    |
| S123    | Green    |
| I131    | Green    |
| S134    | Green    |
| V135    | Green    |
| D136    | Green    |
| T137    | Green    |
| I140    | Green    |
| L176    | Green    |
| E181    | Green    |
| S182    | Green    |
| K183    | Green    |
| S191    | Green    |
| F207    | Green    |
| T214    | Green    |
| V229    | Green    |
| S230    | Green    |
| I233    | Green    |
| A239    | Green    |
| E243    | Green    |
| I258    | Green    |



● Molecule 1: Proton-gated ion channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.76Å 132.51Å 160.52Å 90.00° 102.72° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-3.10) 98.4 (19.97-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.09Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.195 , 0.208 0.212 , 0.223	Depositor DCC
$R_{free}$ test set	3345 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 79.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, LMT, PFL, PLC, ACT

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	0.50	0/2601	0.68	0/3555
1	B	0.51	0/2592	0.70	0/3544
1	C	0.50	0/2592	0.69	0/3544
1	D	0.50	0/2600	0.69	0/3555
1	E	0.50	0/2604	0.69	0/3560
All	All	0.50	0/12989	0.69	0/17758

There are no bond length outliers.

There are no bond angle outliers.

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	2534	0	2557	53	0
1	B	2525	0	2545	80	0
1	C	2525	0	2545	29	0
1	D	2533	0	2550	41	0
1	E	2536	0	2553	67	0
2	A	14	0	25	1	0
2	B	14	0	25	0	0
2	C	14	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	14	0	25	0	0
2	E	26	0	48	5	0
3	A	8	0	6	1	0
3	B	12	0	9	0	0
3	C	4	0	3	0	0
3	D	12	0	9	0	0
3	E	4	0	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
6	A	70	0	111	1	0
6	B	70	0	111	1	0
6	C	70	0	111	3	0
6	D	70	0	111	1	0
6	E	70	0	111	1	0
7	A	26	0	35	44	0
7	B	13	0	17	27	0
7	C	13	0	17	13	0
7	E	13	0	17	7	0
8	A	45	0	0	7	0
8	B	43	0	0	7	0
8	C	34	0	0	5	0
8	D	42	0	0	3	0
8	E	34	0	0	8	0
All	All	13400	0	13569	256	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 10.

