



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 12:24 PM BST

PDB ID : 6TOS  
Title : Crystal structure of the Orexin-1 receptor in complex with GSK1059865  
Authors : Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.  
Deposited on : 2019-12-11  
Resolution : 2.13 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 : 2.13.1  
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) : 2.13.1

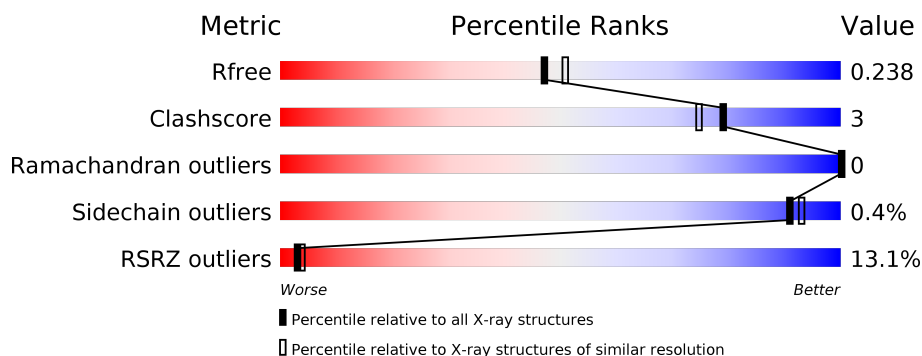
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	336	<div> <div>11%</div> <div>85%</div> <div>10%</div> </div>
1	B	336	<div> <div>13%</div> <div>85%</div> <div>7%</div> <div>9%</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	CIT	A	403	-	-	-	X
6	SOG	A	411	-	-	-	X
6	SOG	B	410	-	-	-	X
6	SOG	B	413	-	-	-	X
6	SOG	B	418	-	-	-	X
8	PGW	B	404	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5708 atoms, of which 46 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 Orexin receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	2	0
			2444	1626	404	397	17			
1	B	307	Total	C	N	O	S	0	2	0
			2458	1631	412	398	17			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU	ARG	engineered mutation	UNP O43613
A	194	ALA	ASN	engineered mutation	UNP O43613
A	198	ALA	LEU	engineered mutation	UNP O43613
A	211	ALA	TYR	engineered mutation	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	VAL	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ASN	deletion	UNP O43613
A	?	-	TRP	deletion	UNP O43613
A	?	-	LYS	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	SER	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP O43613
A	?	-	GLU	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	SER	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	GLU	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	PHE	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	304	VAL	LEU	engineered mutation	UNP O43613
A	339	ALA	CYS	engineered mutation	UNP O43613
A	375	TRP	CYS	engineered mutation	UNP O43613
A	376	TRP	CYS	engineered mutation	UNP O43613
A	381	ALA	-	expression tag	UNP O43613
A	382	ALA	-	expression tag	UNP O43613
A	383	ALA	-	expression tag	UNP O43613
A	384	HIS	-	expression tag	UNP O43613
A	385	HIS	-	expression tag	UNP O43613
A	386	HIS	-	expression tag	UNP O43613
A	387	HIS	-	expression tag	UNP O43613
A	388	HIS	-	expression tag	UNP O43613
A	389	HIS	-	expression tag	UNP O43613
A	390	HIS	-	expression tag	UNP O43613
A	391	HIS	-	expression tag	UNP O43613
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered mutation	UNP O43613
B	162	LEU	ARG	engineered mutation	UNP O43613
B	194	ALA	ASN	engineered mutation	UNP O43613
B	198	ALA	LEU	engineered mutation	UNP O43613

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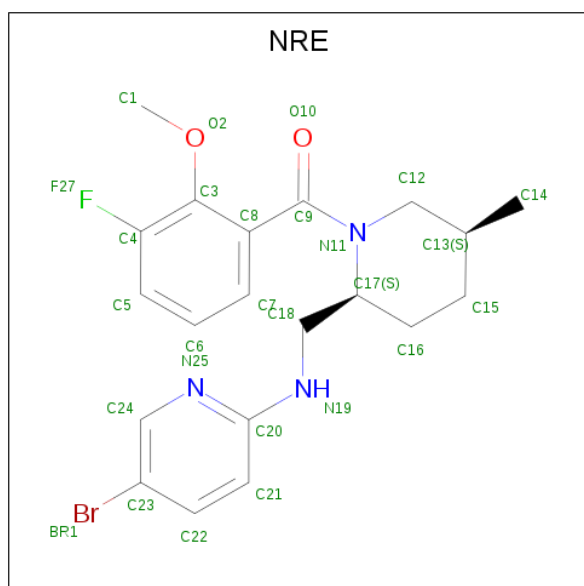
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	PHE	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	304	VAL	LEU	engineered mutation	UNP O43613
B	339	ALA	CYS	engineered mutation	UNP O43613
B	375	TRP	CYS	engineered mutation	UNP O43613
B	376	TRP	CYS	engineered mutation	UNP O43613
B	381	ALA	-	expression tag	UNP O43613
B	382	ALA	-	expression tag	UNP O43613
B	383	ALA	-	expression tag	UNP O43613
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613

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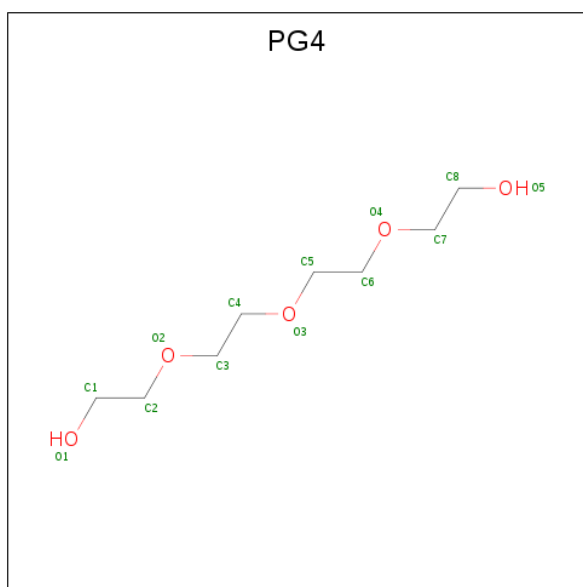
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is [(2 {S},5 {S})-2-[(5-bromanylpyridin-2-yl)amino]methyl]-5-methyl-piperidin-1-yl]-(3-fluoranyl-2-methoxy-phenyl)methanone (three-letter code: NRE) (formula: C<sub>20</sub>H<sub>23</sub>BrFN<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



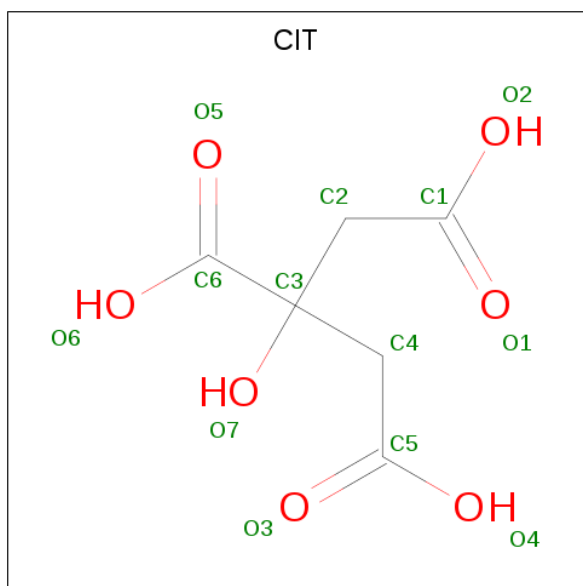
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	F	H	N	O		
2	A	1	50	1	20	1	23	3	2	0	0
2	B	1	50	1	20	1	23	3	2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		

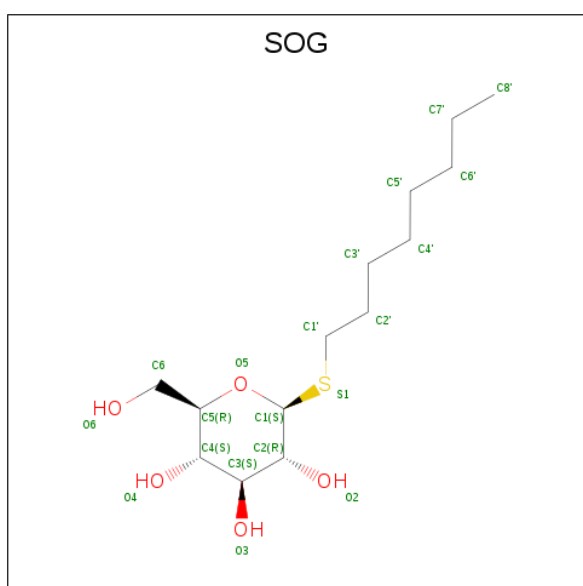
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





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		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula:  $C_{14}H_{28}O_5S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 20 14 5 1	0	0
6	A	1	Total C O S 20 14 5 1	0	0
6	A	1	Total C 5 5	0	0
6	A	1	Total C 8 8	0	0
6	A	1	Total C O S 20 14 5 1	0	0
6	A	1	Total C O S 14 8 5 1	0	0
6	A	1	Total C O S 20 14 5 1	0	0
6	A	1	Total C O S 14 8 5 1	0	0
6	A	1	Total C S 8 7 1	0	0
6	A	1	Total C O S 18 12 5 1	0	0
6	A	1	Total C S 6 5 1	0	0
6	A	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 13 7 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C S 10 9 1	0	0
6	B	1	Total C S 5 4 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C 6 6	0	0
6	B	1	Total C S 6 5 1	0	0
6	B	1	Total C O S 15 9 5 1	0	0

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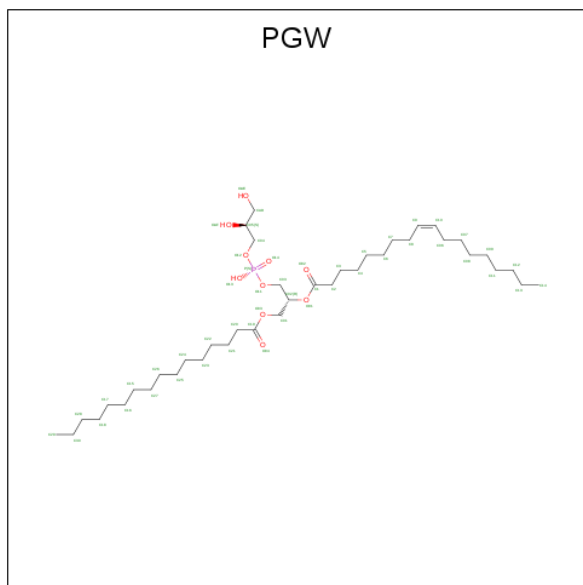
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0
6	B	1	Total C O S 20 14 5 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

- Molecule 8 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O P 51 40 10 1	0	0
8	B	1	Total C O P 51 40 10 1	0	0

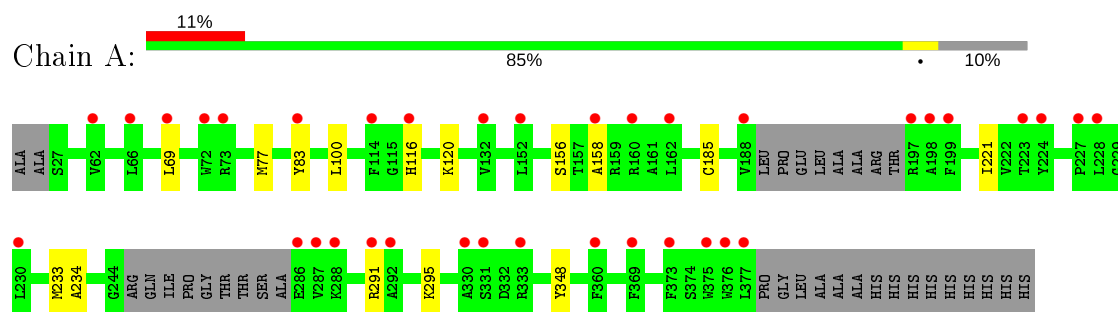
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	67	Total 67	O 67	0	0
9	B	84	Total 84	O 84	0	0

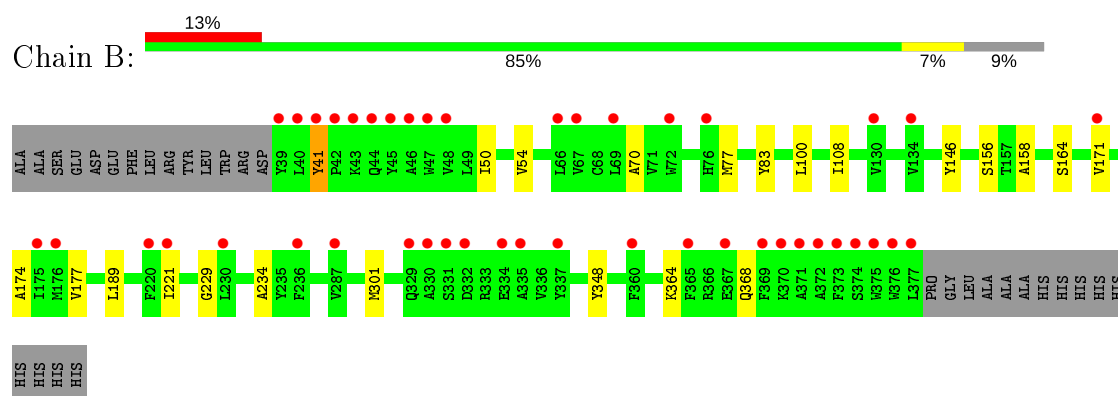
### 3 Residue-property plots [i](#)

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

- Molecule 1: Orexin receptor type 1



- Molecule 1: Orexin receptor type 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.69Å 146.19Å 71.51Å 90.00° 112.43° 90.00°	Depositor
Resolution (Å)	30.47 – 2.13 49.03 – 2.12	Depositor EDS
% Data completeness (in resolution range)	71.1 (30.47-2.13) 82.9 (49.03-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.46 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.193 , 0.218 0.215 , 0.238	Depositor DCC
$R_{free}$ test set	3031 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: SOG, NA, NRE, PGW, PG4, SO4, CIT

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	0.54	0/2520	0.63	1/3432 (0.0%)
1	B	0.56	1/2534 (0.0%)	0.62	1/3456 (0.0%)
All	All	0.55	1/5054 (0.0%)	0.63	2/6888 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	TYR	C-N	8.76	1.50	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	LEU	N-CA-C	-5.53	96.06	111.00
1	A	77	MET	CB-CA-C	-5.33	99.74	110.40

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	2444	0	2490	10	0
1	B	2458	0	2530	19	0
2	A	27	23	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	23	0	0	0
3	A	9	0	11	0	0
4	A	26	0	10	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	173	0	225	4	0
6	B	224	0	305	7	0
7	A	1	0	0	0	0
8	B	102	0	152	7	0
9	A	67	0	0	0	0
9	B	84	0	0	1	0
All	All	5662	46	5723	31	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 3.