All (256) 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:241:LEU:CD2	7:B:510:PFL:H82	1.33	1.55
1:D:207:PHE:HB3	1:E:267[B]:PHE:CE1	1.40	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:404:PLC:H73	8:C:516:HOH:O	1.15	1.31
1:E:265:PHE:HB3	8:E:518:HOH:O	1.17	1.28
7:A:511:PFL:C11	1:B:243:GLU:HG3	1.67	1.25
1:E:111:LEU:HB2	8:E:501:HOH:O	1.32	1.24
1:A:201:ILE:HD13	7:A:511:PFL:O1	1.11	1.22
1:D:207:PHE:CB	1:E:267[B]:PHE:CE1	2.27	1.17
1:A:201:ILE:CD1	7:A:511:PFL:O1	1.93	1.14
7:A:511:PFL:H111	1:B:243:GLU:OE1	1.44	1.13
1:B:241:LEU:CD2	7:B:510:PFL:C8	2.26	1.13
8:D:538:HOH:O	7:E:409:PFL:H111	1.49	1.10
1:B:241:LEU:HD21	7:B:510:PFL:C8	1.82	1.09
1:D:207:PHE:HB3	1:E:267[B]:PHE:CZ	1.88	1.08
1:C:315:PHE:C	8:C:516:HOH:O	1.95	1.05
1:D:207:PHE:HB3	1:E:267[B]:PHE:CD1	1.92	1.05
7:A:511:PFL:H113	1:B:243:GLU:HG3	1.30	1.04
7:A:510:PFL:H91	8:E:524:HOH:O	1.60	1.00
1:D:207:PHE:CB	1:E:267[B]:PHE:CZ	2.44	1.00
1:B:238:ALA:CB	7:B:510:PFL:H123	1.94	0.98
1:B:241:LEU:CG	7:B:510:PFL:H82	1.94	0.98
1:B:241:LEU:HD21	7:B:510:PFL:H82	0.97	0.96
1:A:243:GLU:CD	7:A:510:PFL:H83	1.84	0.96
7:C:408:PFL:HC5	1:D:239:ALA:CB	1.96	0.95
1:A:248:LYS:HE2	8:A:636:HOH:O	1.66	0.95
1:B:39:VAL:HB	8:B:636:HOH:O	1.68	0.94
1:B:241:LEU:HD23	7:B:510:PFL:H82	1.47	0.94
7:C:408:PFL:C11	1:D:243:GLU:HG3	1.99	0.92
1:B:238:ALA:HB1	7:B:510:PFL:C12	1.99	0.92
1:A:243:GLU:HB3	8:A:629:HOH:O	1.70	0.91
6:C:404:PLC:C7	8:C:516:HOH:O	1.85	0.91
1:E:62:ARG:CG	1:E:62:ARG:HH11	1.83	0.90
1:B:238:ALA:CB	7:B:510:PFL:C12	2.48	0.90
8:A:609:HOH:O	1:E:196:SER:HB3	1.74	0.87
1:E:263:TYR:O	1:E:267[B]:PHE:CD2	2.27	0.87
7:C:408:PFL:H113	1:D:243:GLU:HG3	1.55	0.86
1:E:62:ARG:HG3	1:E:62:ARG:HH11	1.43	0.84
7:A:511:PFL:C11	1:B:243:GLU:CG	2.51	0.84
1:B:37:PHE:CE2	1:B:39:VAL:CG2	2.61	0.84
1:B:239:ALA:O	1:B:243:GLU:HG2	1.78	0.83
1:B:201:ILE:HG12	7:B:510:PFL:HC7	1.59	0.83
7:C:408:PFL:HC5	1:D:239:ALA:HB1	1.61	0.81
7:C:408:PFL:HC5	1:D:239:ALA:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:HB3	8:B:634:HOH:O	1.81	0.79
1:A:239:ALA:HB1	7:A:510:PFL:H82	1.65	0.79
7:C:408:PFL:C11	1:D:243:GLU:CG	2.61	0.79
7:A:511:PFL:HC5	1:B:239:ALA:HB3	1.65	0.78
1:B:238:ALA:HB1	7:B:510:PFL:H123	1.63	0.77
1:A:136:ASP:OD1	1:E:63:VAL:HB	1.84	0.77
7:A:511:PFL:HC5	1:B:239:ALA:CB	2.14	0.77
1:D:207:PHE:CD2	1:E:267[B]:PHE:CE2	2.73	0.76
1:B:138:ARG:HB2	8:B:620:HOH:O	1.84	0.76
1:B:37:PHE:HE2	1:B:39:VAL:CG2	1.98	0.75
1:D:207:PHE:HB2	1:E:267[B]:PHE:CZ	2.22	0.75
1:D:10:PRO:HB2	1:D:12:ALA:O	1.86	0.75
1:A:10:PRO:HB2	1:A:12:ALA:O	1.87	0.74
1:B:10:PRO:HB2	1:B:12:ALA:O	1.88	0.74
7:C:408:PFL:H113	1:D:243:GLU:CG	2.18	0.73
1:A:243:GLU:OE1	7:A:510:PFL:H83	1.88	0.72
1:C:10:PRO:HB2	1:C:12:ALA:O	1.89	0.72
1:E:111:LEU:CB	8:E:501:HOH:O	2.09	0.71
1:E:263:TYR:HB3	1:E:267[B]:PHE:HE2	1.55	0.71
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.25	0.71
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.26	0.71
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.72	0.70
1:B:238:ALA:HB1	7:B:510:PFL:H121	1.73	0.70
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.56	0.70
1:A:131:ILE:HD13	3:A:504:ACT:H2	1.74	0.70
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.26	0.70
1:B:37:PHE:HE2	1:B:39:VAL:HG21	1.57	0.70
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.26	0.70
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.57	0.70
1:E:111:LEU:HD22	8:E:501:HOH:O	1.90	0.69
1:D:207:PHE:HD2	1:E:267[B]:PHE:CE2	2.09	0.69
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.74	0.69
1:E:77:ARG:O	1:E:131:ILE:HG22	1.92	0.69
7:C:408:PFL:H111	1:D:243:GLU:HG3	1.73	0.68
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.76	0.68
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.27	0.68
1:A:204:PRO:HB2	7:A:511:PFL:H82	1.76	0.68
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.57	0.68
1:A:196:SER:CB	8:B:634:HOH:O	2.37	0.68
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.57	0.68
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:407:LMT:H92	2:E:401:LMT:H72	1.76	0.68
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.57	0.68
7:A:511:PFL:H111	1:B:243:GLU:CD	2.12	0.68
1:E:239:ALA:CB	7:E:409:PFL:HC5	2.24	0.68
1:D:5:VAL:HG12	1:D:72:TRP:HB2	1.75	0.67
1:E:239:ALA:HB3	7:E:409:PFL:HC5	1.77	0.67
1:B:37:PHE:CE2	1:B:39:VAL:HG21	2.29	0.67
1:B:238:ALA:CB	7:B:510:PFL:H121	2.23	0.66
1:B:238:ALA:HB2	7:B:510:PFL:C12	2.25	0.66
1:A:239:ALA:CB	7:A:510:PFL:HC3	2.26	0.66
1:A:238:ALA:HB2	7:A:511:PFL:H91	1.78	0.65
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.78	0.65
1:E:5:VAL:HG12	1:E:72:TRP:HB2	1.77	0.65
7:B:510:PFL:H122	7:B:510:PFL:O1	1.97	0.65
1:C:5:VAL:HG12	1:C:72:TRP:HB2	1.78	0.65
1:E:239:ALA:HB1	7:E:409:PFL:H112	1.78	0.64
1:B:201:ILE:HG23	7:B:510:PFL:O1	1.97	0.64
7:A:510:PFL:H112	1:E:204:PRO:HB2	1.80	0.63
1:B:241:LEU:HD23	7:B:510:PFL:C8	2.13	0.63
1:B:136:ASP:OD1	1:B:179:ARG:NH2	2.33	0.62
1:D:230:SER:CB	1:E:229:VAL:HG11	2.30	0.61
7:A:511:PFL:H112	1:B:243:GLU:HG3	1.78	0.61
1:A:201:ILE:HA	7:A:511:PFL:H83	1.82	0.61
7:A:511:PFL:H112	1:B:239:ALA:HB1	1.81	0.61
1:B:193:GLN:O	8:B:601:HOH:O	2.16	0.60
7:B:510:PFL:C12	7:B:510:PFL:O1	2.50	0.60
1:E:111:LEU:CD2	8:E:501:HOH:O	2.48	0.60
1:A:134:SER:HA	1:A:140:ILE:HD12	1.84	0.59
1:A:236:ILE:HG23	7:A:510:PFL:HC5	1.84	0.59
7:C:408:PFL:H111	1:D:243:GLU:CG	2.31	0.59
1:C:292:THR:HG23	8:C:515:HOH:O	2.03	0.58
7:C:408:PFL:H112	1:D:239:ALA:HB1	1.84	0.58
7:A:510:PFL:H81	8:A:629:HOH:O	2.02	0.58
1:B:238:ALA:CA	7:B:510:PFL:H123	2.34	0.58
1:A:244:THR:HG21	2:E:402:LMT:H21	1.86	0.58
1:E:214:THR:HG22	6:E:407:PLC:H3'1	1.86	0.58
7:A:510:PFL:H113	1:E:201:ILE:HA	1.86	0.58
1:C:134:SER:HA	1:C:140:ILE:HD12	1.86	0.58
1:E:62:ARG:NH1	1:E:62:ARG:HG3	2.14	0.58
1:E:62:ARG:HG2	1:E:62:ARG:HH11	1.65	0.58
7:A:510:PFL:H121	1:E:238:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ILE:HD11	8:E:507:HOH:O	2.04	0.57
1:B:37:PHE:CE2	1:B:39:VAL:HG23	2.39	0.56
1:E:263:TYR:O	1:E:267[B]:PHE:HD2	1.85	0.55
1:E:37:PHE:CE2	1:E:39:VAL:CG2	2.89	0.54
1:E:134:SER:HA	1:E:140:ILE:HD12	1.89	0.54
1:B:230:SER:CB	1:C:229:VAL:HG11	2.38	0.54
1:D:176:LEU:HB3	1:D:181:GLU:HG3	1.90	0.54
1:A:237:ALA:HA	2:A:501:LMT:H92	1.90	0.54
1:B:134:SER:HA	1:B:140:ILE:HD12	1.90	0.54
7:C:408:PFL:C11	1:D:243:GLU:HG2	2.37	0.54
1:B:241:LEU:HD21	7:B:510:PFL:C7	2.38	0.53
1:B:241:LEU:CG	7:B:510:PFL:C8	2.76	0.53
1:B:201:ILE:HG12	7:B:510:PFL:C7	2.33	0.53
1:D:230:SER:HB3	1:E:229:VAL:CG1	2.38	0.53
1:D:5:VAL:CG1	1:D:72:TRP:HB2	2.39	0.53
1:B:201:ILE:CG1	7:B:510:PFL:HC7	2.35	0.53
1:A:239:ALA:HB3	7:A:510:PFL:HC3	1.90	0.53
1:D:134:SER:HA	1:D:140:ILE:HD12	1.91	0.53
7:A:511:PFL:HC3	1:B:236:ILE:HG23	1.91	0.52
1:A:61:VAL:HG12	1:A:63:VAL:H	1.75	0.52
1:D:207:PHE:C	1:E:267[B]:PHE:CE1	2.83	0.52
7:A:510:PFL:H92	1:E:204:PRO:HG2	1.92	0.52
1:E:12:ALA:O	1:E:13:ASP:HB3	2.09	0.52
1:A:230:SER:CB	1:B:229:VAL:HG11	2.40	0.52
1:B:258:ILE:HD13	1:B:310:LEU:HD13	1.92	0.51
1:E:208:ILE:HD13	1:E:234:ALA:HB3	1.92	0.51
1:C:208:ILE:HD13	1:C:234:ALA:HB3	1.91	0.51
1:A:263:TYR:HE2	7:A:510:PFL:H93	1.74	0.51
7:A:511:PFL:H111	1:B:243:GLU:CG	2.34	0.51
1:E:258:ILE:HD13	1:E:310:LEU:HD13	1.93	0.51
1:B:205:MET:HE2	1:B:238:ALA:HB1	1.92	0.51
1:C:258:ILE:HD13	1:C:310:LEU:HD13	1.92	0.51
1:A:258:ILE:HD13	1:A:310:LEU:HD13	1.91	0.51
7:A:511:PFL:HC5	1:B:239:ALA:HB1	1.92	0.50
1:C:27:CYS:HB3	1:C:157:LEU:HD13	1.93	0.50
1:D:207:PHE:C	1:E:267[B]:PHE:HE1	2.15	0.50
1:A:263:TYR:CE2	7:A:510:PFL:H93	2.45	0.50
1:D:258:ILE:HD13	1:D:310:LEU:HD13	1.93	0.50
1:A:5:VAL:HG22	1:A:72:TRP:HB2	1.94	0.50
1:C:5:VAL:CG1	1:C:72:TRP:HB2	2.41	0.49
1:A:241:LEU:HD22	1:B:240:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:TYR:HE2	7:E:409:PFL:H123	1.78	0.49
1:C:82:GLU:HG3	1:C:109:ARG:HB3	1.94	0.49
8:D:511:HOH:O	7:E:409:PFL:H121	2.12	0.49
1:E:173:ASN:HB3	1:E:180:LEU:HD11	1.95	0.49
1:E:5:VAL:CG1	1:E:72:TRP:HB2	2.41	0.48
7:A:510:PFL:C8	8:A:629:HOH:O	2.59	0.48
1:C:201:ILE:HA	7:C:408:PFL:HC7	1.95	0.48
1:C:176:LEU:HB3	1:C:181:GLU:HG3	1.96	0.48
1:C:196:SER:HB3	8:D:517:HOH:O	2.13	0.48
1:B:241:LEU:HG	7:B:510:PFL:C8	2.43	0.48
1:E:237:ALA:HA	2:E:402:LMT:H92	1.95	0.48
1:A:196:SER:HA	8:B:634:HOH:O	2.13	0.48
1:A:236:ILE:O	7:A:510:PFL:HC4	2.14	0.48
1:A:229:VAL:HG11	1:E:230:SER:CB	2.43	0.48
1:B:63:VAL:HG21	1:C:136:ASP:OD2	2.14	0.48
1:C:292:THR:CG2	8:C:515:HOH:O	2.61	0.47
1:E:176:LEU:HB3	1:E:181:GLU:HG3	1.96	0.47
1:E:263:TYR:O	1:E:267[B]:PHE:CE2	2.67	0.47
1:B:131:ILE:HD12	1:B:183:LYS:HB2	1.95	0.47
1:D:230:SER:CB	1:E:229:VAL:CG1	2.93	0.47
1:B:208:ILE:HD13	1:B:234:ALA:HB3	1.96	0.47
1:D:131:ILE:HD12	1:D:183:LYS:HB2	1.97	0.47
1:B:148:LYS:HE3	1:C:177:GLU:HB3	1.97	0.47
1:A:151:LYS:NZ	8:A:604:HOH:O	2.47	0.46
1:B:28:TYR:HA	1:B:157:LEU:HD12	1.97	0.46
1:E:27:CYS:HB3	1:E:157:LEU:HD13	1.97	0.46
1:A:82:GLU:HG3	1:A:109:ARG:HB3	1.97	0.46
1:E:136:ASP:OD2	1:E:179:ARG:NH2	2.48	0.46
2:E:401:LMT:H42	2:E:402:LMT:H62	1.97	0.46
1:A:141:VAL:HG12	8:A:613:HOH:O	2.15	0.46
1:A:173:ASN:HB3	1:A:180:LEU:HD11	1.96	0.46
1:B:238:ALA:HA	7:B:510:PFL:H123	1.98	0.46
7:A:511:PFL:C11	1:B:243:GLU:CD	2.80	0.45
1:E:7:PRO:CG	1:E:137:THR:OG1	2.64	0.45
1:B:160:TRP:CE3	1:B:190:ILE:HD12	2.51	0.45
2:C:407:LMT:H72	2:E:401:LMT:H52	1.98	0.45
1:A:239:ALA:HB1	7:A:510:PFL:HC3	1.97	0.45
1:A:238:ALA:HB2	7:A:511:PFL:C9	2.45	0.45
1:B:123:SER:HA	1:B:191:SER:HA	1.99	0.44
1:C:7:PRO:CG	1:C:137:THR:OG1	2.66	0.44
1:C:26[B]:GLU:HB2	1:C:40:ASN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:HB3	1:B:180:LEU:HD11	1.99	0.44
1:C:230:SER:CB	1:D:229:VAL:HG11	2.48	0.44
7:C:408:PFL:H123	1:D:263:TYR:HE2	1.83	0.44
1:B:7:PRO:CG	1:B:137:THR:OG1	2.66	0.44
1:D:82:GLU:HG3	1:D:109:ARG:HB3	1.99	0.44
1:B:176:LEU:HB3	1:B:181:GLU:HG3	1.99	0.44
1:A:26[B]:GLU:HB2	1:A:40:ASN:HB3	1.99	0.44
1:A:240:ILE:HG13	7:A:510:PFL:C4	2.48	0.44
1:A:232:LEU:HD21	1:E:208:ILE:HG22	1.99	0.44
1:A:236:ILE:HG23	7:A:510:PFL:C5	2.46	0.43
1:B:214:THR:HG22	6:B:507:PLC:H3'1	1.99	0.43
1:D:214:THR:HG22	6:D:407:PLC:H3'1	2.00	0.43
1:E:239:ALA:HB1	7:E:409:PFL:HC5	1.99	0.43
1:C:214:THR:HG22	6:C:405:PLC:H3'1	2.00	0.43
1:A:200:ASN:O	7:A:511:PFL:H10	2.18	0.43
1:C:123:SER:HA	1:C:191:SER:HA	2.01	0.43
1:A:214:THR:HG22	6:A:507:PLC:H3'1	2.01	0.42
1:A:61:VAL:CG1	1:A:63:VAL:O	2.67	0.42
1:B:238:ALA:HB2	7:B:510:PFL:H123	1.86	0.42
1:E:123:SER:HA	1:E:191:SER:HA	2.01	0.42
1:C:173:ASN:HB3	1:C:180:LEU:HD11	2.01	0.42
1:A:240:ILE:HG12	1:E:241:LEU:HD22	2.01	0.42
1:B:239:ALA:O	1:B:243:GLU:CG	2.60	0.42
1:B:230:SER:HB3	1:C:229:VAL:CG1	2.49	0.42
1:B:53:ALA:HA	1:B:96:PRO:O	2.19	0.42
1:A:123:SER:HA	1:A:191:SER:HA	2.02	0.42
7:A:511:PFL:H113	1:B:243:GLU:CG	2.23	0.42
1:B:243:GLU:H	1:B:243:GLU:HG2	1.72	0.42
1:D:123:SER:HA	1:D:191:SER:HA	2.01	0.42
1:B:37:PHE:CD2	1:B:39:VAL:HG23	2.54	0.42
1:E:55:ASP:O	1:E:59:SER:HB2	2.19	0.42
1:A:24:LEU:HD22	1:A:39:VAL:CG2	2.50	0.41
7:A:511:PFL:HC4	1:B:236:ILE:O	2.20	0.41
7:A:511:PFL:C11	1:B:243:GLU:OE1	2.37	0.41
1:E:160:TRP:CE3	1:E:190:ILE:HD12	2.55	0.41
7:A:511:PFL:C4	1:B:240:ILE:HG13	2.50	0.41
1:D:7:PRO:CG	1:D:137:THR:OG1	2.68	0.41
1:D:207:PHE:CD2	1:E:267[B]:PHE:CZ	3.08	0.41
1:A:204:PRO:HG2	7:A:511:PFL:H122	2.02	0.41
1:E:131:ILE:HD12	1:E:183:LYS:HB2	2.03	0.41
1:E:235:HIS:HB2	8:E:507:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:PRO:HG2	1:E:137:THR:OG1	2.21	0.41
1:B:201:ILE:HG12	7:B:510:PFL:C8	2.50	0.41
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.93	0.41
1:B:126:LEU:HA	8:B:609:HOH:O	2.20	0.40
1:A:230:SER:HB3	1:B:229:VAL:CG1	2.51	0.40
1:A:82:GLU:HG3	1:A:109:ARG:HD3	2.02	0.40
1:C:233:ILE:HA	1:C:236:ILE:HD12	2.03	0.40
1:C:7:PRO:HG2	1:C:137:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/317 (98%)	298 (96%)	13 (4%)	0	100	100
1	B	310/317 (98%)	300 (97%)	10 (3%)	0	100	100
1	C	310/317 (98%)	299 (96%)	11 (4%)	0	100	100
1	D	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
1	E	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
All	All	1553/1585 (98%)	1499 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	280/282 (99%)	276 (99%)	4 (1%)	67	86
1	B	279/282 (99%)	277 (99%)	2 (1%)	84	93
1	C	279/282 (99%)	275 (99%)	4 (1%)	67	86
1	D	280/282 (99%)	275 (98%)	5 (2%)	59	82
1	E	280/282 (99%)	274 (98%)	6 (2%)	53	79
All	All	1398/1410 (99%)	1377 (98%)	21 (2%)	65	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ILE
1	A	233	ILE
1	A	245	ASN
1	A	304	LEU
1	B	17	THR
1	B	304	LEU
1	C	17	THR
1	C	27	CYS
1	C	208	ILE
1	C	304	LEU
1	D	17	THR
1	D	39	VAL
1	D	131	ILE
1	D	233	ILE
1	D	304	LEU
1	E	17	THR
1	E	62	ARG
1	E	147	GLU
1	E	233	ILE
1	E	243	GLU
1	E	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	83	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 12 are monoatomic - leaving 36 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
7	PFL	A	510	-	13,13,13	0.33	0	18,18,18	0.76	0
2	LMT	D	401	-	13,13,36	0.77	0	12,12,47	0.50	0
6	PLC	D	407	-	22,22,41	0.55	0	20,20,49	0.48	0
6	PLC	B	508	-	11,11,41	0.46	0	10,10,49	0.62	0
6	PLC	E	408	-	11,11,41	0.44	0	10,10,49	0.61	0
3	ACT	D	409	-	1,3,3	5.09	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	5.18	1 (100%)	0,3,3	0.00	-
3	ACT	B	502	-	1,3,3	3.89	1 (100%)	0,3,3	0.00	-
3	ACT	B	509	-	1,3,3	6.45	1 (100%)	0,3,3	0.00	-
6	PLC	A	508	-	11,11,41	0.45	0	10,10,49	0.62	0
2	LMT	A	501	-	13,13,36	0.67	0	12,12,47	0.50	0
6	PLC	A	506	-	33,33,41	1.04	2 (6%)	39,41,49	1.07	2 (5%)
6	PLC	D	406	-	33,33,41	1.09	3 (9%)	39,41,49	1.09	2 (5%)
6	PLC	E	406	-	33,33,41	1.06	2 (6%)	39,41,49	1.08	2 (5%)
6	PLC	C	406	-	11,11,41	0.43	0	10,10,49	0.68	0
7	PFL	B	510	-	13,13,13	0.42	0	18,18,18	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	A	502	-	1,3,3	4.36	1 (100%)	0,3,3	0.00	-
7	PFL	C	408	-	13,13,13	0.28	0	18,18,18	0.49	0
7	PFL	A	511	-	13,13,13	0.51	0	18,18,18	0.65	1 (5%)
6	PLC	C	404	-	33,33,41	1.00	2 (6%)	39,41,49	1.14	3 (7%)
3	ACT	C	401	-	1,3,3	6.22	1 (100%)	0,3,3	0.00	-
3	ACT	D	402	-	1,3,3	5.29	1 (100%)	0,3,3	0.00	-
2	LMT	C	407	-	13,13,36	0.69	0	12,12,47	0.59	0
6	PLC	A	507	-	22,22,41	0.54	0	20,20,49	0.54	0
6	PLC	D	408	-	11,11,41	0.39	0	10,10,49	0.64	0
3	ACT	D	404	-	1,3,3	4.09	1 (100%)	0,3,3	0.00	-
7	PFL	E	409	-	13,13,13	0.21	0	18,18,18	0.50	0
2	LMT	E	401	-	11,11,36	0.76	0	10,10,47	0.35	0
2	LMT	B	501	-	13,13,36	0.61	0	12,12,47	0.88	1 (8%)
3	ACT	B	504	-	1,3,3	5.92	1 (100%)	0,3,3	0.00	-
2	LMT	E	402	-	13,13,36	0.76	0	12,12,47	0.49	0
6	PLC	B	507	-	22,22,41	0.56	0	20,20,49	0.48	0
6	PLC	B	506	-	33,33,41	1.11	2 (6%)	39,41,49	1.05	2 (5%)
6	PLC	E	407	-	22,22,41	0.61	0	20,20,49	0.51	0
3	ACT	E	403	-	1,3,3	3.37	1 (100%)	0,3,3	0.00	-
6	PLC	C	405	-	22,22,41	0.60	0	20,20,49	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PFL	A	510	-	-	3/8/8/8	0/1/1/1
2	LMT	D	401	-	-	0/11/11/61	-
6	PLC	D	407	-	-	8/18/18/45	-
6	PLC	B	508	-	-	1/9/9/45	-
6	PLC	E	408	-	-	1/9/9/45	-
6	PLC	A	508	-	-	1/9/9/45	-
2	LMT	A	501	-	-	1/11/11/61	-
6	PLC	A	506	-	-	20/37/37/45	-
6	PLC	D	406	-	-	21/37/37/45	-
6	PLC	E	406	-	-	20/37/37/45	-
6	PLC	C	406	-	-	1/9/9/45	-
7	PFL	B	510	-	-	6/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PFL	C	408	-	-	0/8/8/8	0/1/1/1
7	PFL	A	511	-	-	3/8/8/8	0/1/1/1
6	PLC	C	404	-	-	23/37/37/45	-
2	LMT	C	407	-	-	0/11/11/61	-
6	PLC	A	507	-	-	6/18/18/45	-
6	PLC	D	408	-	-	0/9/9/45	-
7	PFL	E	409	-	-	0/8/8/8	0/1/1/1
2	LMT	E	401	-	-	0/9/9/61	-
2	LMT	B	501	-	-	2/11/11/61	-
2	LMT	E	402	-	-	1/11/11/61	-
6	PLC	B	507	-	-	6/18/18/45	-
6	PLC	B	506	-	-	22/37/37/45	-
6	PLC	E	407	-	-	8/18/18/45	-
6	PLC	C	405	-	-	6/18/18/45	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	509	ACT	CH3-C	6.45	1.56	1.48
3	C	401	ACT	CH3-C	6.22	1.56	1.48
3	B	504	ACT	CH3-C	5.92	1.56	1.48
3	D	402	ACT	CH3-C	5.29	1.55	1.48
3	A	504	ACT	CH3-C	5.18	1.55	1.48
3	D	409	ACT	CH3-C	5.09	1.55	1.48
3	A	502	ACT	CH3-C	4.36	1.54	1.48
3	D	404	ACT	CH3-C	4.09	1.54	1.48
3	B	502	ACT	CH3-C	3.89	1.53	1.48
3	E	403	ACT	CH3-C	3.37	1.53	1.48
6	D	406	PLC	O2-C'	3.00	1.42	1.34
6	B	506	PLC	O2-C'	2.89	1.42	1.34
6	E	406	PLC	O2-C'	2.79	1.42	1.34
6	A	506	PLC	O2-C'	2.62	1.41	1.34
6	C	404	PLC	O2-C'	2.52	1.41	1.34
6	B	506	PLC	O3-CB	2.25	1.39	1.33
6	E	406	PLC	C3-C2	2.11	1.57	1.50
6	D	406	PLC	P-O4P	2.07	1.67	1.59
6	C	404	PLC	O3-CB	2.06	1.39	1.33
6	A	506	PLC	O3-CB	2.02	1.39	1.33
6	D	406	PLC	O3-CB	2.00	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	406	PLC	C2-O2-C'	4.27	128.31	117.79
6	A	506	PLC	C2-O2-C'	3.78	127.10	117.79
6	C	404	PLC	C2-O2-C'	3.78	127.09	117.79
6	B	506	PLC	C2-O2-C'	3.77	127.08	117.79
6	E	406	PLC	C2-O2-C'	3.58	126.61	117.79
6	C	404	PLC	C3-C2-C1	3.44	119.93	111.79
6	E	406	PLC	C3-C2-C1	3.38	119.78	111.79
6	D	406	PLC	C3-C2-C1	3.27	119.51	111.79
6	A	506	PLC	C3-C2-C1	3.20	119.37	111.79
6	B	506	PLC	C3-C2-C1	2.80	118.41	111.79
6	C	404	PLC	C8-N-C7	-2.74	101.93	108.97
2	B	501	LMT	C3-C2-C1	-2.10	104.19	113.49
7	A	511	PFL	O1-C1-C6	-2.02	115.08	120.63