The worst 5 of 31 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:234:ALA:HB2	8:B:404:PGW:H7A	1.62	0.79
1:B:174:ALA:HB1	8:B:405:PGW:H8	1.78	0.65
1:B:77:MET:HE1	1:B:368:GLN:HG3	1.80	0.64
1:B:156:SER:HB2	6:B:416:SOG:H5'1	1.80	0.62
1:B:41:TYR:HA	1:B:108:ILE:O	2.01	0.60

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	298/336 (89%)	293 (98%)	5 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/336 (91%)	302 (98%)	5 (2%)	0	100	100
All	All	605/672 (90%)	595 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	257/279 (92%)	255 (99%)	2 (1%)	81	85
1	B	258/279 (92%)	258 (100%)	0	100	100
All	All	515/558 (92%)	513 (100%)	2 (0%)	91	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	156	SER

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	350	ASN
1	A	368	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 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	$\# Z  > 2$
6	SOG	B	419	-	20,20,20	0.32	0	24,25,25	0.38	0
6	SOG	A	410	-	7,7,20	0.12	0	6,6,25	0.09	0
6	SOG	B	412	-	20,20,20	0.31	0	24,25,25	0.41	0
6	SOG	A	407	-	20,20,20	0.40	0	24,25,25	0.36	0
2	NRE	A	401	-	29,29,29	1.28	4 (13%)	35,40,40	1.51	4 (11%)
6	SOG	B	415	-	15,15,20	0.39	0	18,20,25	0.51	0
6	SOG	B	409	-	20,20,20	0.46	0	24,25,25	0.65	0
6	SOG	A	417	-	5,5,20	0.30	0	3,4,25	0.18	0
6	SOG	A	408	-	20,20,20	0.35	0	24,25,25	0.44	0
6	SOG	A	416	-	18,18,20	0.33	0	22,23,25	0.67	1 (4%)
6	SOG	B	414	-	5,5,20	0.33	0	3,4,25	0.12	0
6	SOG	A	409	-	4,4,20	0.15	0	3,3,25	0.20	0
6	SOG	B	417	-	20,20,20	0.35	0	24,25,25	0.29	0
3	PG4	A	402	-	8,8,12	0.18	0	7,7,11	0.23	0
6	SOG	A	411	-	20,20,20	0.33	0	24,25,25	0.44	0
4	CIT	A	403	-	3,12,12	0.59	0	3,17,17	0.94	0
8	PGW	B	405	-	50,50,50	0.30	0	53,56,56	0.36	0
6	SOG	A	413	-	20,20,20	0.40	0	24,25,25	0.62	0
5	SO4	B	402	-	4,4,4	0.22	0	6,6,6	0.39	0
8	PGW	B	404	-	50,50,50	0.32	0	53,56,56	0.35	0
6	SOG	A	414	-	14,14,20	0.32	0	18,19,25	0.81	1 (5%)
6	SOG	B	416	-	8,8,20	0.21	0	7,7,25	0.41	0
6	SOG	B	406	-	20,20,20	0.31	0	24,25,25	0.51	0
2	NRE	B	401	-	29,29,29	1.23	4 (13%)	35,40,40	1.45	4 (11%)
5	SO4	A	405	-	4,4,4	0.26	0	6,6,6	0.43	0
6	SOG	A	415	-	7,7,20	0.23	0	6,6,25	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SOG	B	407	-	12,13,20	0.60	0	16,18,25	0.46	0
6	SOG	A	418	-	20,20,20	0.36	0	24,25,25	0.32	0
6	SOG	B	418	-	20,20,20	0.37	0	24,25,25	0.40	0
6	SOG	A	412	-	14,14,20	0.44	0	18,19,25	0.90	2 (11%)
6	SOG	B	408	-	20,20,20	0.41	0	24,25,25	0.78	1 (4%)
4	CIT	A	404	-	3,12,12	0.65	0	3,17,17	0.73	0
5	SO4	B	403	-	4,4,4	0.19	0	6,6,6	0.39	0
6	SOG	B	410	-	9,9,20	0.20	0	8,8,25	0.10	0
6	SOG	B	420	-	20,20,20	0.31	0	24,25,25	0.33	0
6	SOG	B	411	-	4,4,20	0.39	0	3,3,25	0.08	0
5	SO4	A	406	-	4,4,4	0.08	0	6,6,6	0.19	0
6	SOG	B	413	-	5,5,20	0.15	0	4,4,25	0.09	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
6	SOG	B	419	-	-	7/11/31/31	0/1/1/1
6	SOG	A	410	-	-	5/5/5/31	-
6	SOG	B	412	-	-	4/11/31/31	0/1/1/1
6	SOG	A	407	-	-	4/11/31/31	0/1/1/1
2	NRE	A	401	-	-	1/15/28/28	0/3/3/3
6	SOG	B	415	-	-	3/6/26/31	0/1/1/1
6	SOG	B	409	-	-	10/11/31/31	0/1/1/1
6	SOG	A	408	-	-	4/11/31/31	0/1/1/1
6	SOG	A	416	-	-	4/9/29/31	0/1/1/1
6	SOG	B	414	-	-	1/3/3/31	-
6	SOG	A	409	-	-	1/2/2/31	-
6	SOG	B	417	-	-	10/11/31/31	0/1/1/1
3	PG4	A	402	-	-	5/6/6/10	-
6	SOG	A	411	-	-	5/11/31/31	0/1/1/1
6	SOG	B	418	-	-	8/11/31/31	0/1/1/1
8	PGW	B	405	-	-	29/55/55/55	-
6	SOG	A	413	-	-	8/11/31/31	0/1/1/1
6	SOG	A	417	-	-	0/3/3/31	-
8	PGW	B	404	-	1/1/5/7	29/55/55/55	-
6	SOG	A	414	-	-	2/5/25/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	B	416	-	-	2/6/6/31	-
6	SOG	B	406	-	-	4/11/31/31	0/1/1/1
2	NRE	B	401	-	-	1/15/28/28	0/3/3/3
6	SOG	A	415	-	-	3/5/5/31	-
6	SOG	B	407	-	-	2/4/24/31	0/1/1/1
6	SOG	A	418	-	-	5/11/31/31	0/1/1/1
4	CIT	A	403	-	-	6/6/16/16	-
6	SOG	A	412	-	-	2/5/25/31	0/1/1/1
6	SOG	B	408	-	-	5/11/31/31	0/1/1/1
4	CIT	A	404	-	-	1/6/16/16	-
6	SOG	B	410	-	-	2/7/7/31	-
6	SOG	B	420	-	-	7/11/31/31	0/1/1/1
6	SOG	B	411	-	-	0/2/2/31	-
6	SOG	B	413	-	-	2/3/3/31	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NRE	C17-N11	2.93	1.50	1.47
2	A	401	NRE	C12-N11	2.84	1.50	1.46
2	A	401	NRE	C20-N19	2.81	1.40	1.36
2	B	401	NRE	C12-N11	2.74	1.50	1.46
2	B	401	NRE	C20-N19	2.73	1.40	1.36

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NRE	C1-O2-C3	4.39	126.82	114.78
2	A	401	NRE	C1-O2-C3	3.64	124.76	114.78
2	A	401	NRE	C8-C9-N11	3.32	122.51	117.92
2	A	401	NRE	O10-C9-C8	-3.22	113.57	120.06
2	B	401	NRE	F27-C4-C3	3.00	121.69	117.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	404	PGW	C05

5 of 182 torsion outliers are listed below:

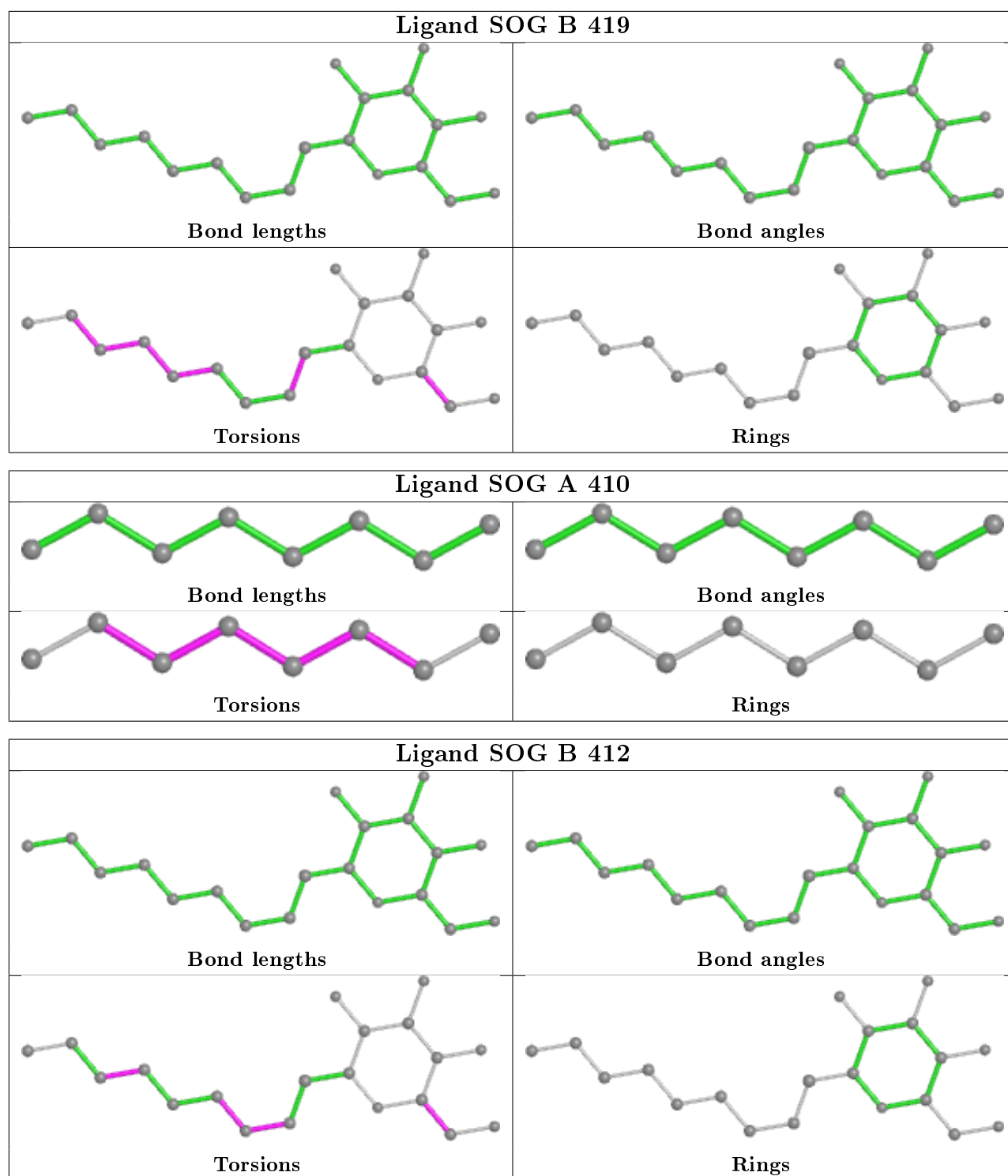
Mol	Chain	Res	Type	Atoms
6	B	419	SOG	C2'-C1'-S1-C1
6	B	409	SOG	C2-C1-S1-C1'
6	B	409	SOG	C2'-C1'-S1-C1
8	B	405	PGW	C03-O11-P-O13
8	B	405	PGW	C04-O12-P-O14