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	406	PLC	C1'-C'-O2-C2
6	D	406	PLC	C4-O4P-P-O2P
6	D	406	PLC	C4-O4P-P-O3P
6	E	406	PLC	C1'-C'-O2-C2
6	E	406	PLC	C1-O3P-P-O1P
6	E	406	PLC	C1-O3P-P-O4P
7	B	510	PFL	C12-C10-C6-C5
6	C	404	PLC	C1'-C'-O2-C2
6	C	404	PLC	C1-O3P-P-O2P
6	C	404	PLC	C1-O3P-P-O4P
6	C	404	PLC	C4-O4P-P-O1P
6	C	404	PLC	C4-O4P-P-O3P
6	A	506	PLC	C1'-C'-O2-C2
6	A	506	PLC	C1-O3P-P-O1P
6	A	506	PLC	C1-O3P-P-O4P
6	B	506	PLC	C1'-C'-O2-C2
6	B	506	PLC	C1-O3P-P-O1P
6	B	506	PLC	C1-O3P-P-O4P
7	B	510	PFL	C12-C10-C6-C1
7	A	510	PFL	C11-C10-C6-C5
7	A	511	PFL	C3-C2-C7-C8
7	B	510	PFL	C3-C2-C7-C8
7	A	510	PFL	C11-C10-C6-C1
7	A	511	PFL	C1-C2-C7-C8
6	D	406	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
6	E	406	PLC	O'-C'-O2-C2
6	C	404	PLC	O'-C'-O2-C2
6	A	506	PLC	O'-C'-O2-C2
6	B	506	PLC	O'-C'-O2-C2
7	B	510	PFL	C3-C2-C7-C9
6	E	406	PLC	C4-C5-N-C8
6	A	506	PLC	C4-C5-N-C8
6	D	406	PLC	C'-C1'-C2'-C3'
6	D	406	PLC	CB-C1B-C2B-C3B
6	E	406	PLC	C'-C1'-C2'-C3'
6	E	406	PLC	CB-C1B-C2B-C3B
6	A	506	PLC	C'-C1'-C2'-C3'
6	A	506	PLC	CB-C1B-C2B-C3B
6	B	506	PLC	C'-C1'-C2'-C3'
6	B	506	PLC	CB-C1B-C2B-C3B
6	C	404	PLC	CB-C1B-C2B-C3B
7	B	510	PFL	C1-C2-C7-C8
6	D	406	PLC	C1-O3P-P-O4P
6	E	406	PLC	C4-O4P-P-O3P
6	A	506	PLC	C4-O4P-P-O3P
6	B	506	PLC	C4-O4P-P-O3P
6	C	404	PLC	C'-C1'-C2'-C3'
7	B	510	PFL	C1-C2-C7-C9
6	E	406	PLC	C4-C5-N-C7
6	C	404	PLC	C4-C5-N-C6
6	C	404	PLC	C4-C5-N-C8
6	A	506	PLC	C4-C5-N-C7
6	B	506	PLC	C4-C5-N-C6
6	B	506	PLC	C4-C5-N-C8
6	B	506	PLC	C3B-C4B-C5B-C6B
6	E	407	PLC	C4'-C5'-C6'-C7'
6	C	405	PLC	C1'-C2'-C3'-C4'
6	A	507	PLC	C1'-C2'-C3'-C4'
6	D	407	PLC	C1'-C2'-C3'-C4'
6	B	507	PLC	C1'-C2'-C3'-C4'
6	E	406	PLC	C4-C5-N-C6
6	C	404	PLC	C4-C5-N-C7
6	A	506	PLC	C4-C5-N-C6
6	B	506	PLC	C4-C5-N-C7
6	C	405	PLC	C5B-C6B-C7B-C8B
6	D	406	PLC	C1B-C2B-C3B-C4B
6	B	506	PLC	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
6	A	506	PLC	C3B-C4B-C5B-C6B
6	E	406	PLC	C3B-C4B-C5B-C6B
6	C	404	PLC	C3B-C4B-C5B-C6B
6	D	406	PLC	C4-C5-N-C6
6	D	406	PLC	C3B-C4B-C5B-C6B
6	D	406	PLC	C4B-C5B-C6B-C7B
6	E	407	PLC	C'-C1'-C2'-C3'
6	A	506	PLC	O3P-C1-C2-O2
6	D	406	PLC	C4-C5-N-C7
6	A	507	PLC	C6'-C7'-C8'-C9'
6	B	507	PLC	C2'-C3'-C4'-C5'
6	D	406	PLC	C1'-C2'-C3'-C4'
6	D	407	PLC	C2'-C3'-C4'-C5'
6	E	407	PLC	C2'-C3'-C4'-C5'
6	A	507	PLC	C2'-C3'-C4'-C5'
6	C	405	PLC	C2'-C3'-C4'-C5'
6	E	406	PLC	C1B-C2B-C3B-C4B
6	B	507	PLC	C6'-C7'-C8'-C9'
6	A	506	PLC	C1B-C2B-C3B-C4B
6	A	507	PLC	C5B-C6B-C7B-C8B
6	C	404	PLC	O3P-C1-C2-O2
7	A	511	PFL	C3-C2-C7-C9
6	C	405	PLC	C6'-C7'-C8'-C9'
6	B	506	PLC	C1'-C2'-C3'-C4'
6	D	407	PLC	C4'-C5'-C6'-C7'
6	D	406	PLC	C4-C5-N-C8
6	A	506	PLC	C1'-C2'-C3'-C4'
6	B	508	PLC	C1'-C2'-C3'-C4'
6	D	406	PLC	O3P-C1-C2-O2
6	E	406	PLC	O3P-C1-C2-O2
6	C	406	PLC	C1'-C2'-C3'-C4'
6	E	408	PLC	C1'-C2'-C3'-C4'
6	E	406	PLC	C1'-C2'-C3'-C4'
6	B	507	PLC	C5B-C6B-C7B-C8B
6	D	407	PLC	C8'-C9'-CA'-CB'
6	C	405	PLC	C8'-C9'-CA'-CB'
6	A	508	PLC	C1'-C2'-C3'-C4'
6	E	407	PLC	C3'-C4'-C5'-C6'
6	D	406	PLC	C1-O3P-P-O1P
6	D	406	PLC	C4-O4P-P-O1P
6	E	406	PLC	C4-O4P-P-O1P
6	C	404	PLC	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	A	506	PLC	C4-O4P-P-O1P
6	B	506	PLC	C4-O4P-P-O1P
6	C	404	PLC	C4B-C5B-C6B-C7B
6	B	506	PLC	C4B-C5B-C6B-C7B
7	A	510	PFL	C12-C10-C6-C5
6	D	406	PLC	O4P-C4-C5-N
6	E	406	PLC	O4P-C4-C5-N
6	C	404	PLC	O4P-C4-C5-N
6	A	506	PLC	O4P-C4-C5-N
6	B	506	PLC	O4P-C4-C5-N
6	A	506	PLC	C4B-C5B-C6B-C7B
6	B	507	PLC	C8'-C9'-CA'-CB'
6	A	507	PLC	C4'-C5'-C6'-C7'
6	E	406	PLC	C3-C2-O2-C'
6	B	506	PLC	C3-C2-O2-C'
6	C	404	PLC	O3P-C1-C2-C3
6	C	404	PLC	C1B-C2B-C3B-C4B
6	B	507	PLC	C4'-C5'-C6'-C7'
6	C	405	PLC	C4'-C5'-C6'-C7'
6	E	406	PLC	C4B-C5B-C6B-C7B
6	A	507	PLC	C8'-C9'-CA'-CB'
6	E	407	PLC	C8'-C9'-CA'-CB'
6	D	407	PLC	CB-C1B-C2B-C3B
6	E	407	PLC	C1'-C2'-C3'-C4'
6	C	404	PLC	C1'-C2'-C3'-C4'
2	B	501	LMT	C9-C10-C11-C12
2	B	501	LMT	C11-C10-C9-C8
6	C	404	PLC	C3-C2-O2-C'
6	A	506	PLC	C3-C2-O2-C'
6	D	407	PLC	C5B-C6B-C7B-C8B
6	E	407	PLC	C5'-C6'-C7'-C8'
2	E	402	LMT	C1-C2-C3-C4
6	D	406	PLC	O3P-C1-C2-C3
6	D	407	PLC	C6'-C7'-C8'-C9'
6	E	407	PLC	C5B-C6B-C7B-C8B
6	B	506	PLC	O3P-C1-C2-O2
6	C	404	PLC	C2B-C1B-CB-O3
6	E	406	PLC	C2B-C1B-CB-O3
6	A	506	PLC	C2B-C1B-CB-O3
6	C	404	PLC	C2B-C1B-CB-OB
6	A	506	PLC	C2B-C1B-CB-OB
6	B	506	PLC	C2B-C1B-CB-O3

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Mol	Chain	Res	Type	Atoms
6	E	406	PLC	C2B-C1B-CB-OB
6	D	407	PLC	C4B-C5B-C6B-C7B
6	B	506	PLC	O2-C'-C1'-C2'
2	A	501	LMT	C1-C2-C3-C4
6	B	506	PLC	C2B-C1B-CB-OB
6	D	406	PLC	C2B-C1B-CB-O3
6	D	406	PLC	O2-C'-C1'-C2'
6	C	404	PLC	O2-C'-C1'-C2'
6	B	506	PLC	O'-C'-C1'-C2'

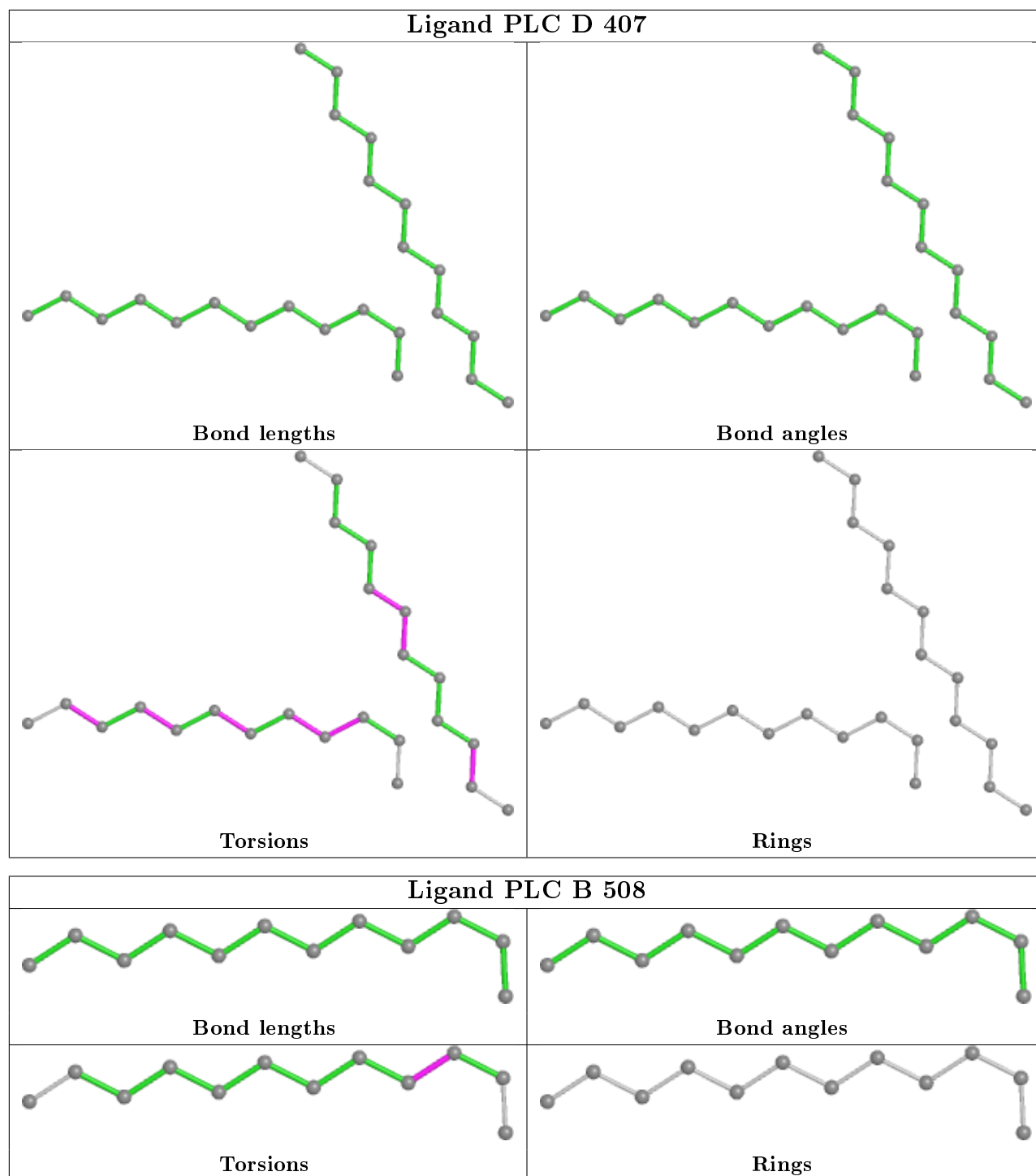
There are no ring outliers.

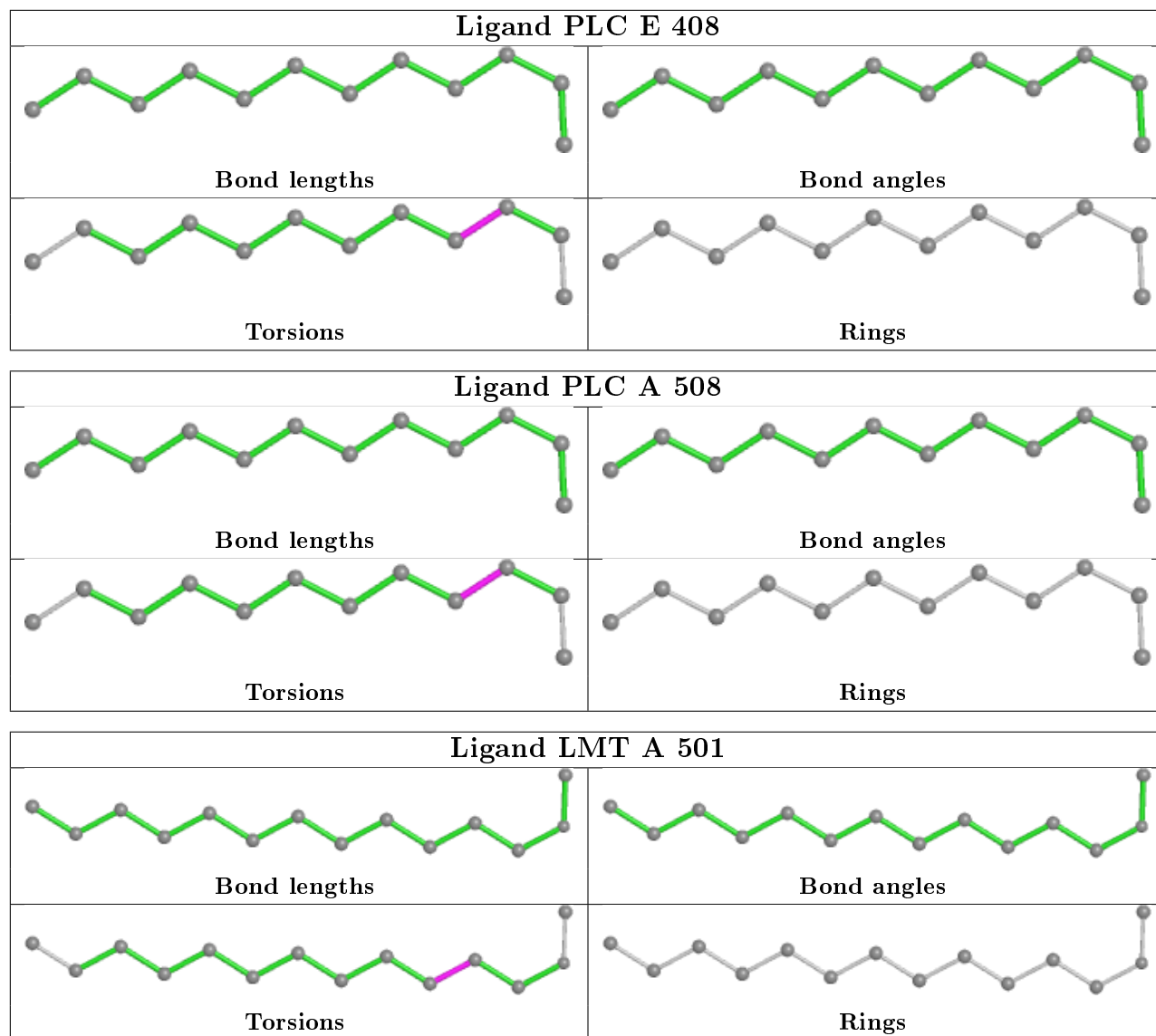
16 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	510	PFL	19	0
6	D	407	PLC	1	0
3	A	504	ACT	1	0
2	A	501	LMT	1	0
7	B	510	PFL	27	0
7	C	408	PFL	13	0
7	A	511	PFL	25	0
6	C	404	PLC	2	0
2	C	407	LMT	2	0
6	A	507	PLC	1	0
7	E	409	PFL	7	0
2	E	401	LMT	3	0
2	E	402	LMT	3	0
6	B	507	PLC	1	0
6	E	407	PLC	1	0
6	C	405	PLC	1	0

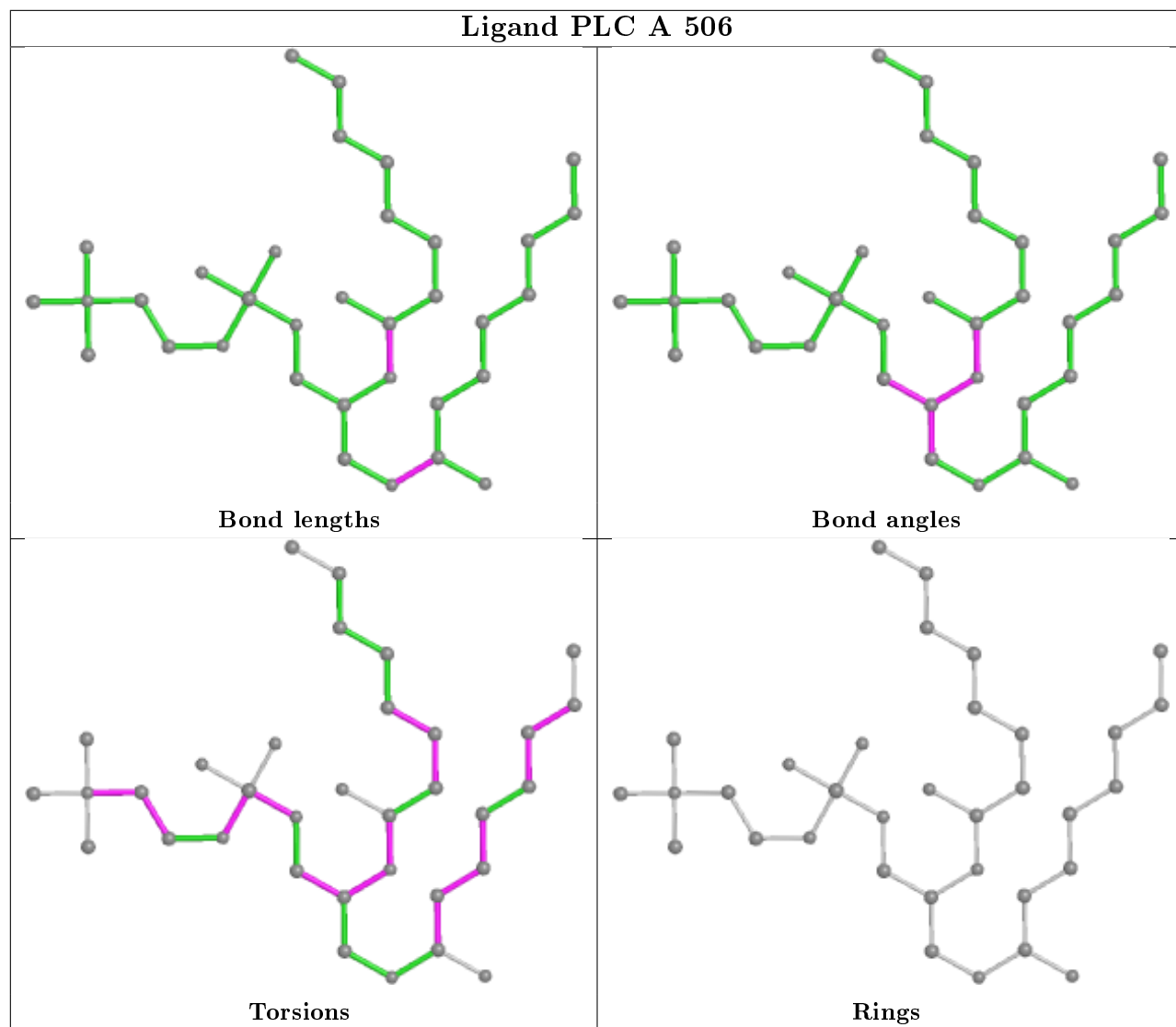
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