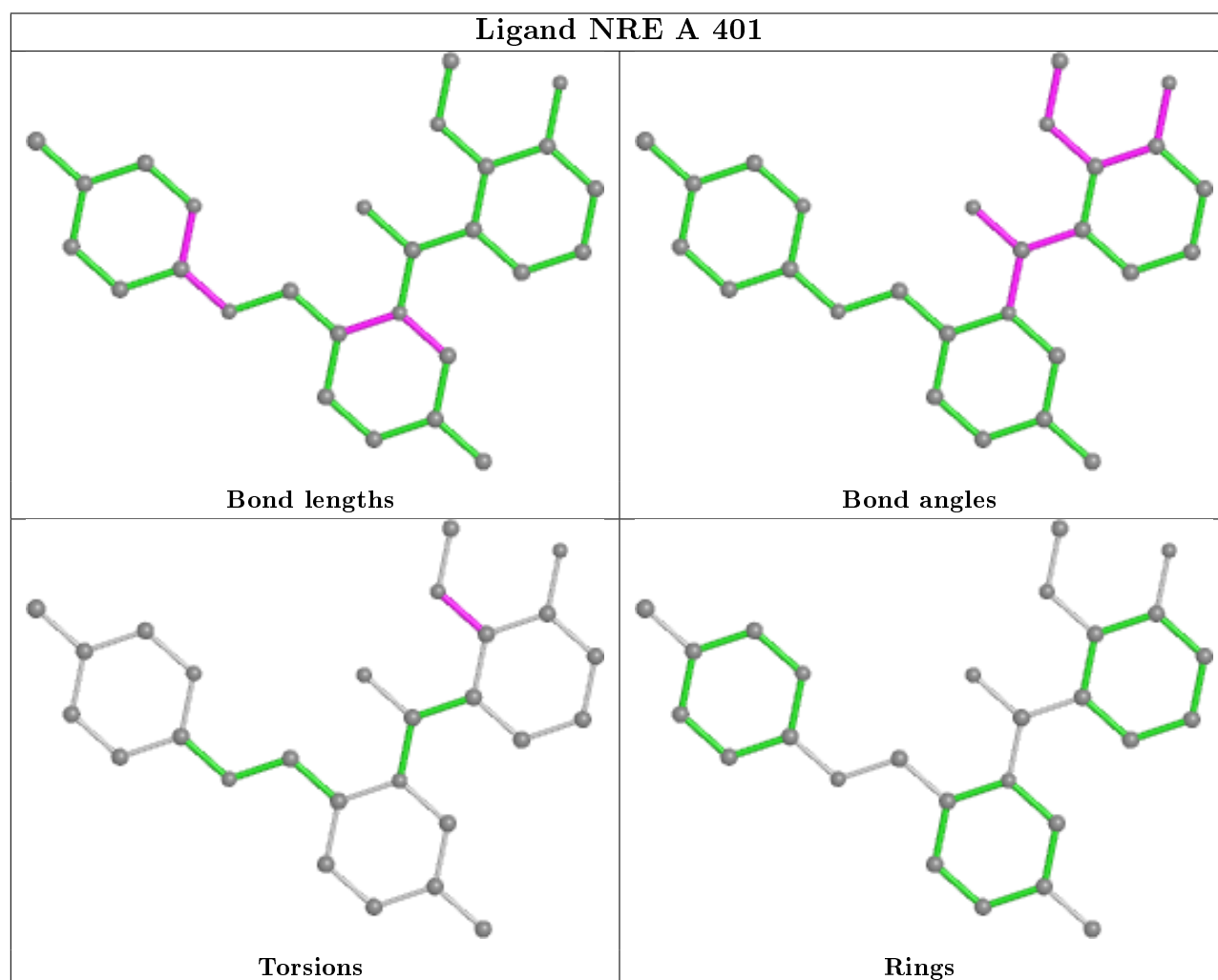
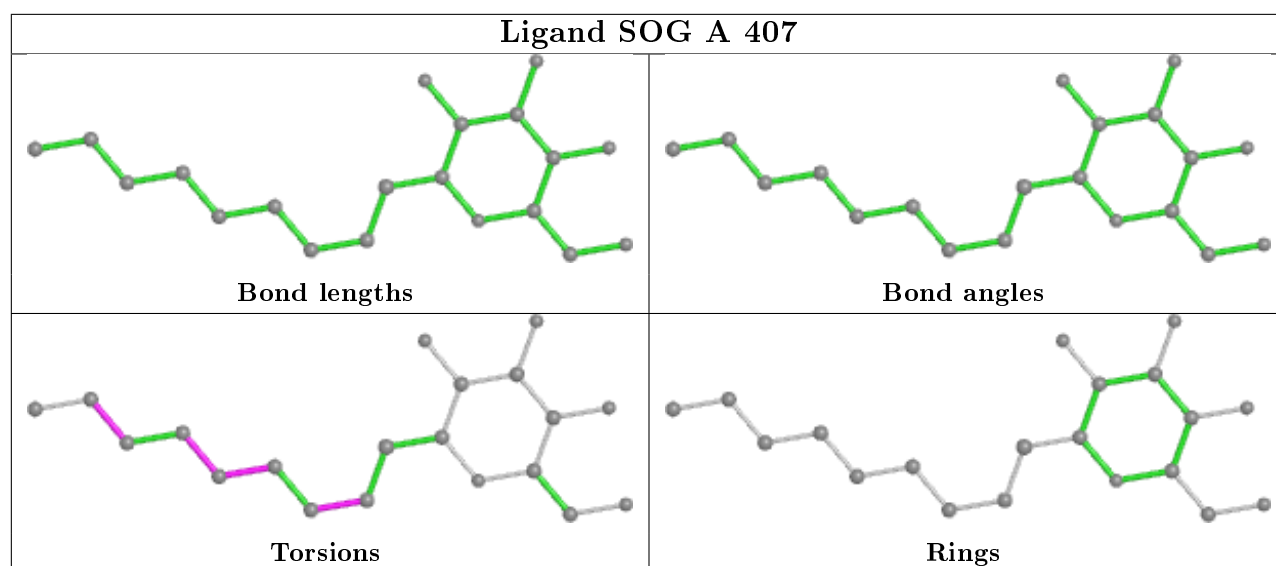
There are no ring outliers.

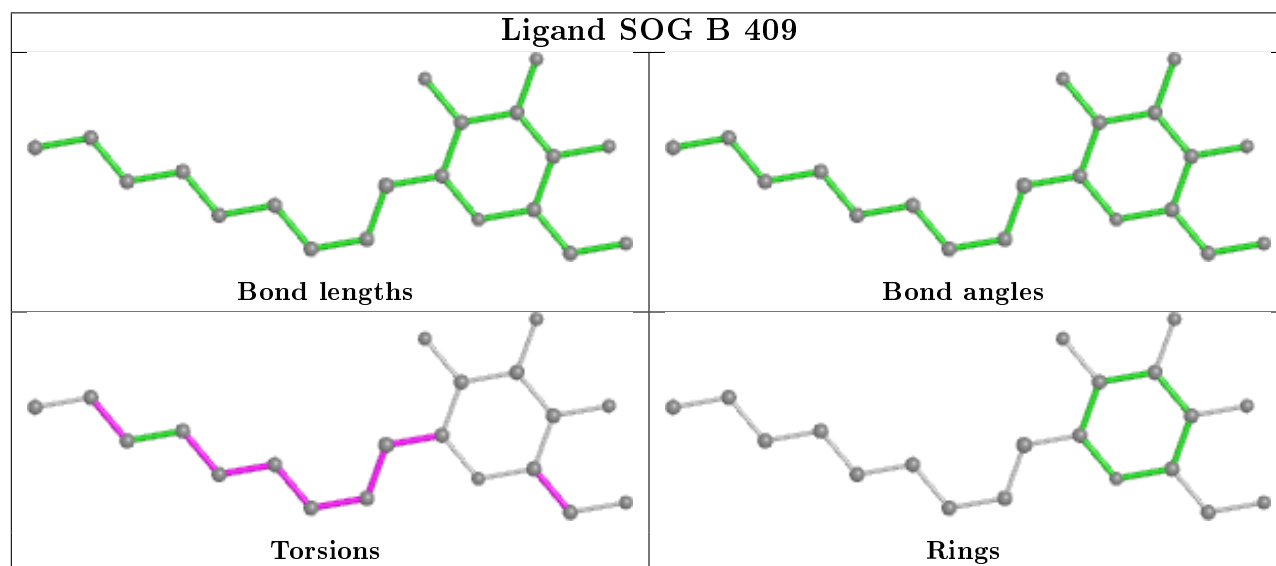
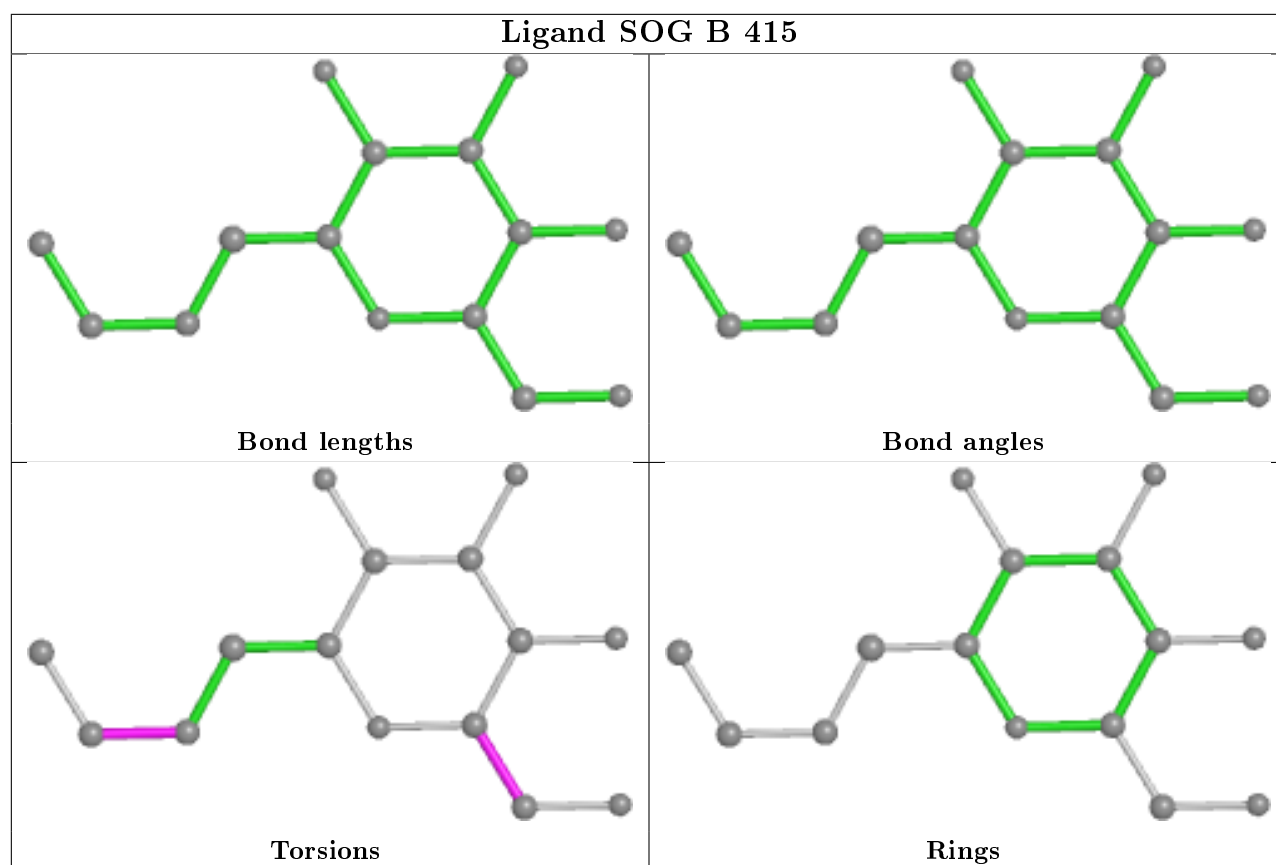
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	412	SOG	2	0
6	A	408	SOG	2	0
8	B	405	PGW	5	0
6	A	413	SOG	1	0
8	B	404	PGW	2	0
6	A	414	SOG	1	0
6	B	416	SOG	3	0
6	B	408	SOG	1	0
6	B	420	SOG	1	0

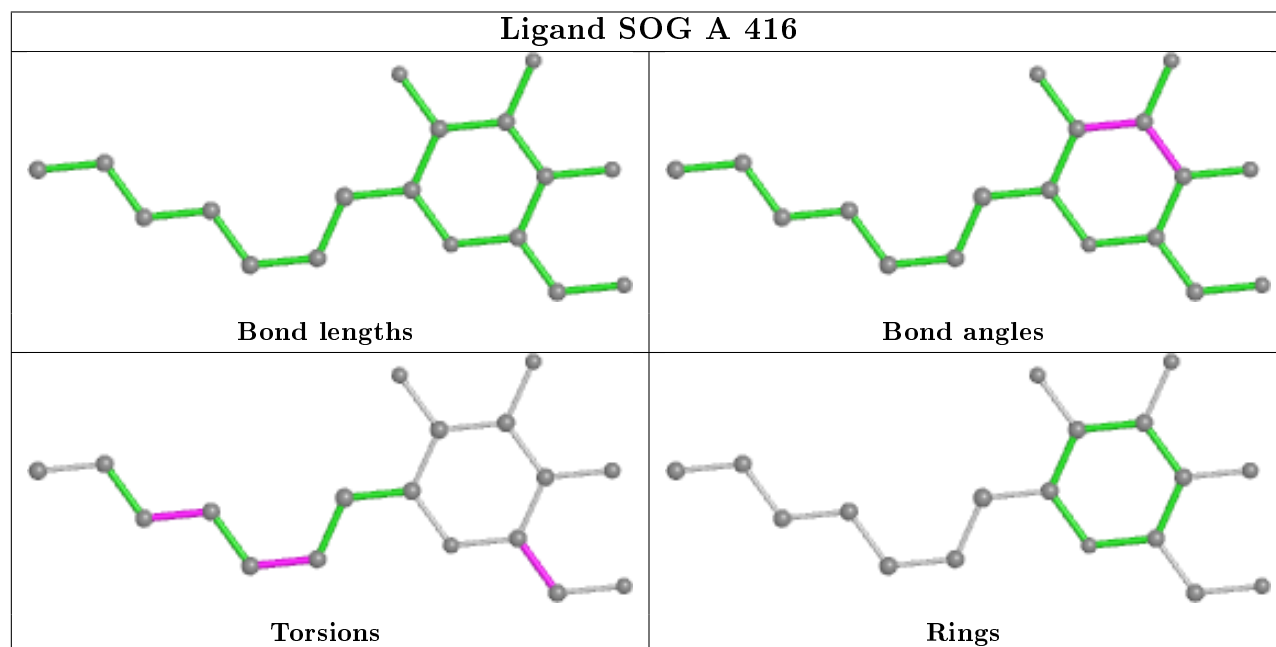
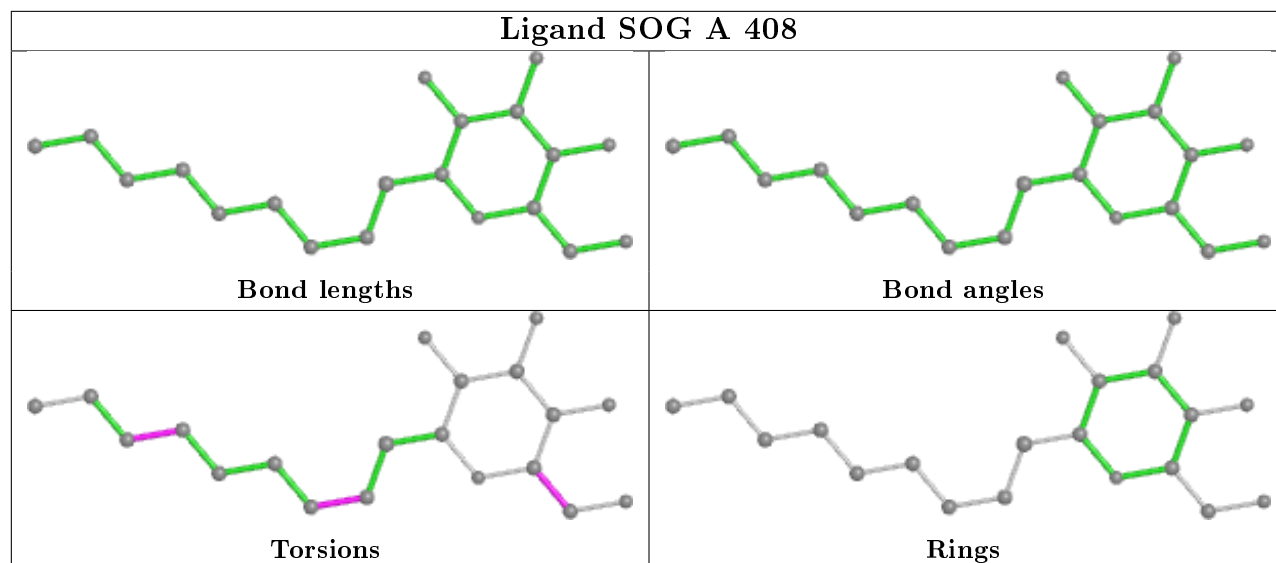
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

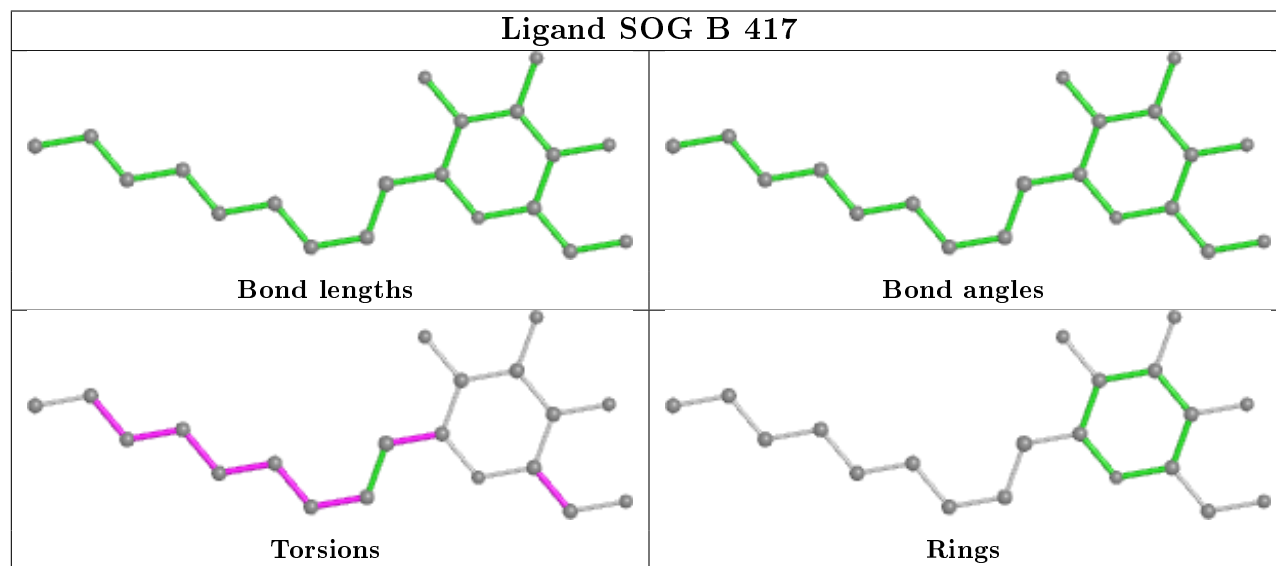
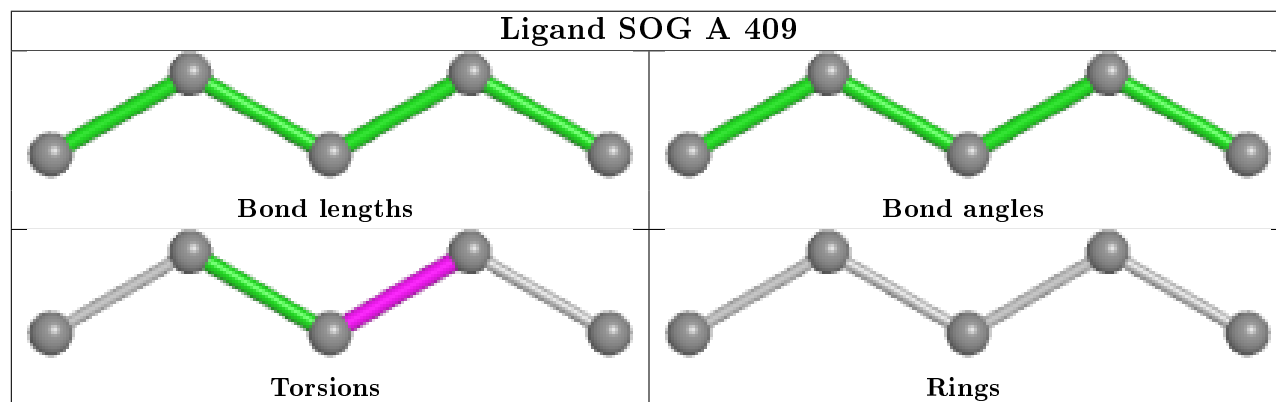
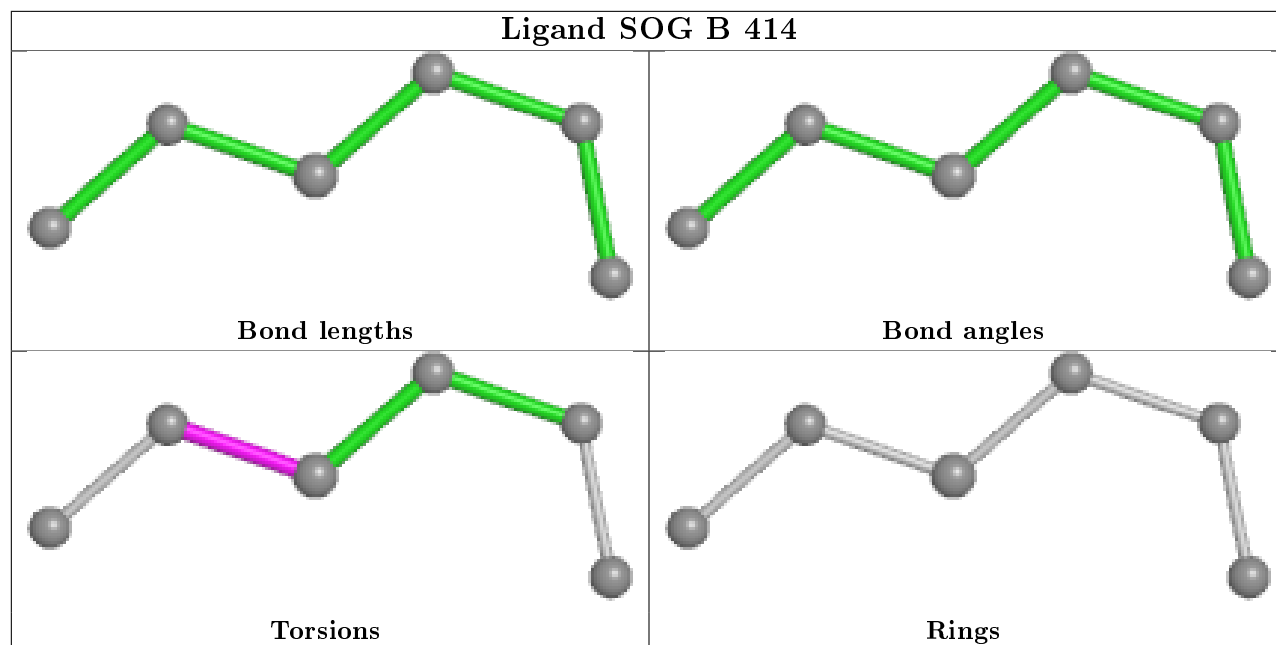