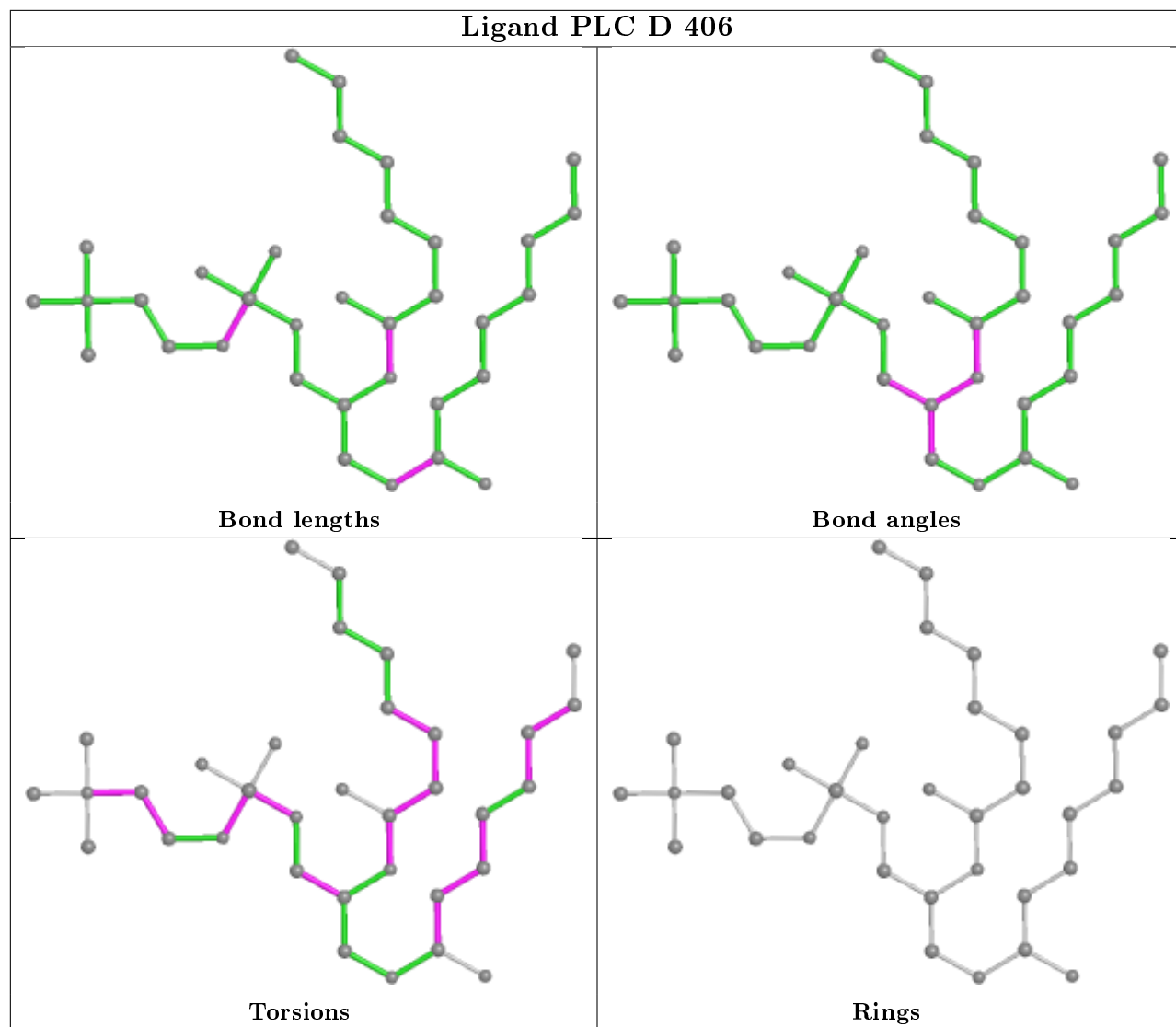




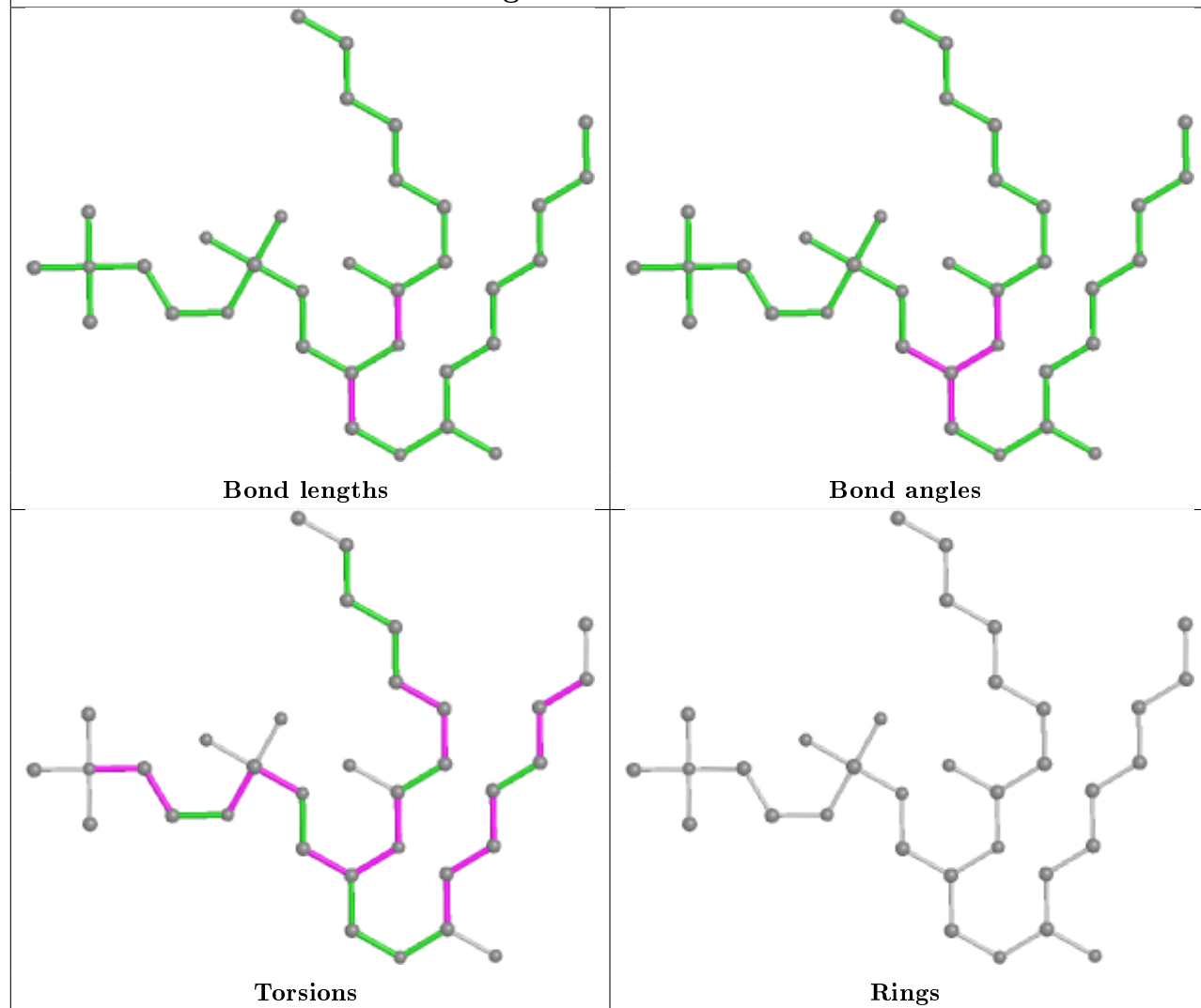




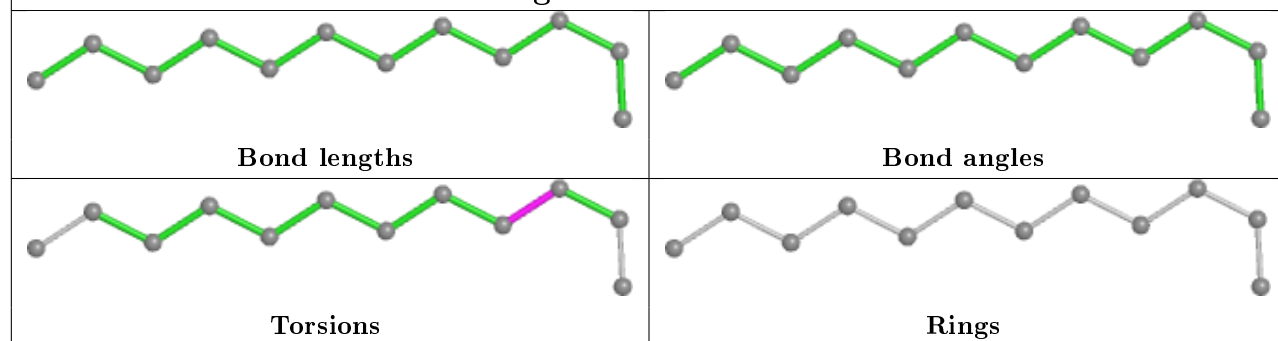
## Ligand PLC D 406



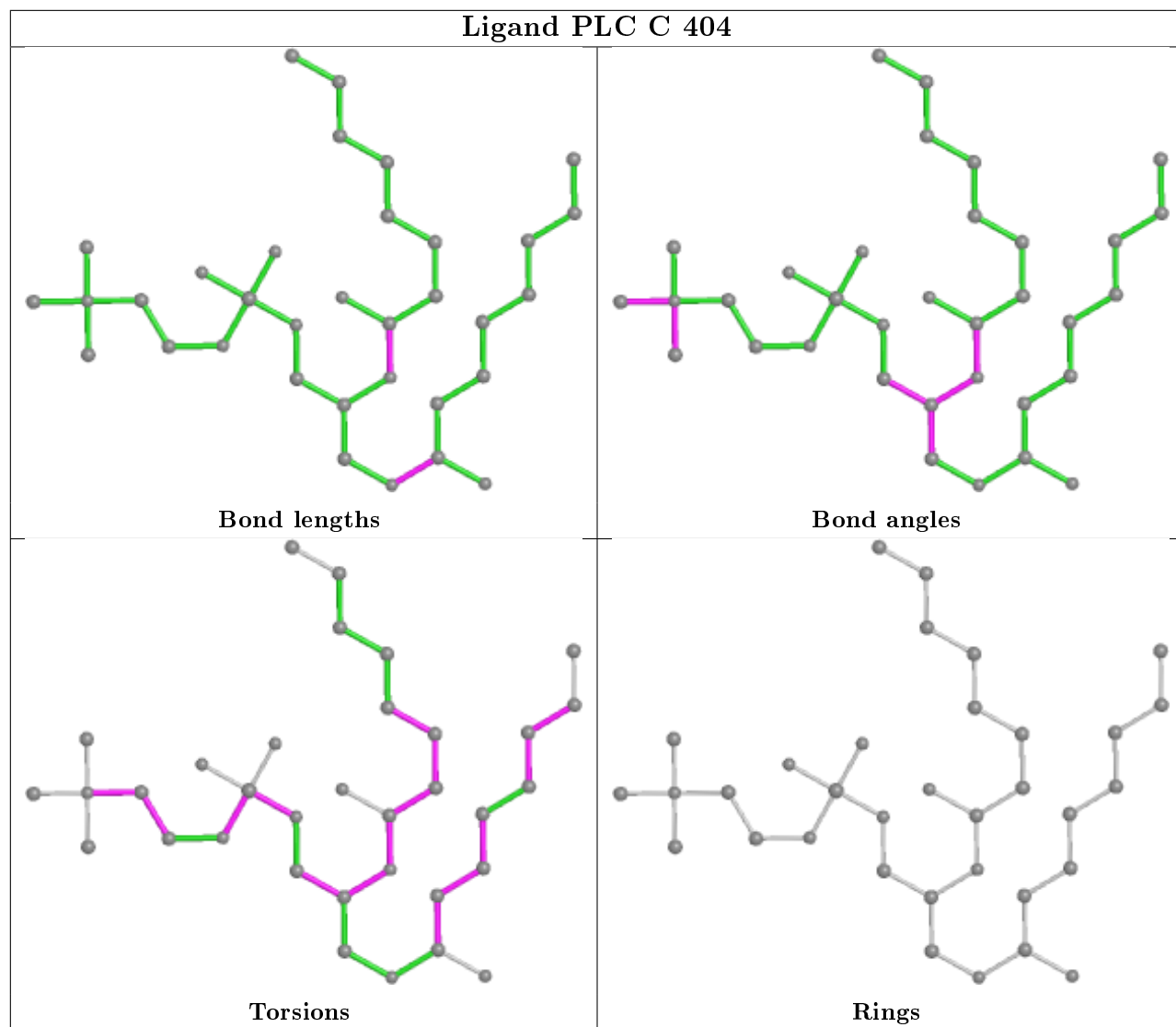
## Ligand PLC E 406

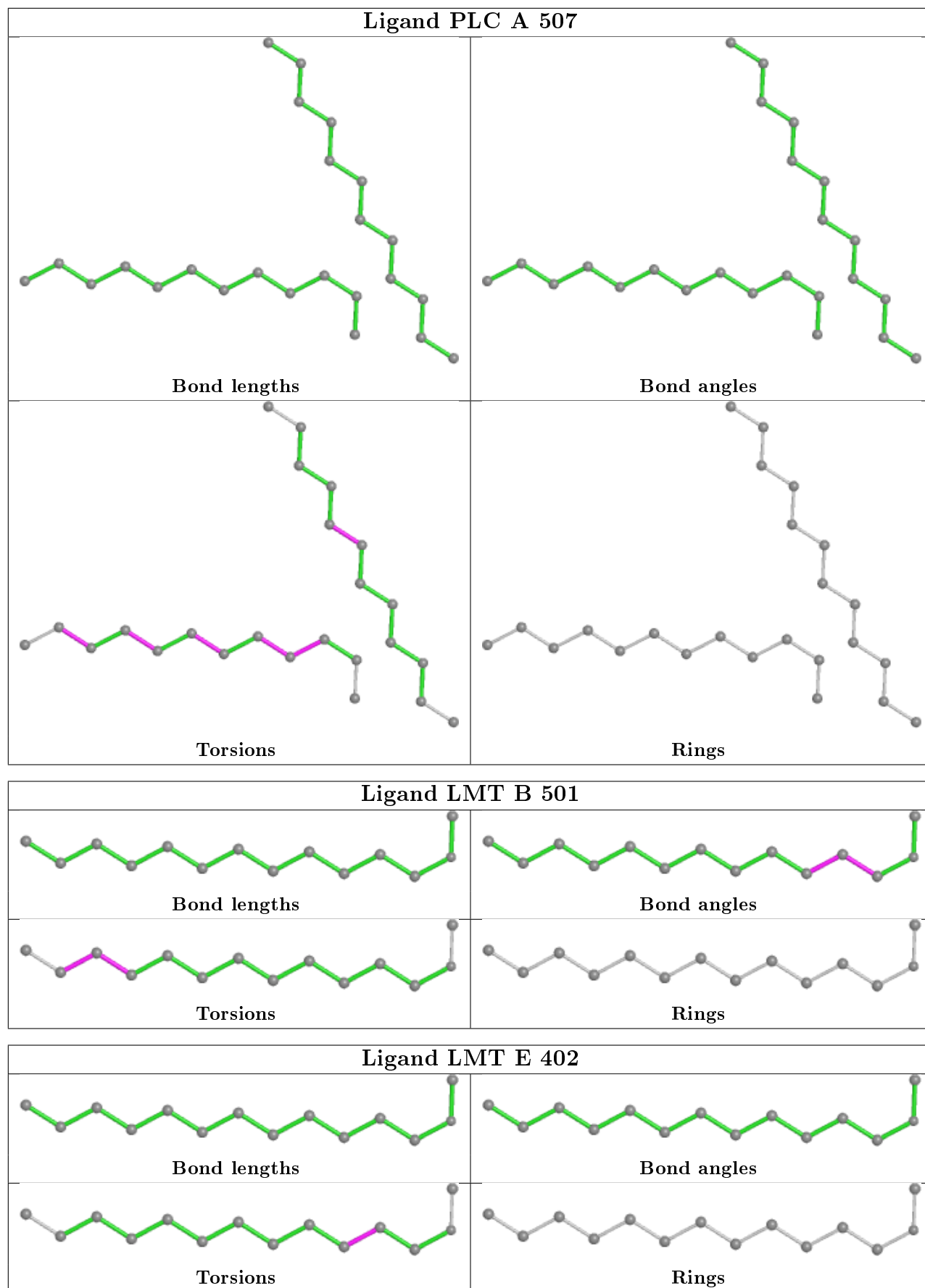


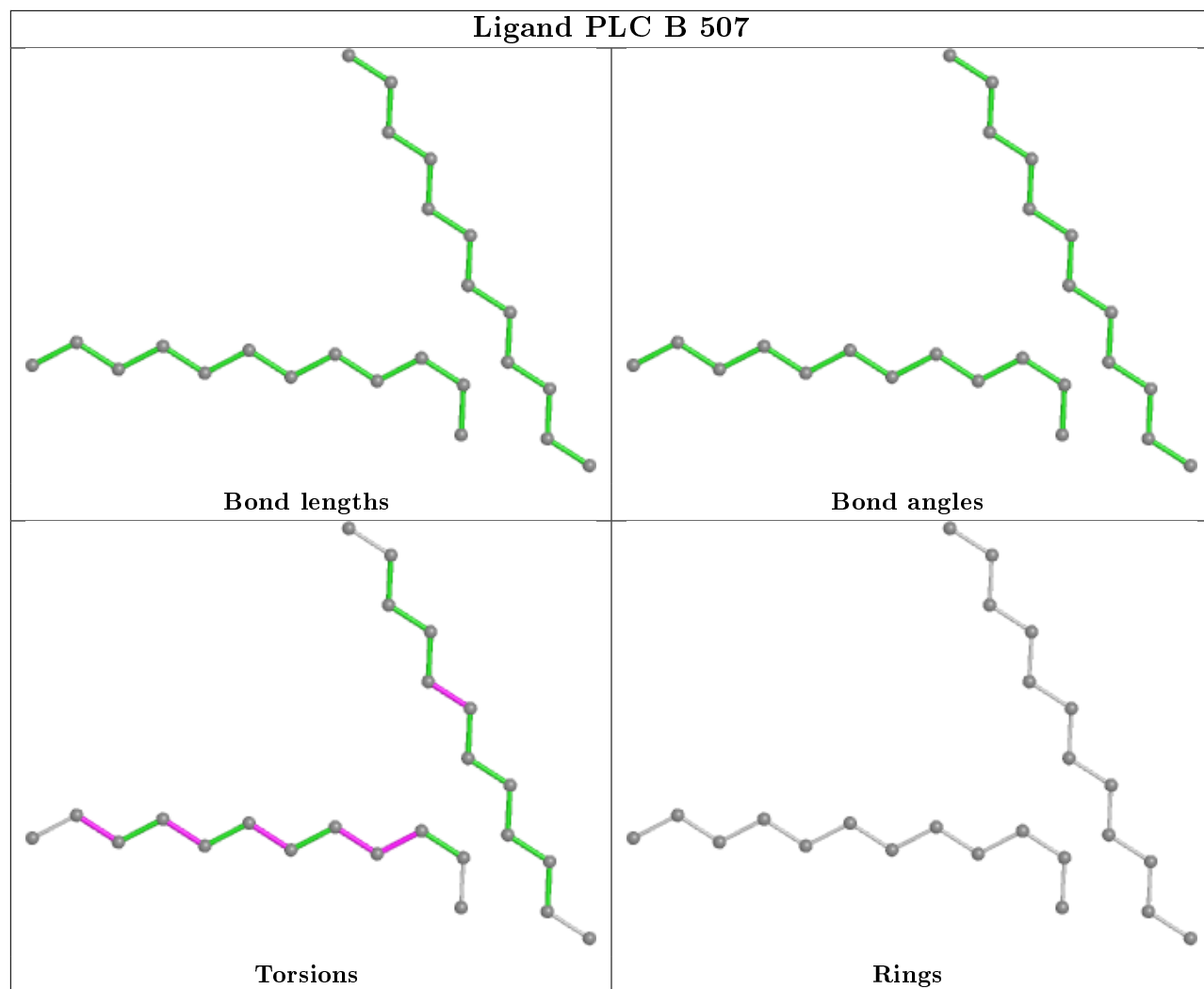
## Ligand PLC C 406



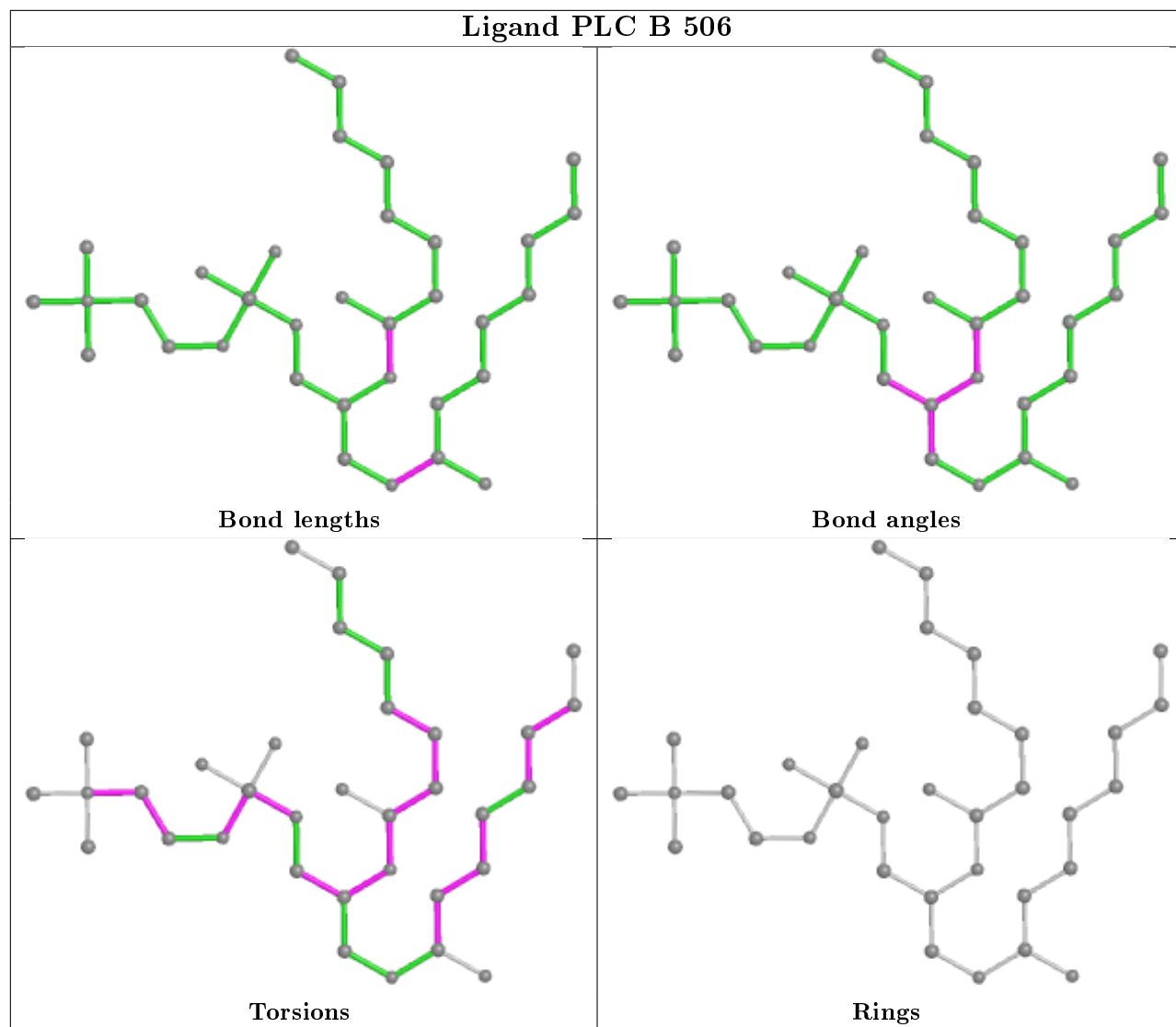
## Ligand PLC C 404

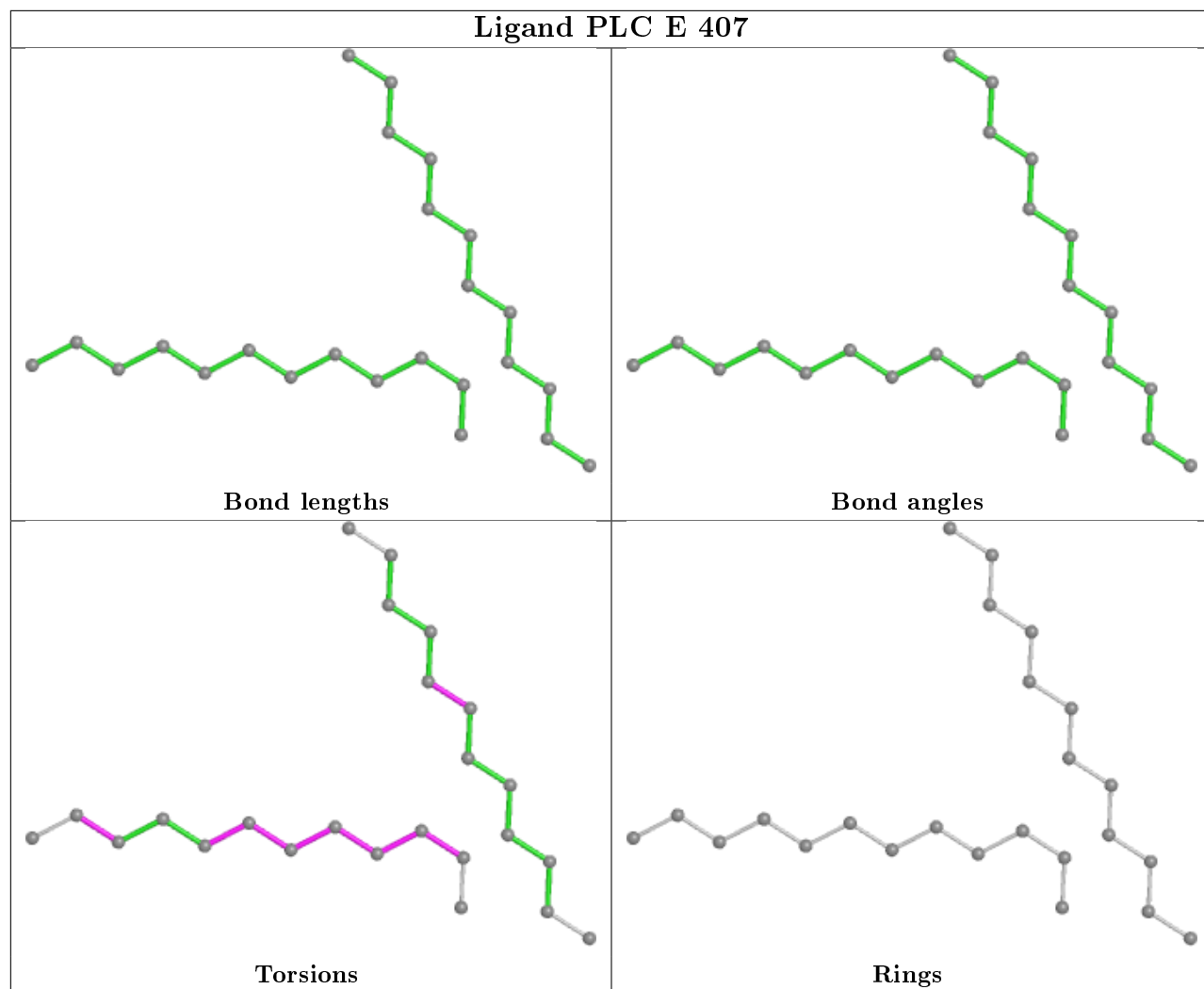




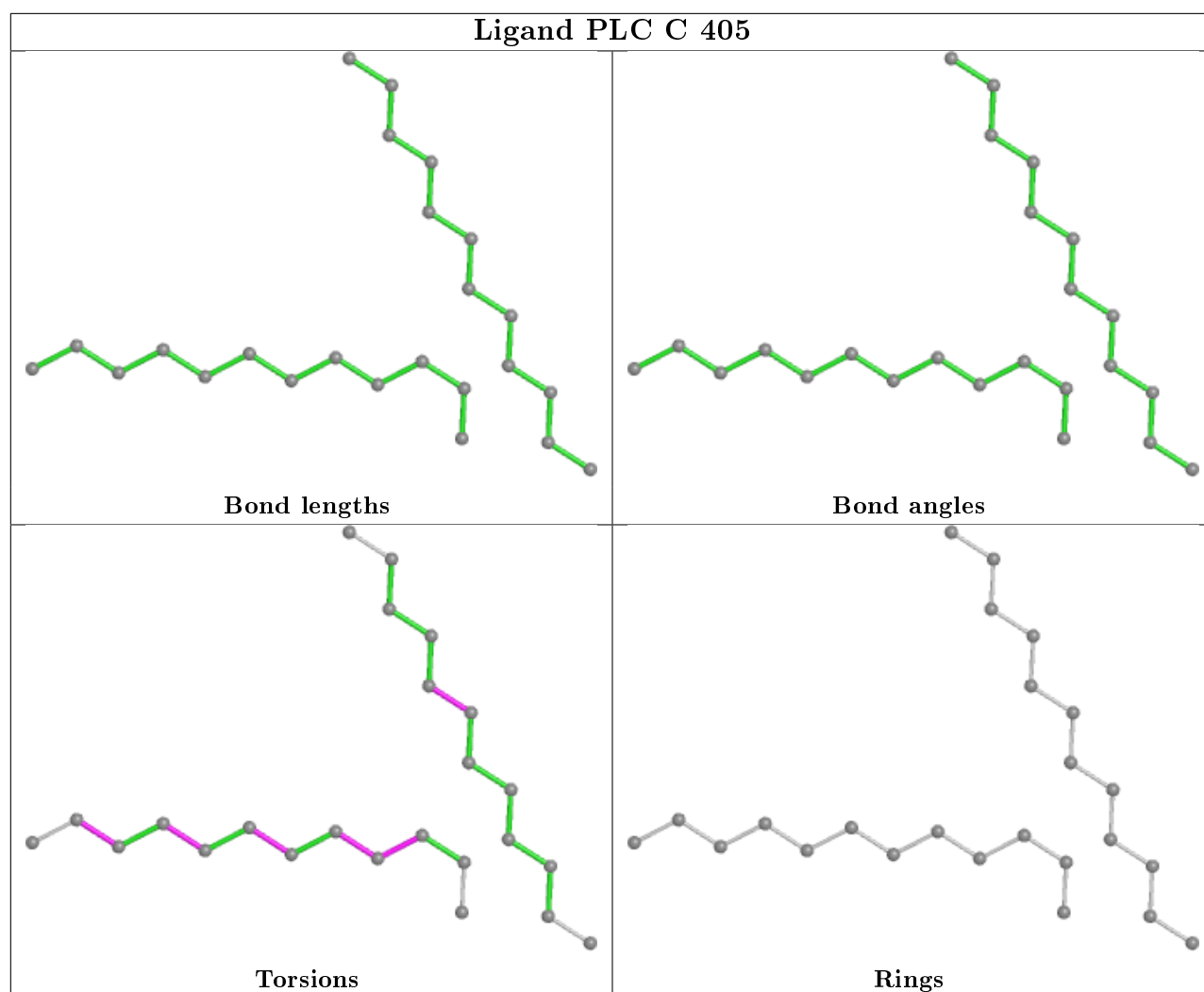


## Ligand PLC B 506









## 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	311/317 (98%)	-0.40	3 (0%) 82 67	53, 76, 122, 170	0
1	B	311/317 (98%)	-0.45	0 100 100	52, 75, 110, 146	0
1	C	311/317 (98%)	-0.37	4 (1%) 77 59	51, 76, 119, 168	0
1	D	311/317 (98%)	-0.43	1 (0%) 94 88	52, 75, 119, 173	0
1	E	311/317 (98%)	-0.39	5 (1%) 72 51	53, 77, 117, 157	0
All	All	1555/1585 (98%)	-0.41	13 (0%) 86 72	51, 76, 118, 173	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	ARG	4.2
1	E	58	ARG	3.8
1	A	57	VAL	3.3
1	D	283	SER	3.2
1	C	13	ASP	3.1
1	E	13	ASP	3.0
1	C	11	ILE	2.7
1	A	59	SER	2.7
1	E	69	GLU	2.5
1	E	12	ALA	2.4
1	A	11	ILE	2.3
1	C	12	ALA	2.3
1	E	170	LYS	2.1

### 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 ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

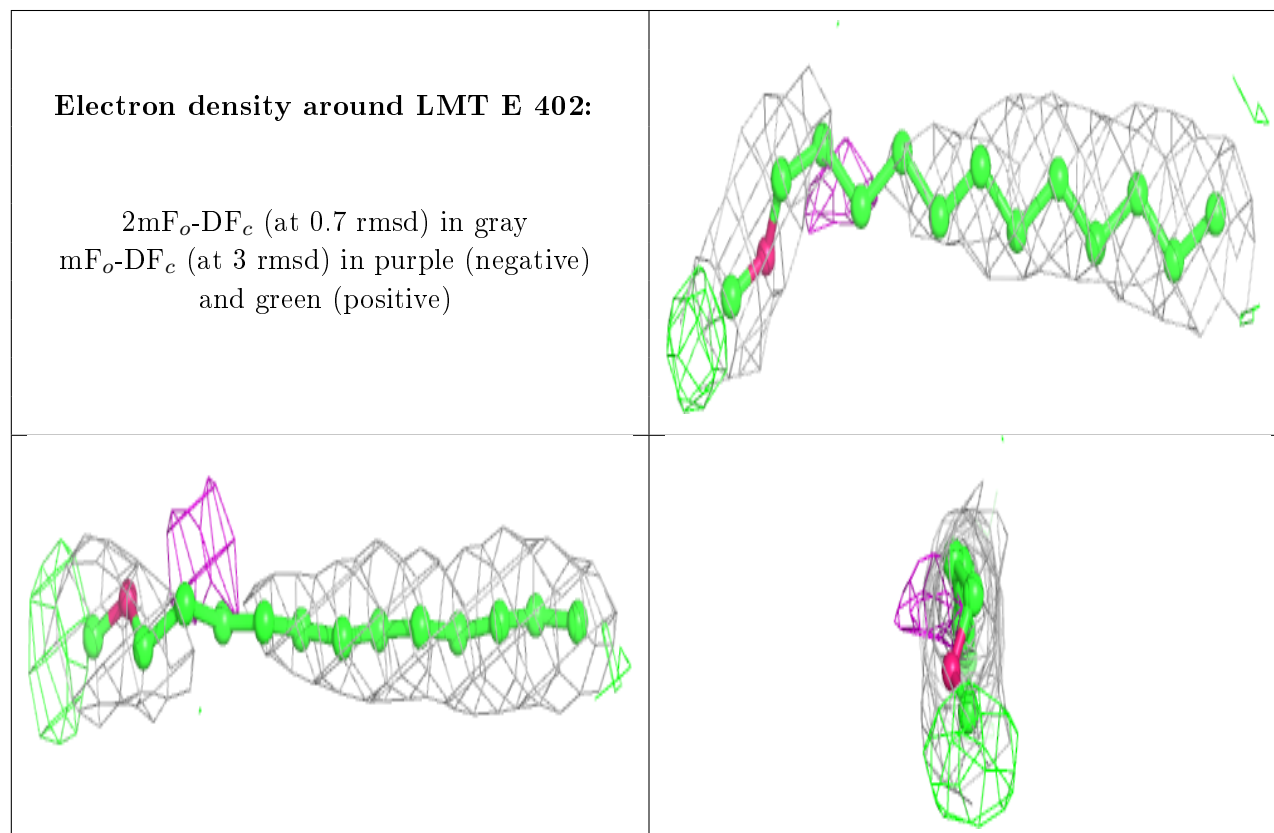
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	B	505	1/1	0.49	0.39	70,70,70,70	0