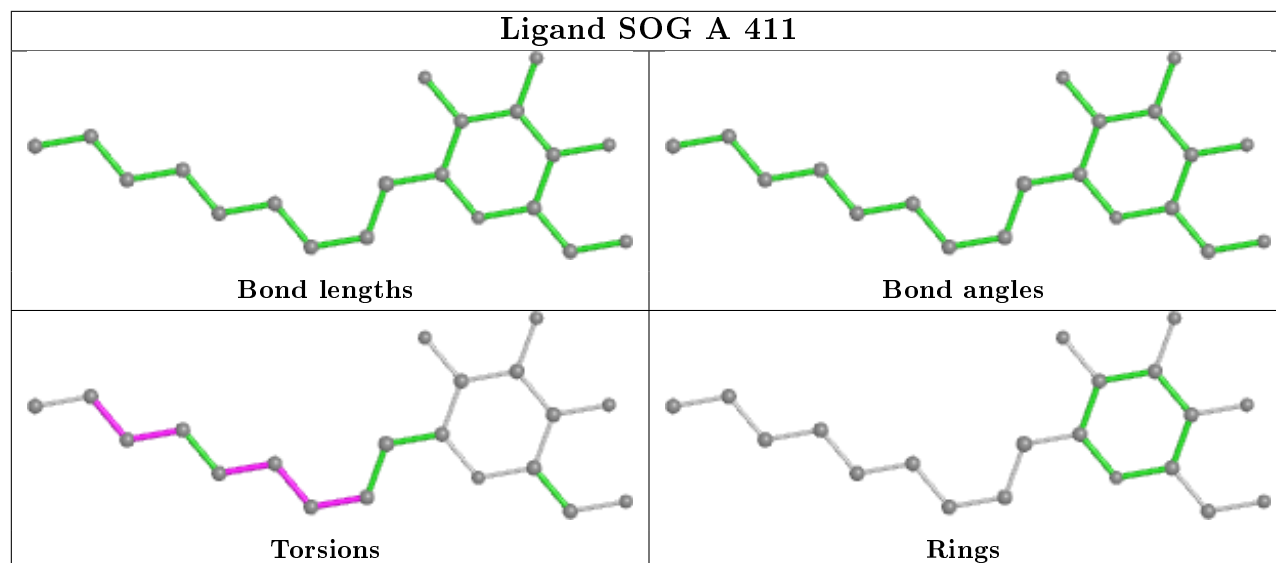




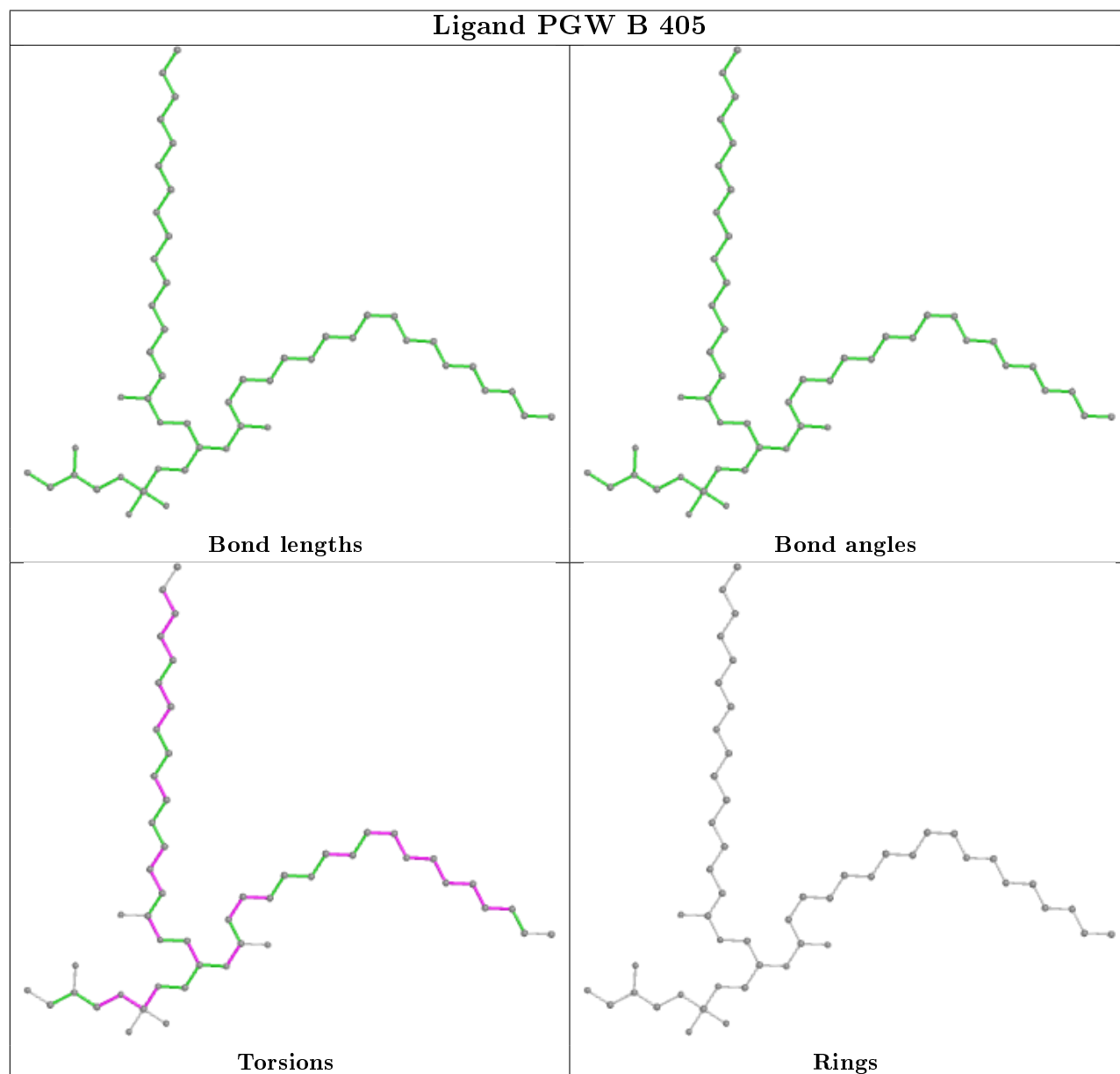




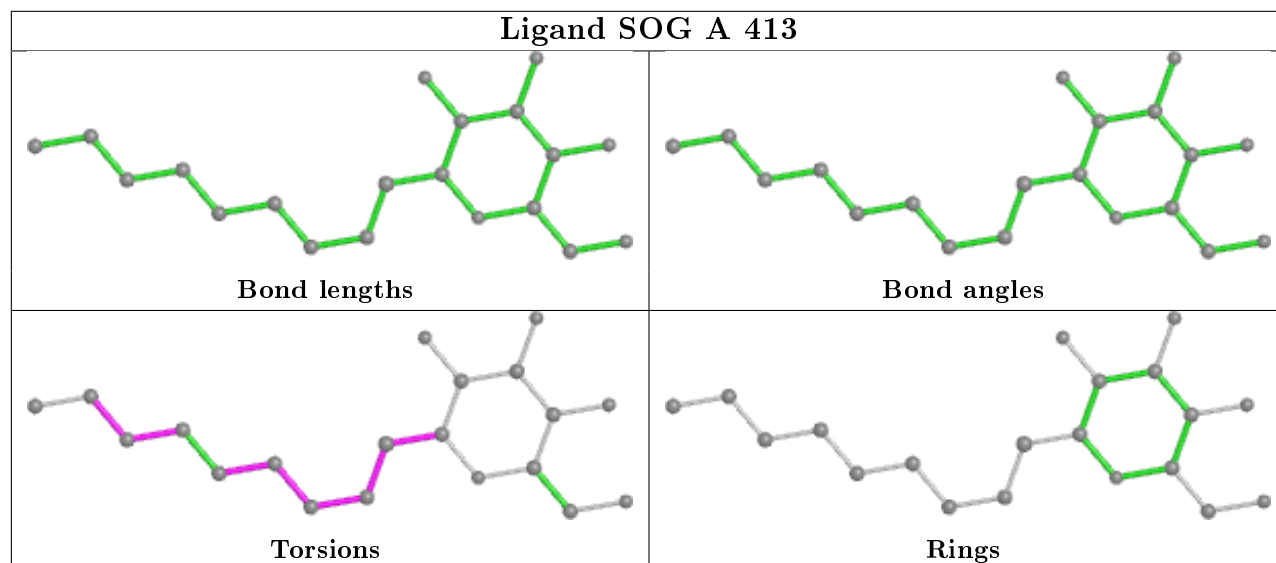
## Ligand SOG A 411



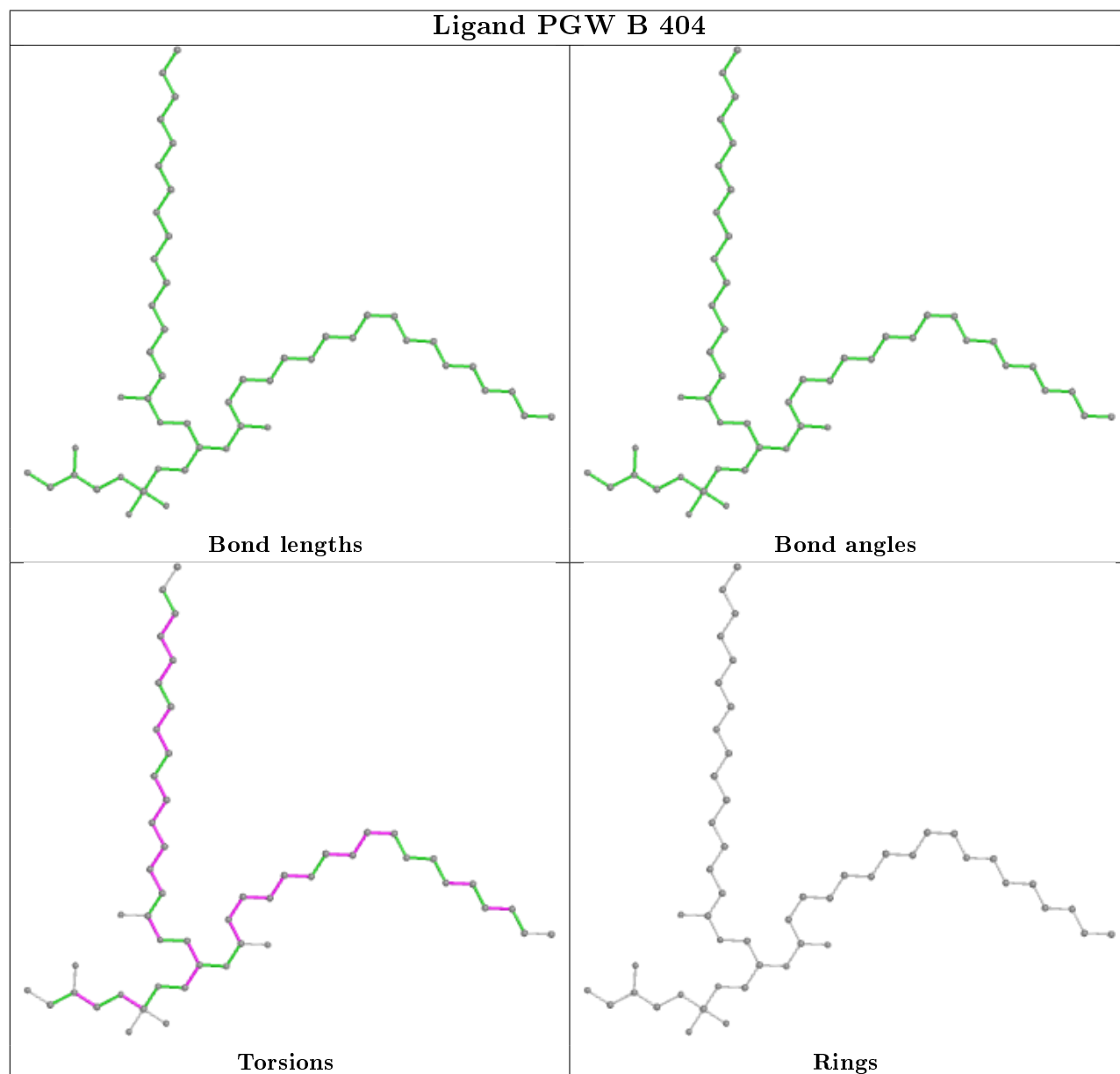
## Ligand PGW B 405

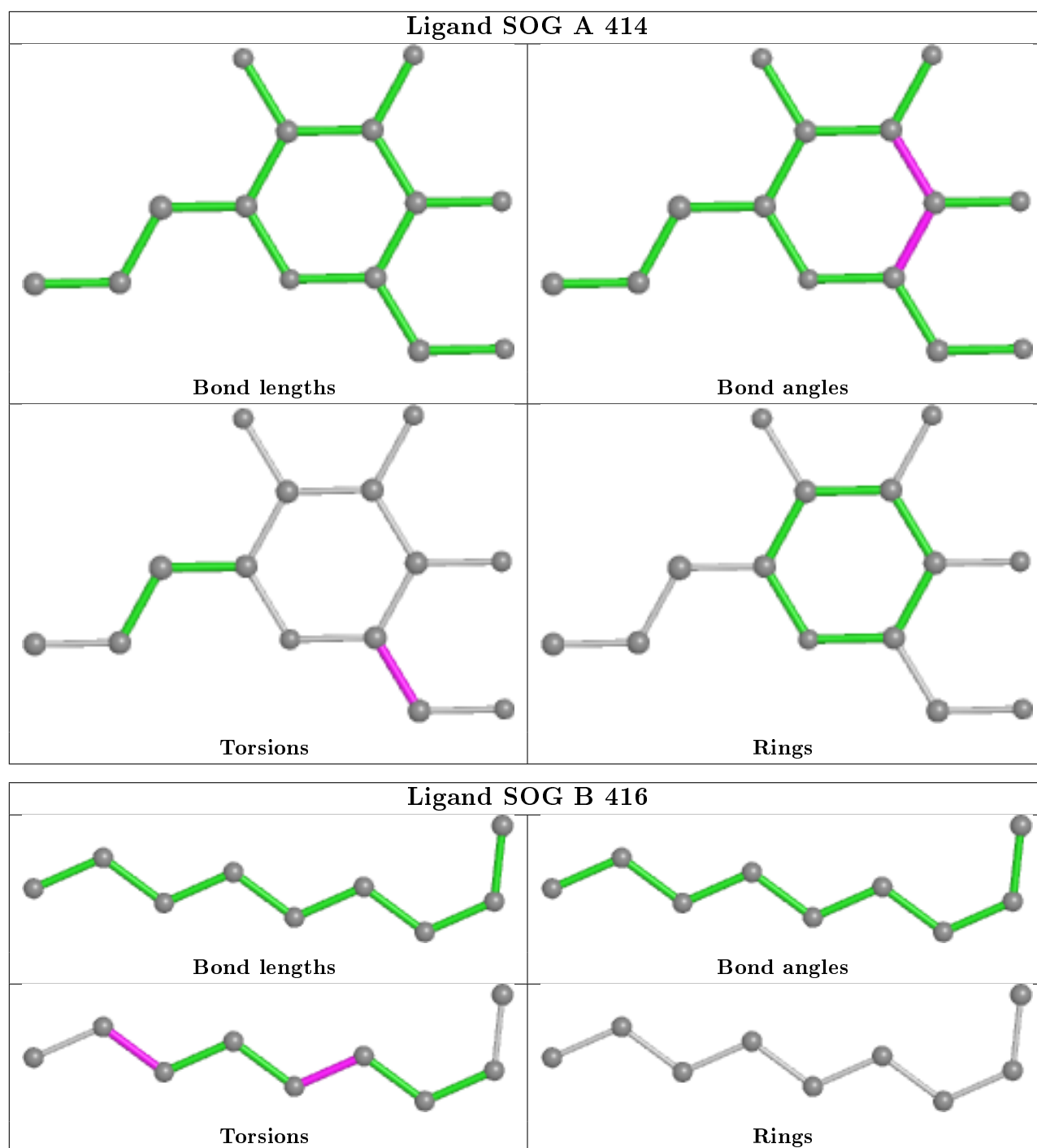


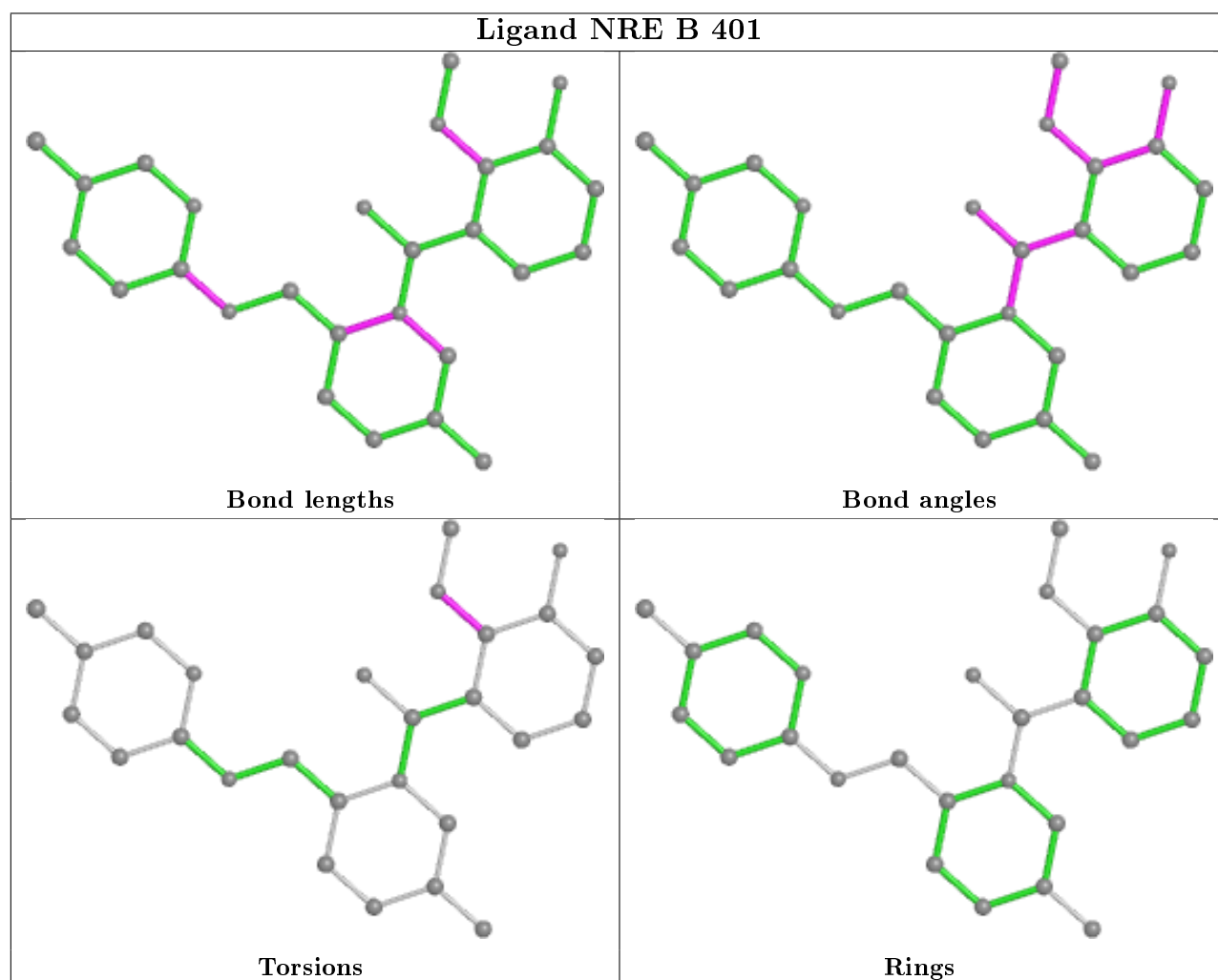
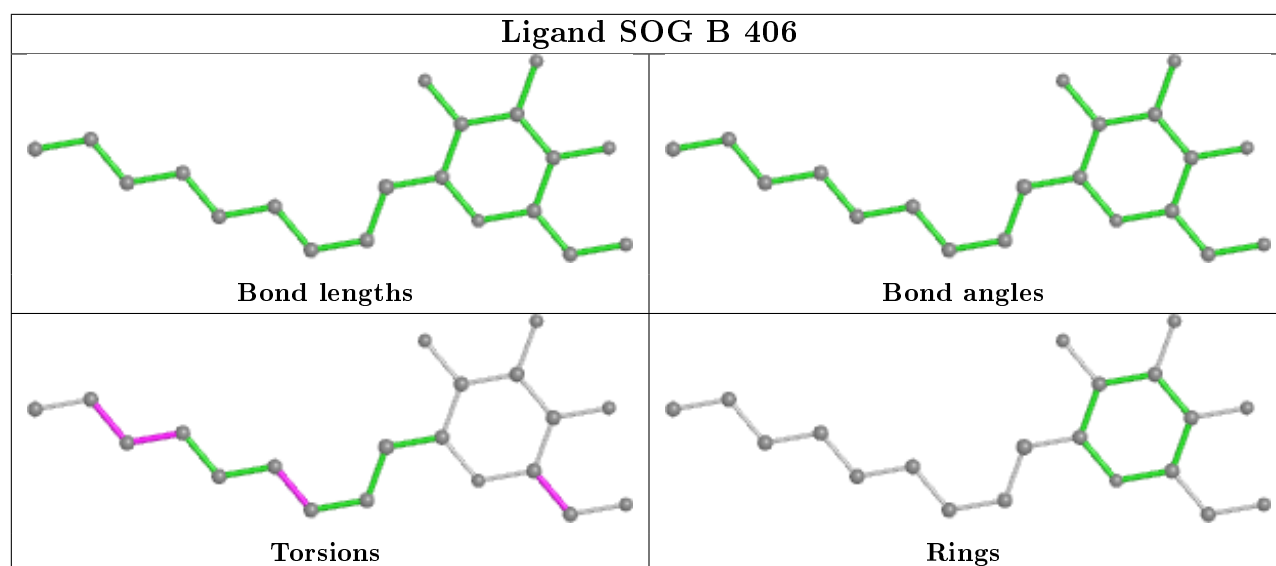
## Ligand SOG A 413

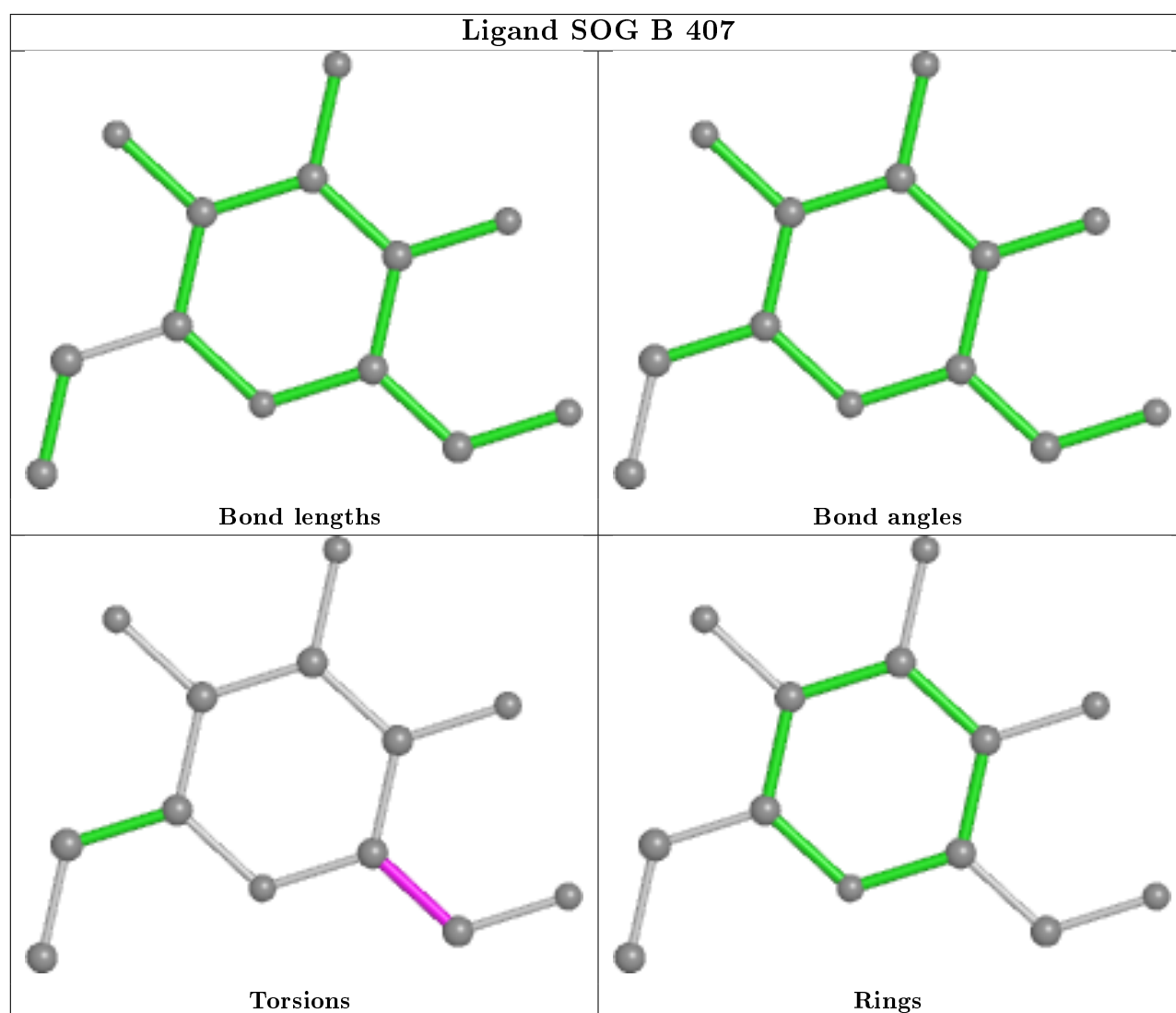
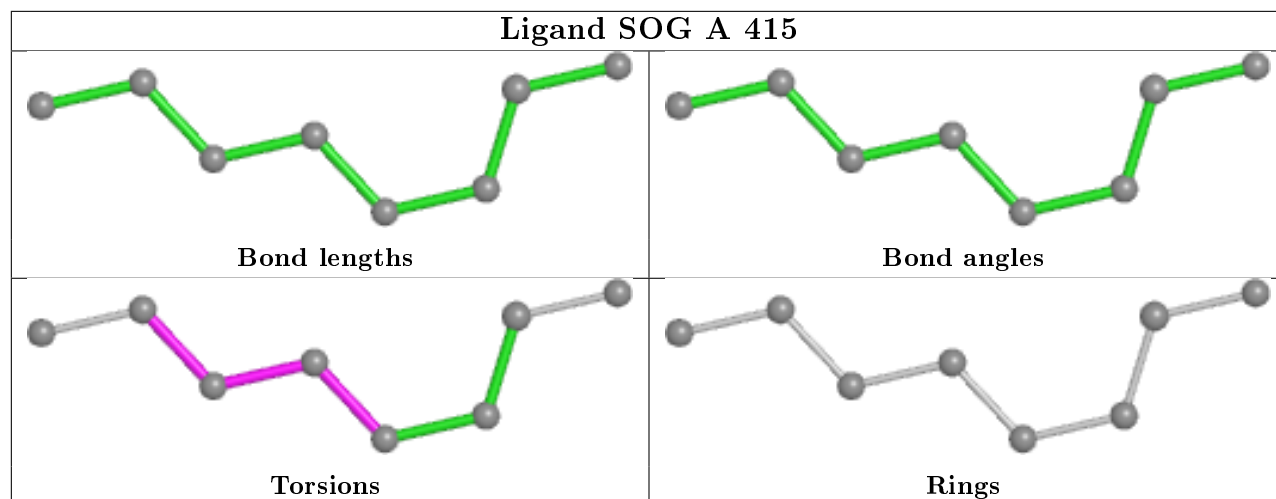