5	NA	E	405	1/1	0.52	0.59	72,72,72,72	0
2	LMT	E	402	14/35	0.54	0.45	71,84,102,103	0
2	LMT	C	407	14/35	0.66	0.37	56,76,102,103	0
2	LMT	A	501	14/35	0.69	0.39	62,76,110,110	0
6	PLC	B	506	34/42	0.69	0.43	95,130,172,174	0
5	NA	E	410	1/1	0.71	0.36	92,92,92,92	0
4	CL	B	503	1/1	0.72	0.55	168,168,168,168	0
6	PLC	E	407	24/42	0.73	0.46	75,90,112,112	0
6	PLC	A	507	24/42	0.73	0.50	78,100,120,121	0
6	PLC	C	405	24/42	0.73	0.38	78,91,101,102	0
6	PLC	D	406	34/42	0.74	0.37	85,129,164,165	0
7	PFL	B	510	13/13	0.74	0.34	138,139,141,142	13
6	PLC	C	404	34/42	0.74	0.36	85,123,169,170	0
6	PLC	B	508	12/42	0.74	0.44	101,102,116,117	0
6	PLC	C	406	12/42	0.74	0.57	98,102,110,110	0
6	PLC	B	507	24/42	0.75	0.46	83,93,107,108	0
6	PLC	D	407	24/42	0.76	0.51	83,104,111,113	0
6	PLC	A	506	34/42	0.77	0.38	89,132,174,175	0
6	PLC	D	408	12/42	0.77	0.31	89,90,113,114	0
7	PFL	A	510	13/13	0.77	0.37	120,128,130,130	0
2	LMT	B	501	14/35	0.78	0.31	74,86,103,103	0
6	PLC	E	406	34/42	0.80	0.40	85,132,170,171	0
6	PLC	A	508	12/42	0.80	0.44	91,95,105,105	0
2	LMT	D	401	14/35	0.81	0.29	77,81,101,102	0
6	PLC	E	408	12/42	0.81	0.48	94,96,111,112	0
7	PFL	E	409	13/13	0.81	0.56	144,149,152,154	0
7	PFL	C	408	13/13	0.81	0.37	145,149,152,154	0
5	NA	A	509	1/1	0.82	0.20	82,82,82,82	0
5	NA	A	505	1/1	0.84	0.16	74,74,74,74	0
5	NA	D	405	1/1	0.86	0.08	81,81,81,81	0
2	LMT	E	401	12/35	0.87	0.28	74,83,89,90	0