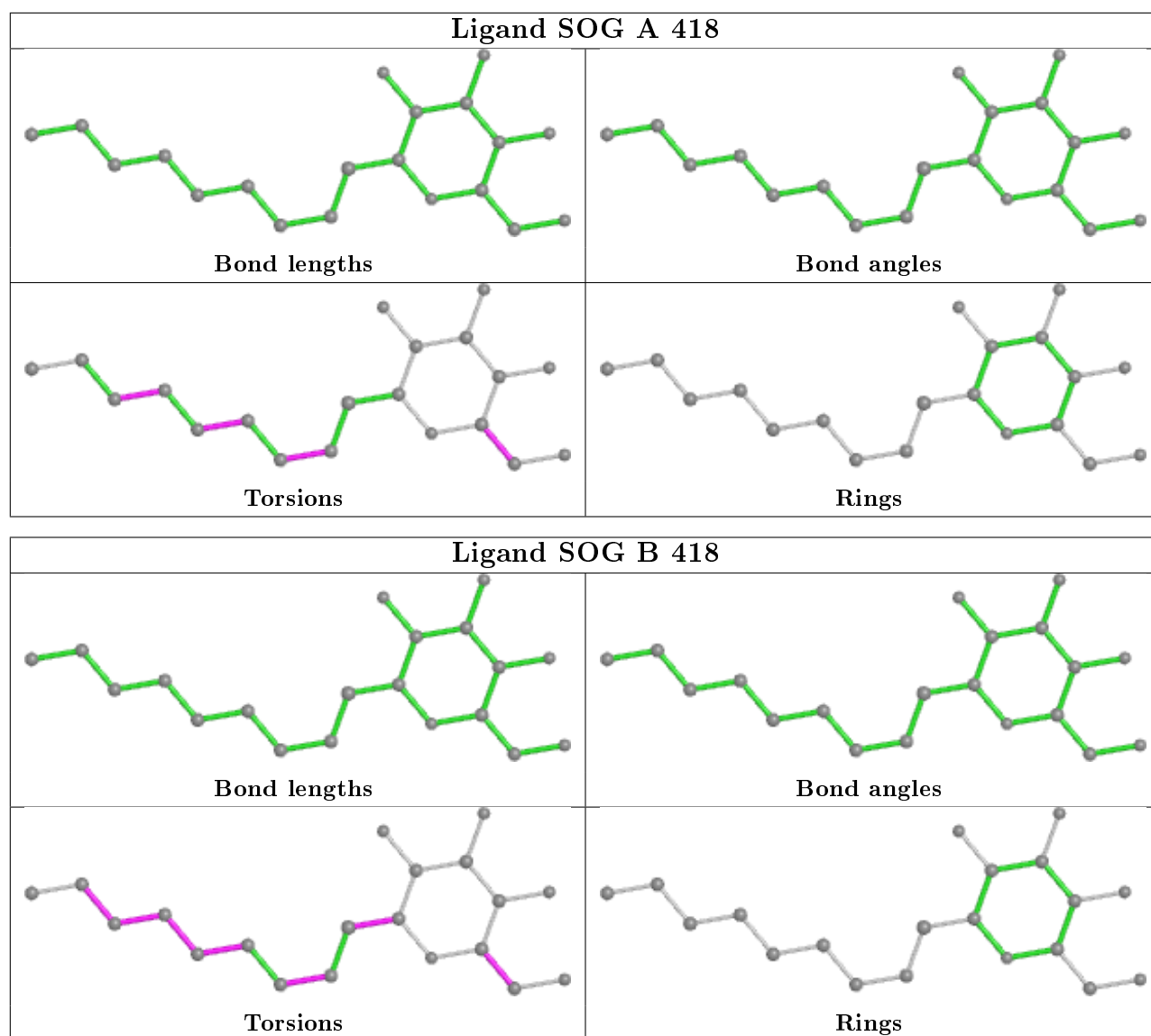
## Ligand PGW B 404



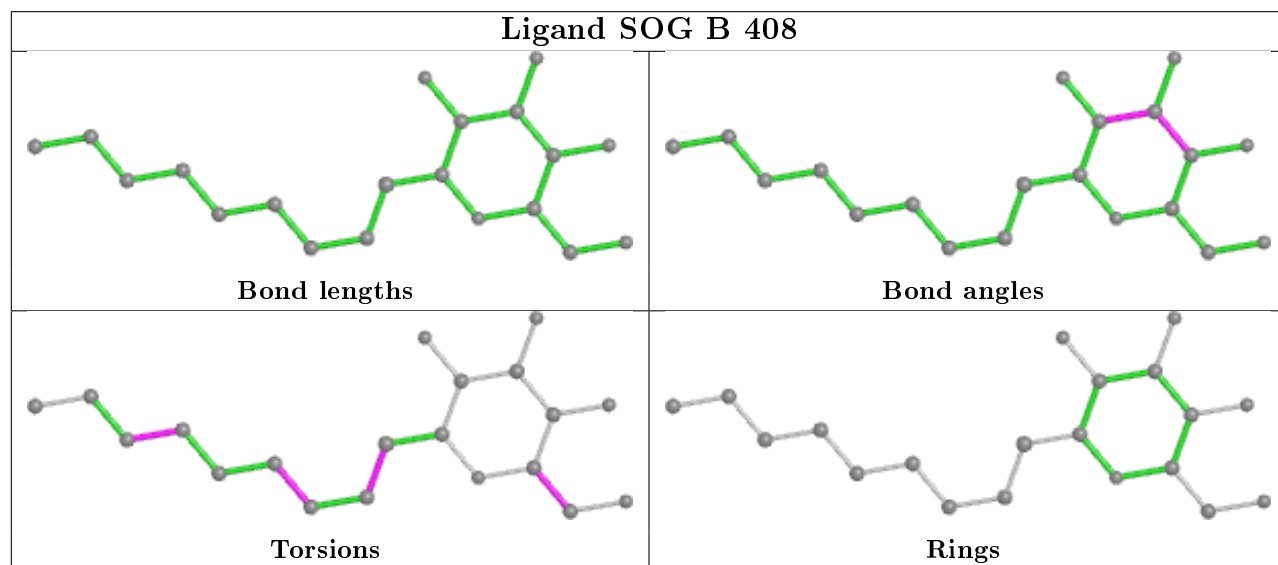
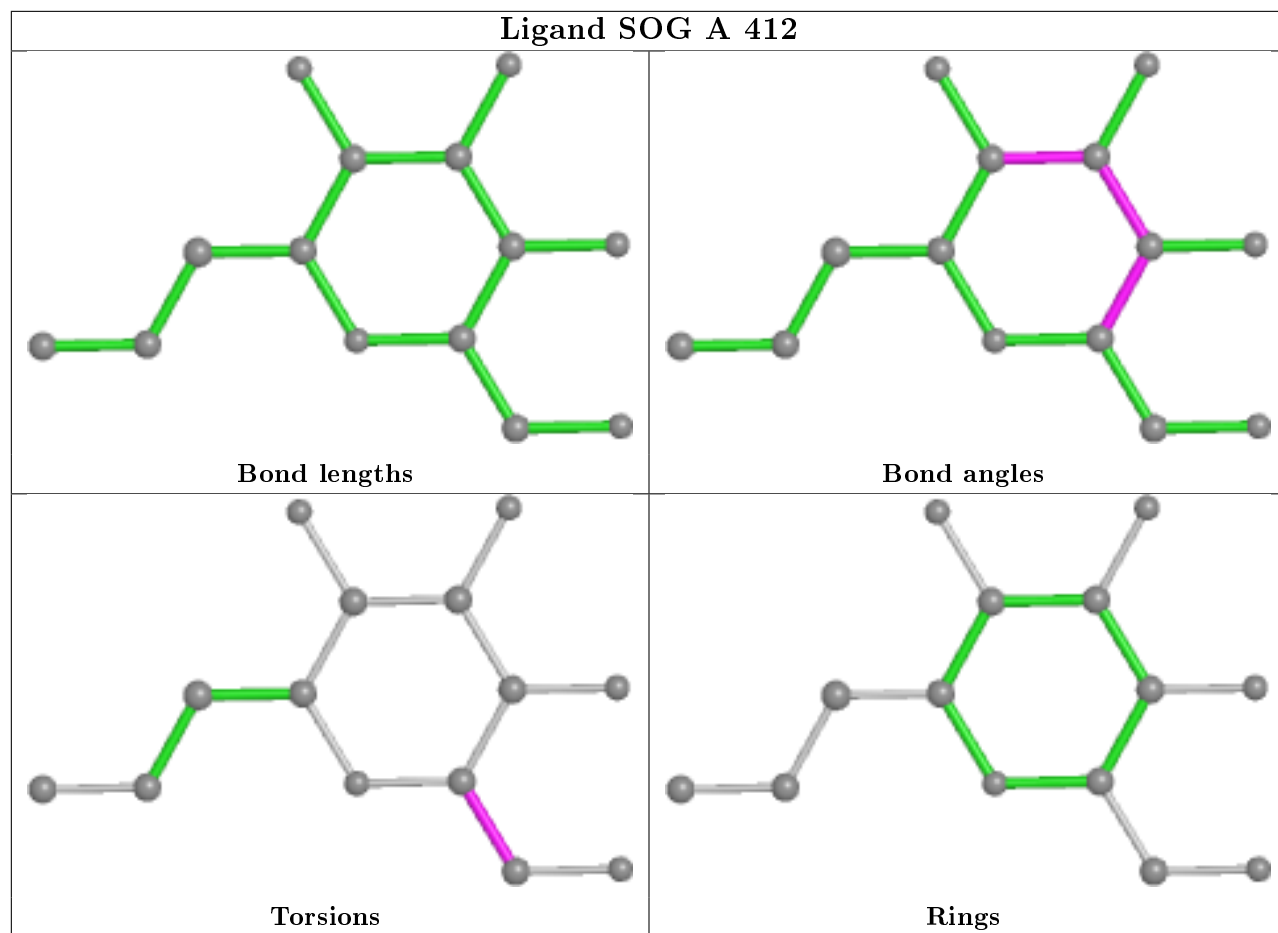


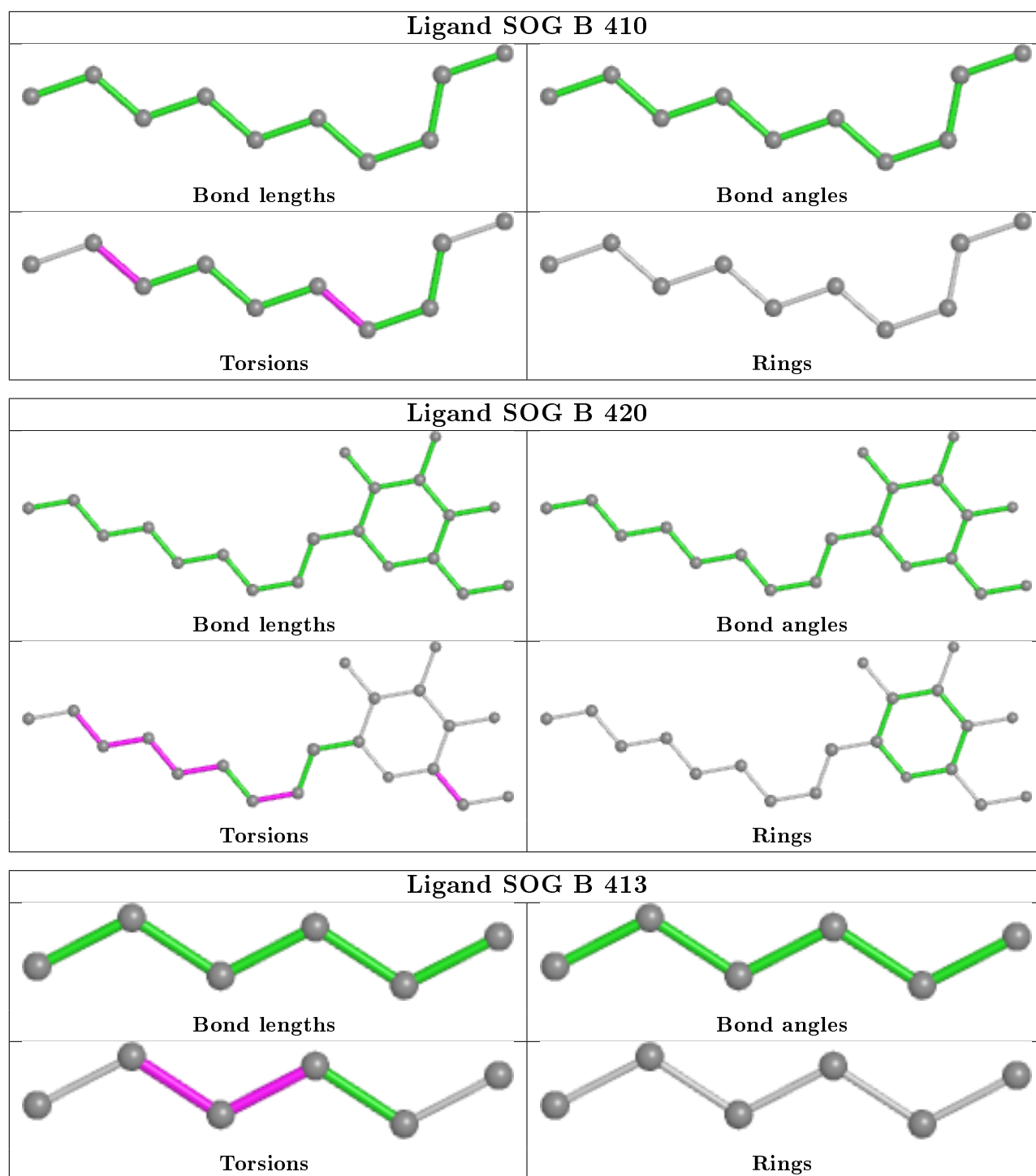












## 5.7 Other polymers [i](#)

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	302/336 (89%)	0.74	36 (11%) 4 5	29, 48, 102, 147	0
1	B	307/336 (91%)	0.93	44 (14%) 2 3	30, 47, 96, 144	0
All	All	609/672 (90%)	0.84	80 (13%) 3 4	29, 47, 100, 147	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	TYR	11.2
1	A	376	TRP	10.6
1	A	377	LEU	9.4
1	B	42	PRO	9.2
1	B	376	TRP	8.9

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

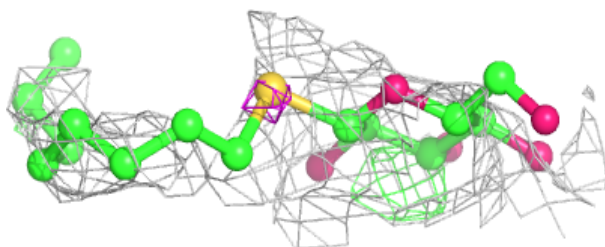
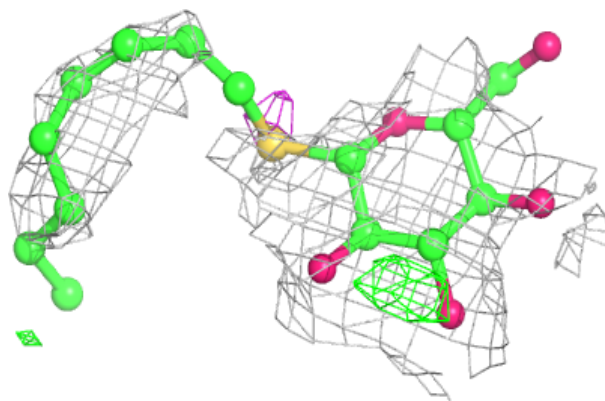
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
6	SOG	B	411	5/20	0.51	0.27	88,89,92,94	0
4	CIT	A	403	13/13	0.55	0.60	134,137,139,139	0
6	SOG	B	417	20/20	0.56	0.29	128,139,143,144	0
6	SOG	A	418	20/20	0.60	0.27	125,135,137,137	0
6	SOG	B	419	20/20	0.61	0.36	77,117,121,122	0
6	SOG	A	417	6/20	0.63	0.26	107,109,109,110	0
4	CIT	A	404	13/13	0.67	0.32	141,145,147,147	0
3	PG4	A	402	9/13	0.67	0.22	92,101,104,105	0
6	SOG	A	413	20/20	0.68	0.23	64,98,101,103	0
6	SOG	A	414	14/20	0.69	0.21	105,113,114,115	0
6	SOG	B	416	9/20	0.70	0.24	62,72,92,97	0
6	SOG	B	418	20/20	0.71	0.54	137,139,140,140	0
6	SOG	B	409	20/20	0.71	0.24	107,113,115,115	0
6	SOG	B	413	6/20	0.73	0.50	65,69,71,71	0
8	PGW	B	404	51/51	0.75	0.28	39,65,110,111	0
6	SOG	B	410	10/20	0.76	0.64	100,101,104,105	0
8	PGW	B	405	51/51	0.76	0.26	39,62,106,112	0
6	SOG	B	414	6/20	0.76	0.23	116,117,118,118	0
6	SOG	A	411	20/20	0.78	0.46	101,102,105,105	0
6	SOG	B	415	15/20	0.78	0.17	110,116,118,119	0
6	SOG	B	407	13/20	0.80	0.20	85,90,92,92	0
6	SOG	B	408	20/20	0.80	0.17	55,89,91,93	0
6	SOG	A	410	8/20	0.80	0.27	71,72,73,74	0
6	SOG	A	407	20/20	0.81	0.27	56,81,88,90	0
6	SOG	A	416	18/20	0.81	0.30	121,125,128,128	0
6	SOG	A	408	20/20	0.82	0.18	94,106,110,111	0
6	SOG	B	420	20/20	0.82	0.29	98,121,125,126	0
5	SO4	A	406	5/5	0.84	0.25	103,105,106,108	0
6	SOG	A	412	14/20	0.86	0.27	78,82,84,84	0
6	SOG	B	412	20/20	0.87	0.20	91,102,105,106	0
6	SOG	A	415	8/20	0.88	0.48	71,80,97,98	0
5	SO4	B	403	5/5	0.91	0.21	91,94,95,96	0
7	NA	A	419	1/1	0.92	0.21	71,71,71,71	0
6	SOG	B	406	20/20	0.93	0.11	42,50,55,56	0
5	SO4	A	405	5/5	0.95	0.15	71,76,78,80	0
2	NRE	B	401	27/27	0.95	0.13	41,43,49,64	0
2	NRE	A	401	27/27	0.95	0.12	42,43,48,60	0
6	SOG	A	409	5/20	0.96	0.13	50,51,56,58	0
5	SO4	B	402	5/5	0.97	0.12	69,70,72,77	0

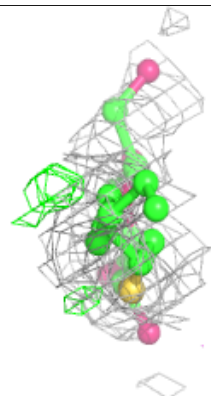
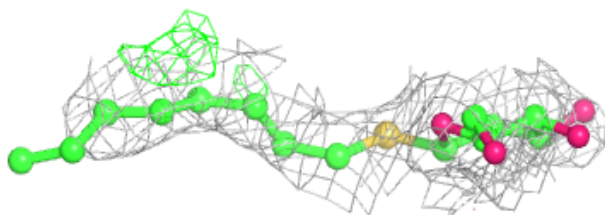
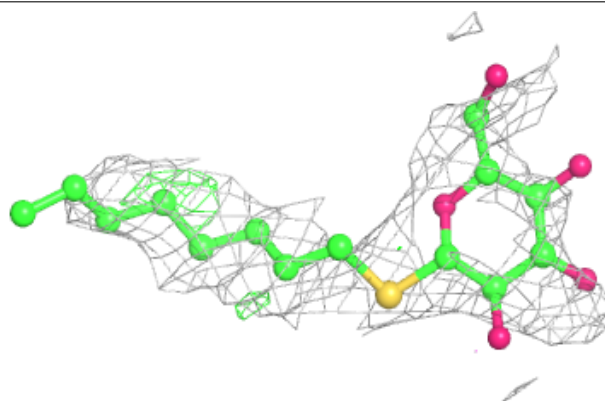
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SOG B 417:**