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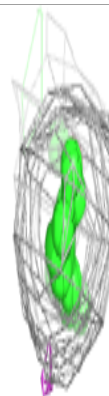
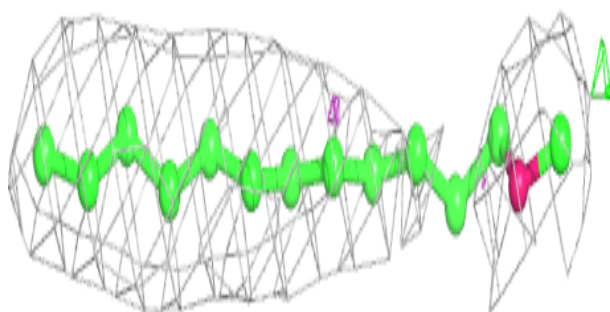
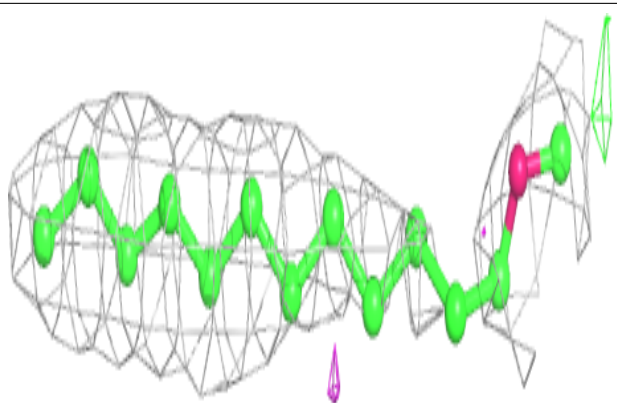
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PFL	A	511	13/13	0.87	0.34	131,139,142,143	0
4	CL	C	402	1/1	0.92	0.15	82,82,82,82	0
3	ACT	D	409	4/4	0.94	0.14	70,71,72,74	0
5	NA	C	403	1/1	0.94	0.14	72,72,72,72	0
4	CL	D	403	1/1	0.94	0.13	68,68,68,68	0
3	ACT	A	502	4/4	0.95	0.16	65,68,69,72	0
3	ACT	C	401	4/4	0.95	0.17	70,73,73,74	0
3	ACT	D	404	4/4	0.96	0.23	64,65,65,65	0
3	ACT	B	502	4/4	0.96	0.32	77,79,80,80	0
3	ACT	E	403	4/4	0.96	0.20	83,86,87,89	0
3	ACT	B	504	4/4	0.96	0.18	81,86,87,87	0
3	ACT	B	509	4/4	0.97	0.13	74,74,76,79	0
3	ACT	A	504	4/4	0.98	0.10	69,71,72,74	0
4	CL	E	404	1/1	0.98	0.13	72,72,72,72	0
3	ACT	D	402	4/4	0.98	0.13	64,64,65,65	0
4	CL	A	503	1/1	0.99	0.14	73,73,73,73	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.

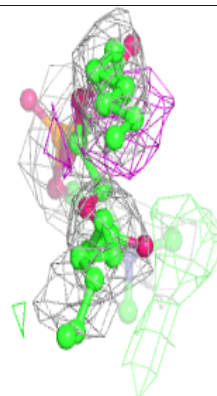
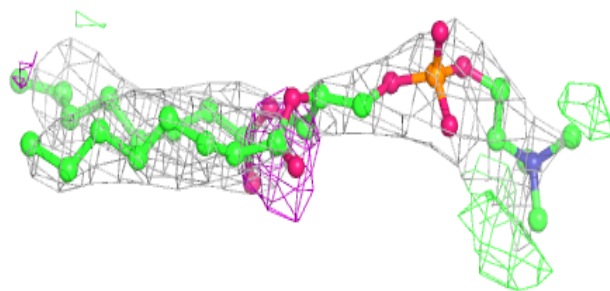
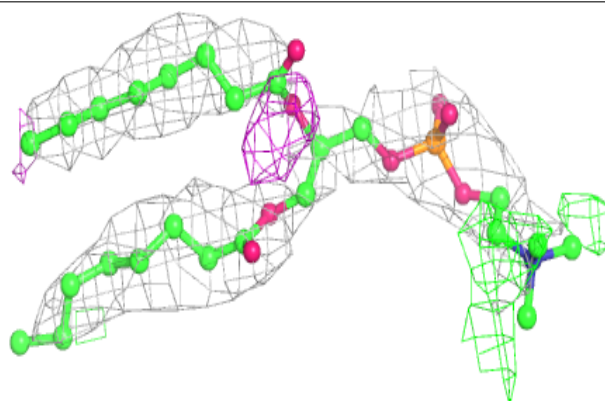


**Electron density around LMT A 501:**

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

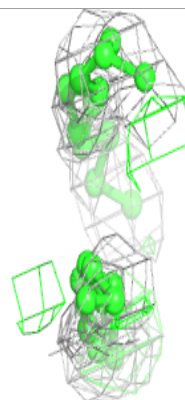
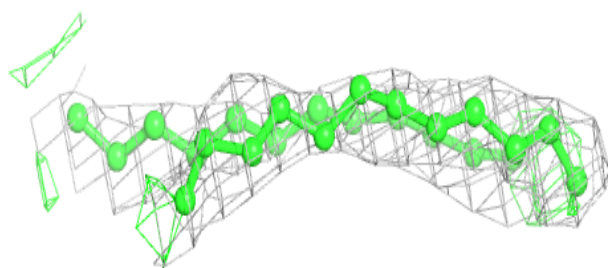
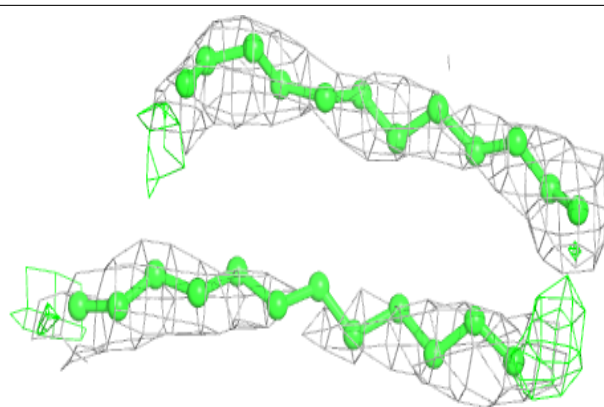
**Electron density around PLC B 506:**

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

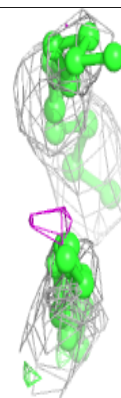
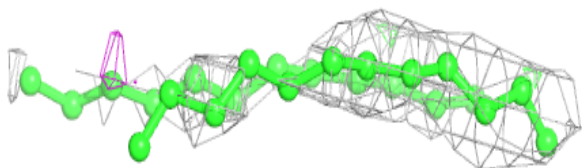
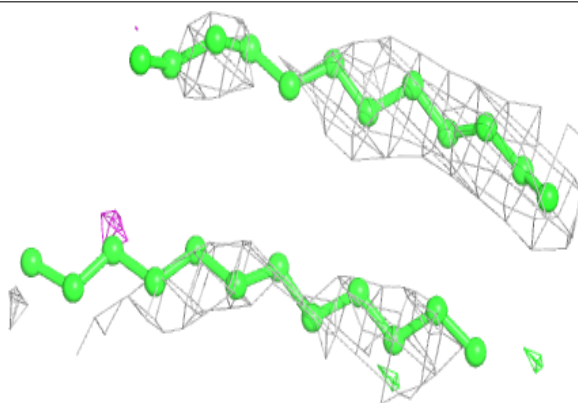


**Electron density around PLC E 407:**

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and green (positive)

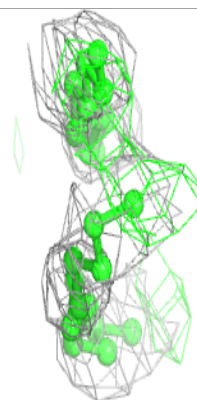
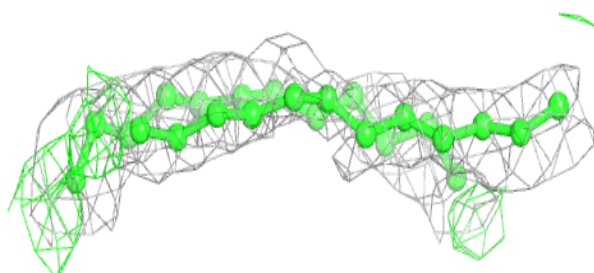
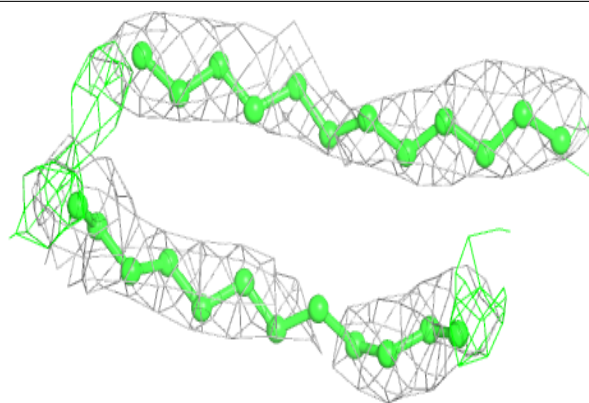
**Electron density around PLC A 507:**

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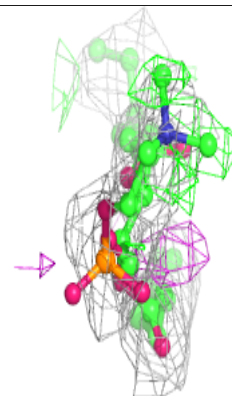
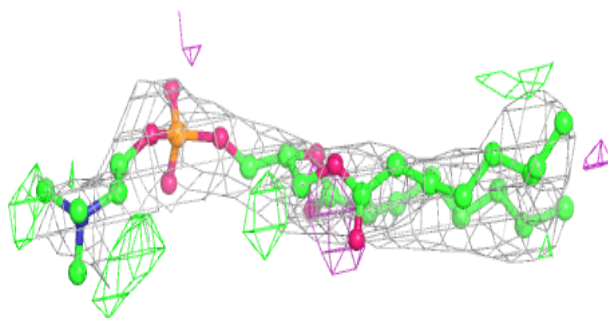
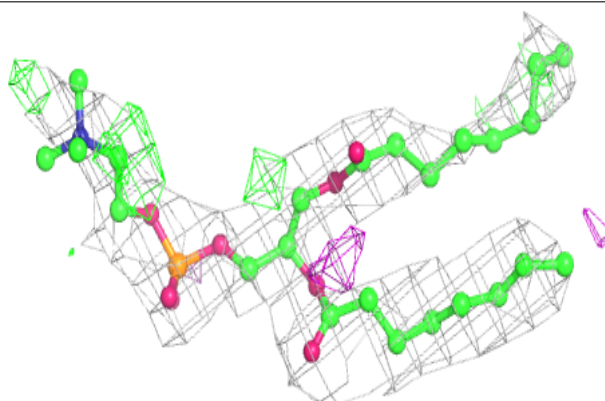


**Electron density around PLC C 405:**

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and green (positive)

**Electron density around PLC D 406:**

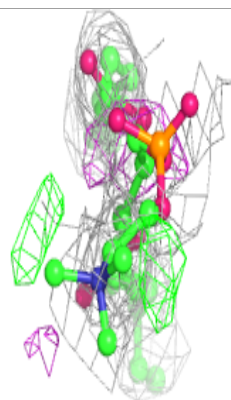
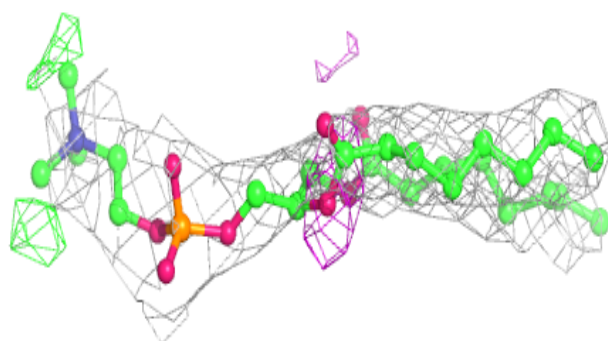
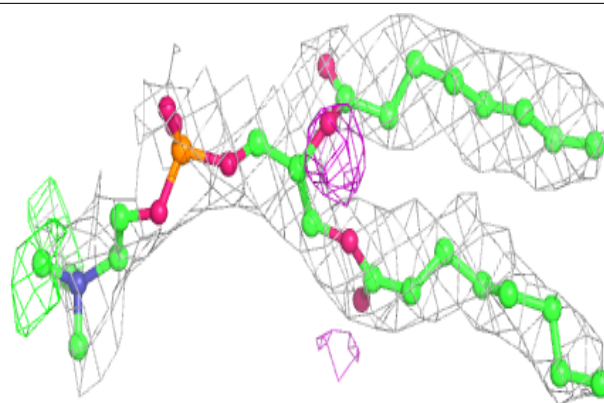
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



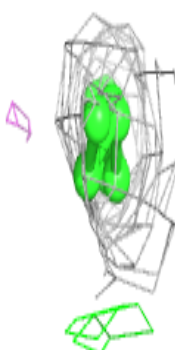
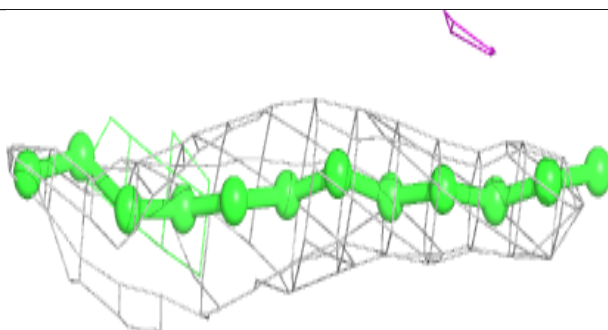
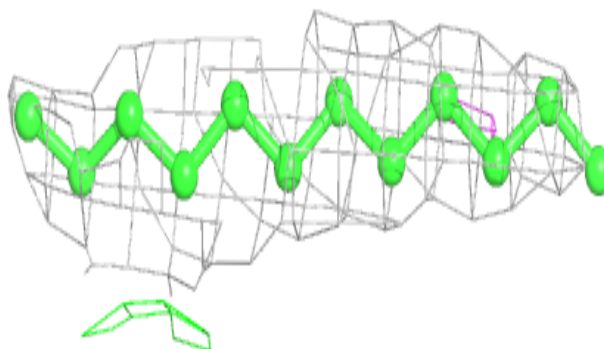


**Electron density around PLC C 404:**

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

**Electron density around PLC B 508:**

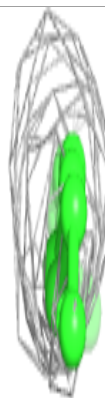
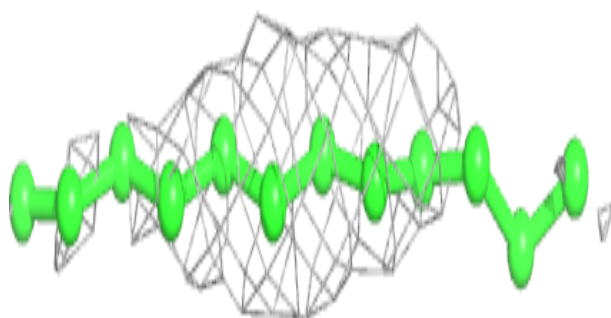
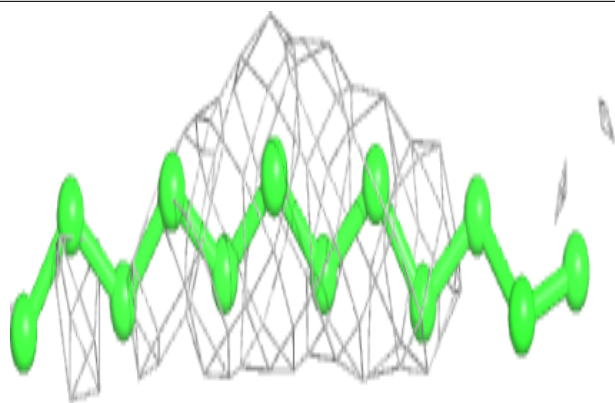
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



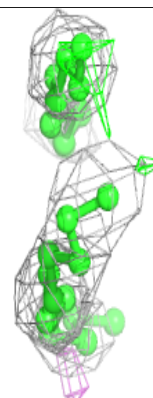
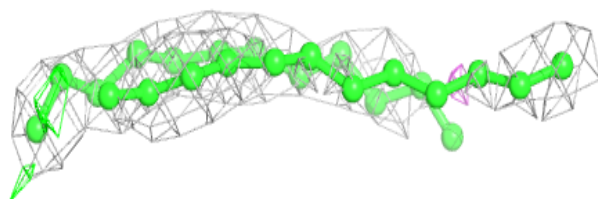
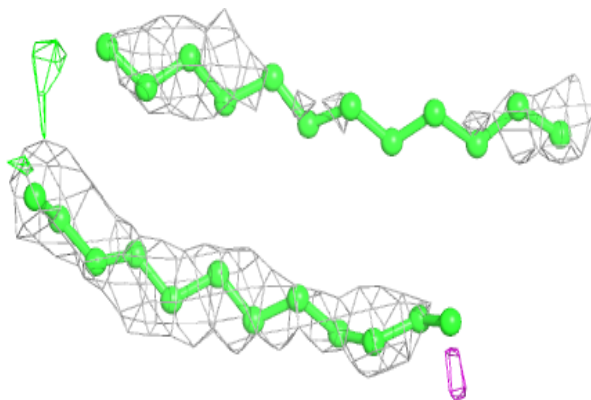


**Electron density around PLC C 406:**

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and green (positive)

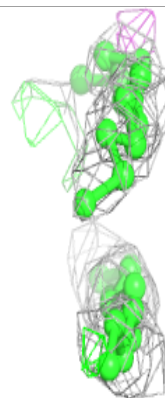
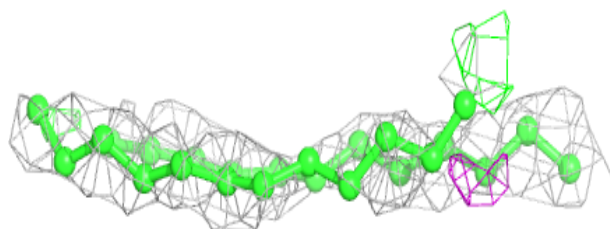
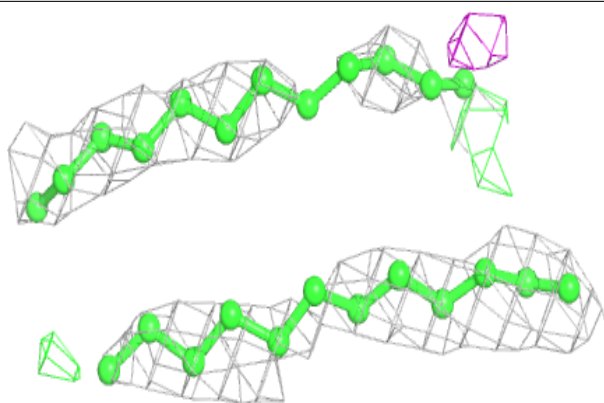
**Electron density around PLC B 507:**

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and green (positive)

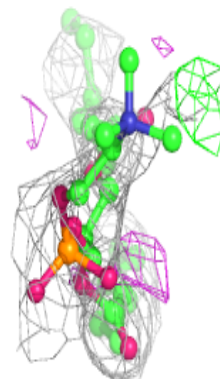
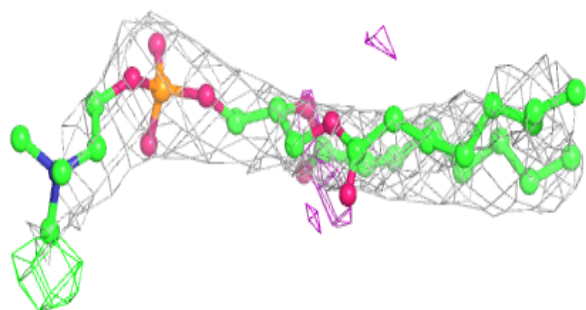
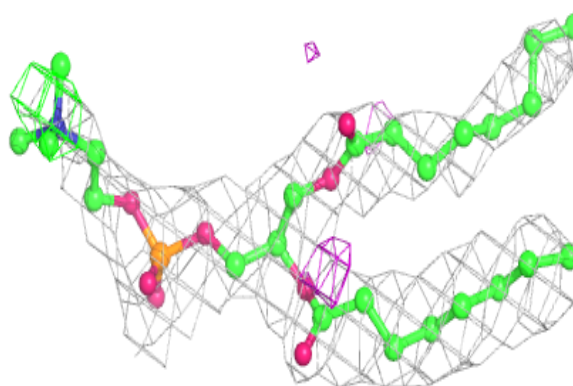


**Electron density around PLC D 407:**

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

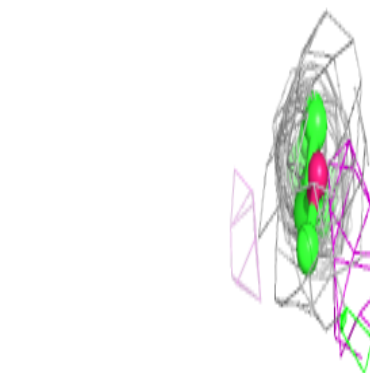
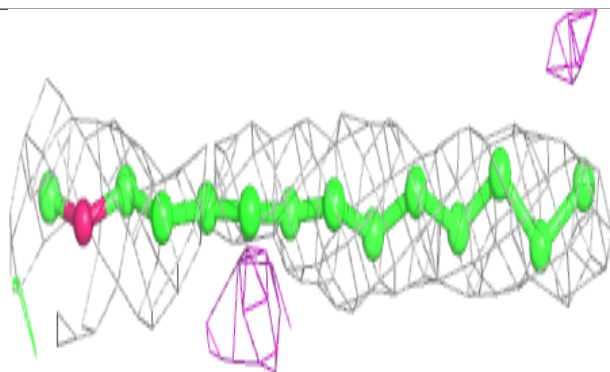
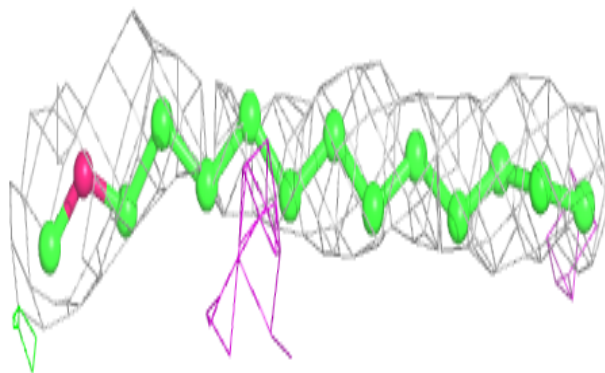
**Electron density around PLC A 506:**

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

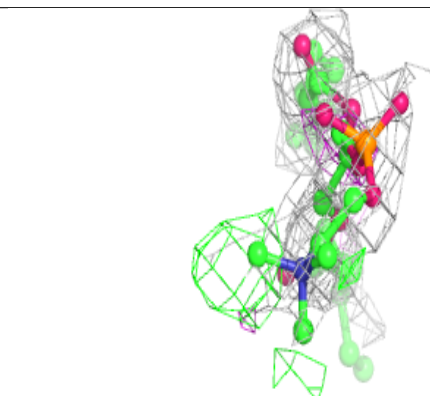
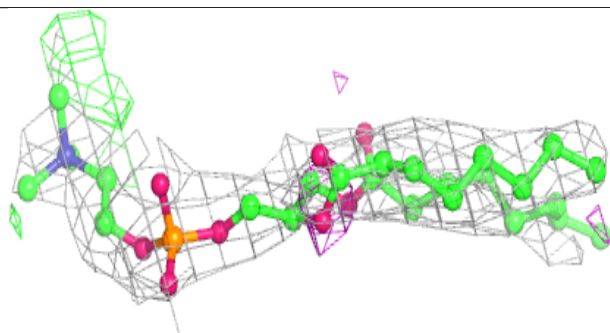
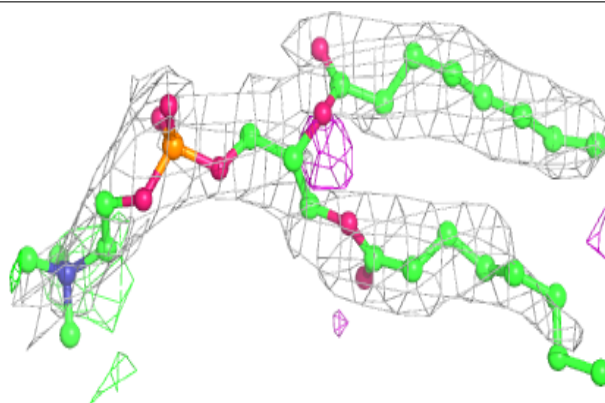


**Electron density around LMT B 501:**

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

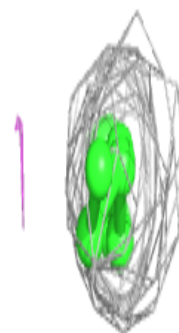
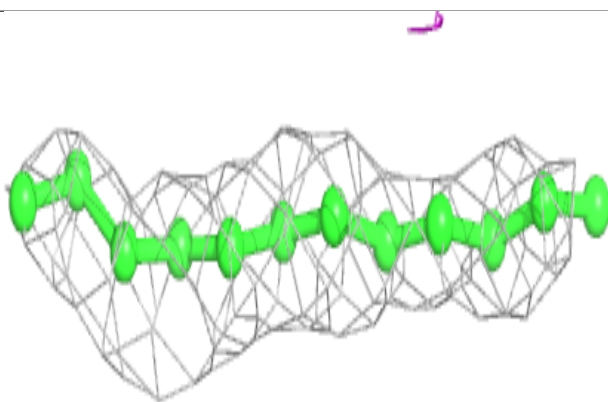
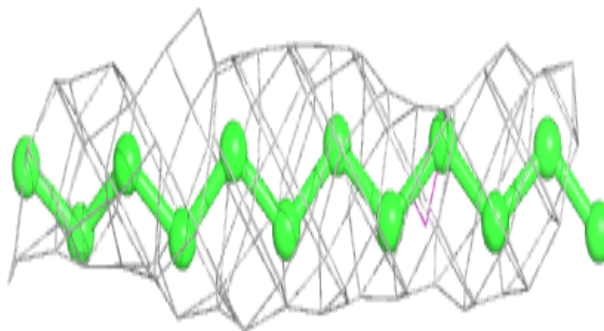
**Electron density around PLC E 406:**

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

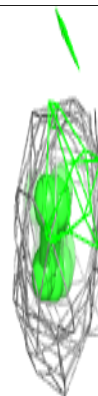
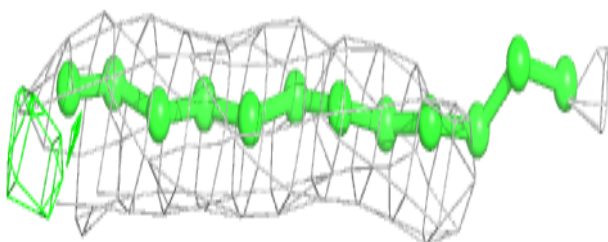
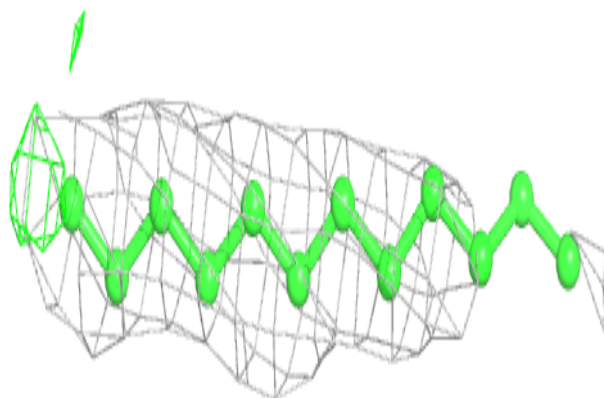


**Electron density around PLC A 508:**

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

**Electron density around PLC E 408:**

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



## 6.5 Other polymers

There are no such residues in this entry.