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

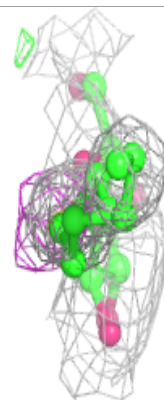
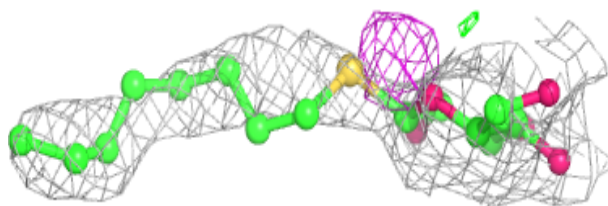
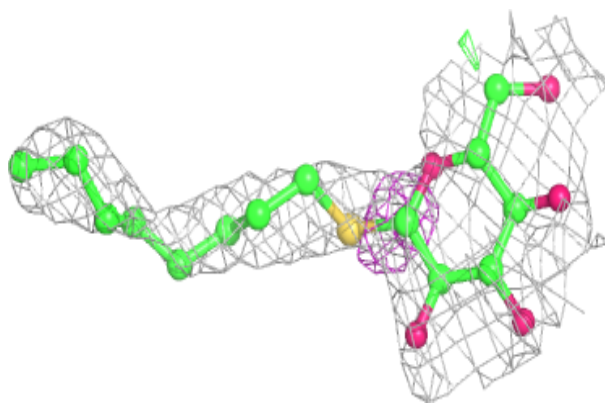
**Electron density around SOG A 418:**

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

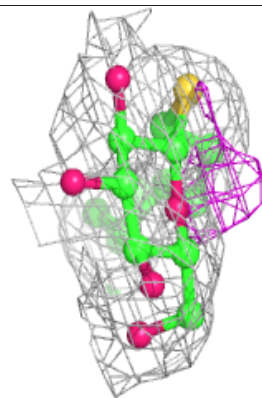
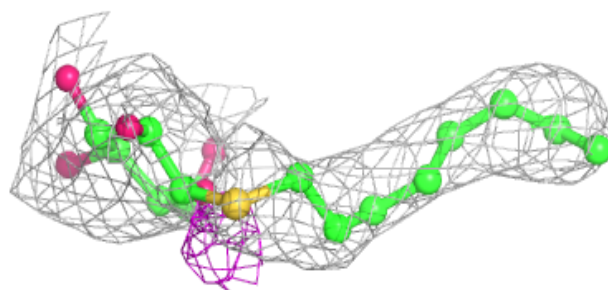
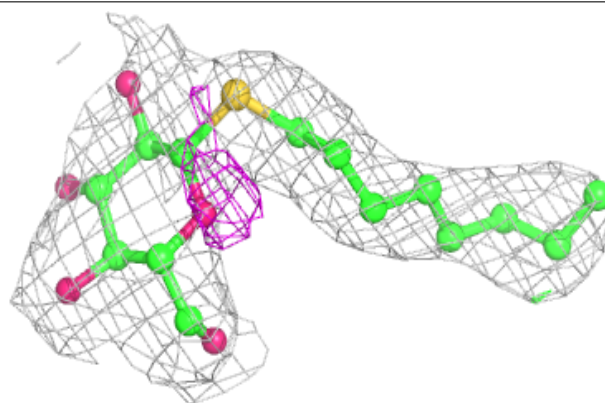


**Electron density around SOG B 419:**

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

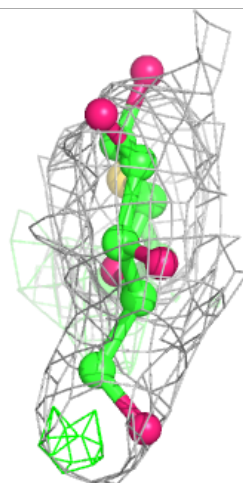
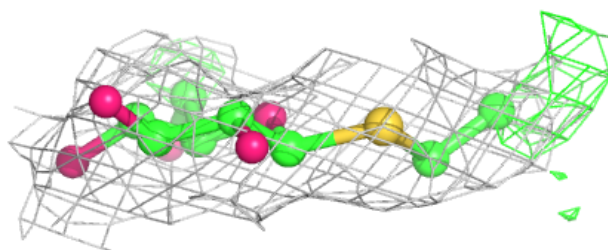
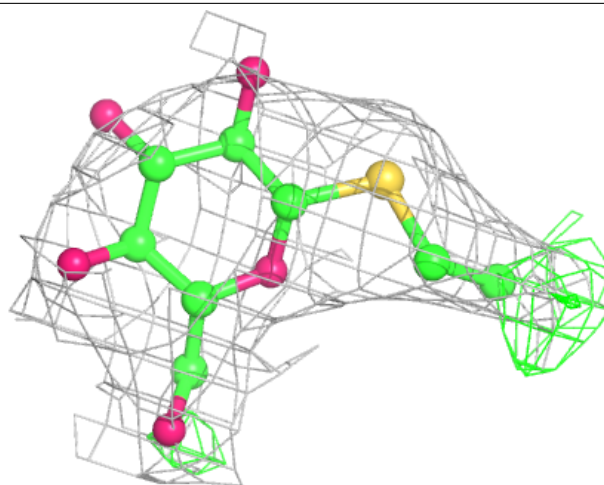
**Electron density around SOG A 413:**

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



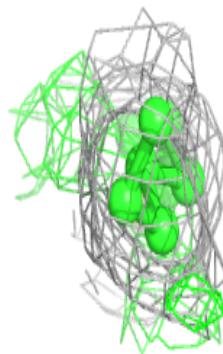
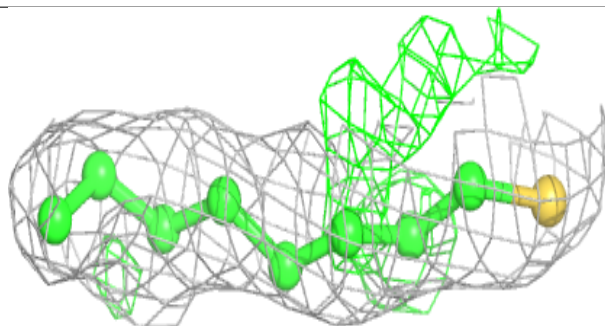
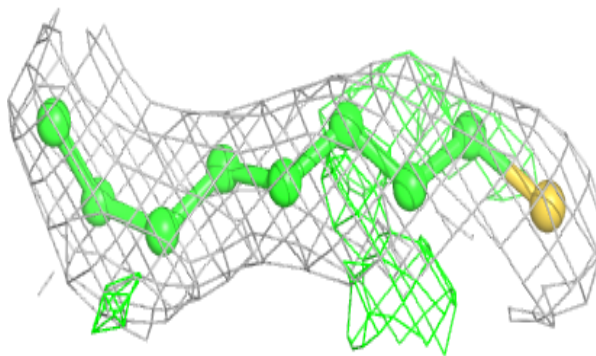
**Electron density around SOG A 414:**

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



**Electron density around SOG B 416:**

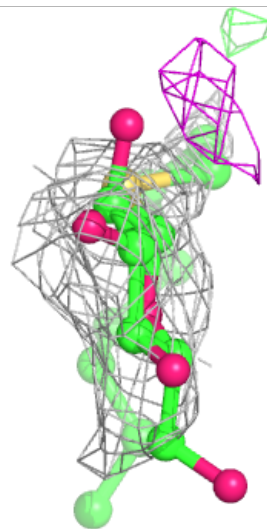
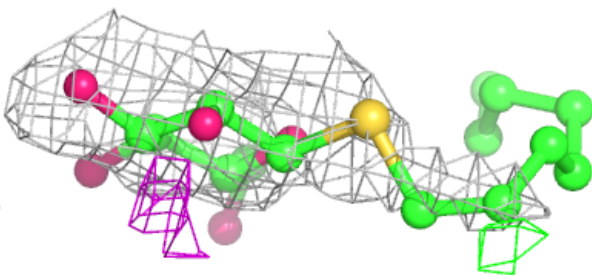
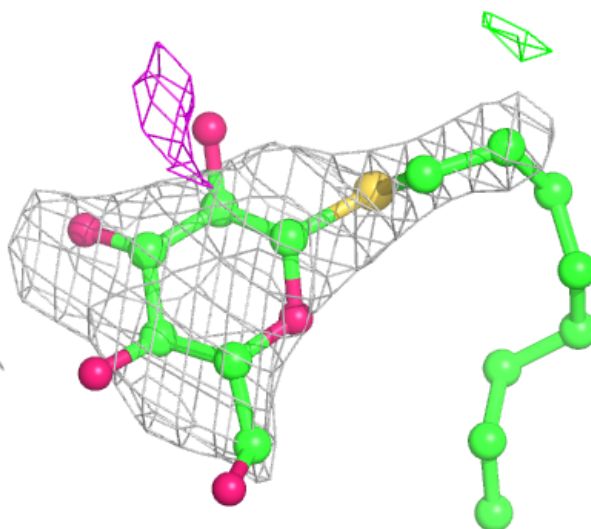
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





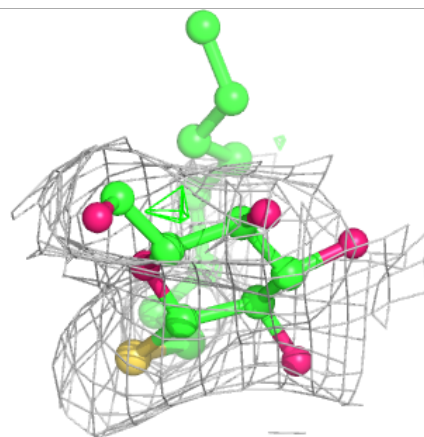
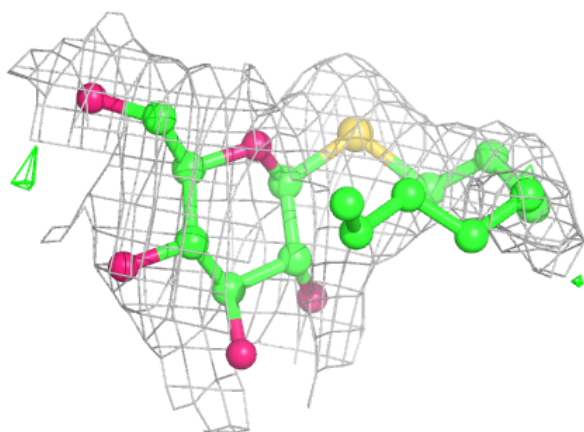
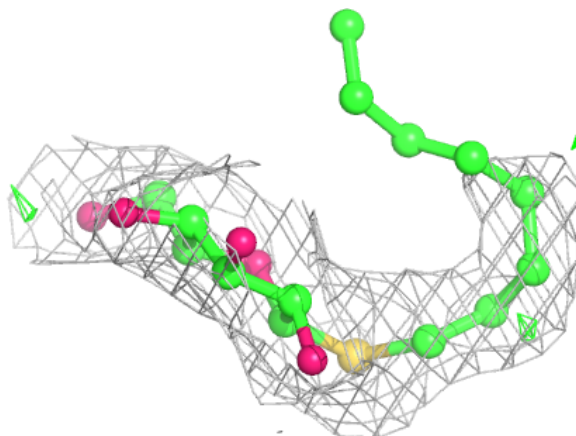
**Electron density around SOG B 418:**

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



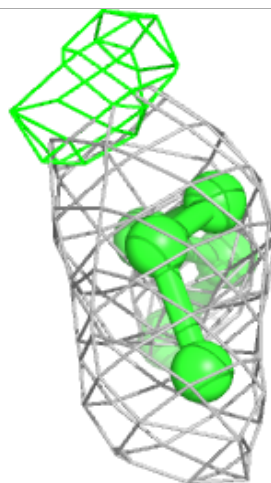
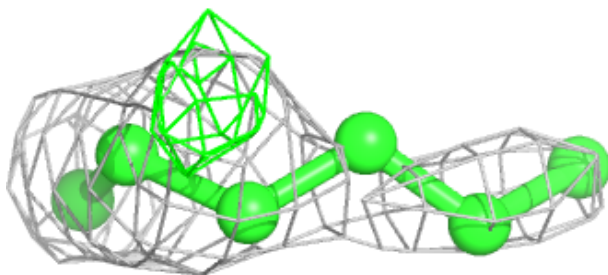
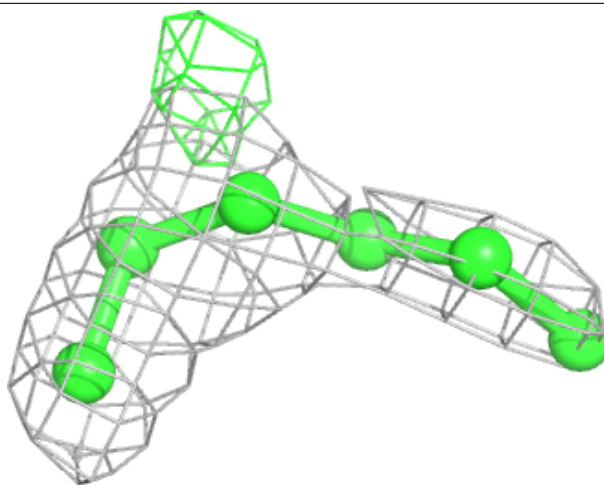
**Electron density around SOG B 409:**

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



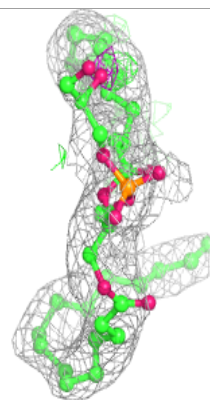
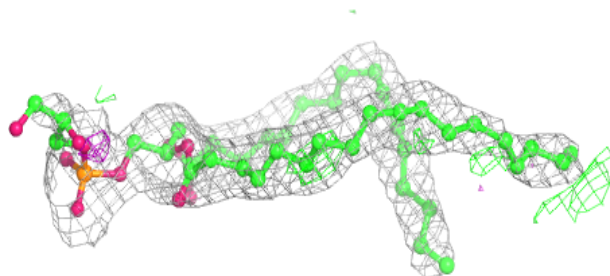
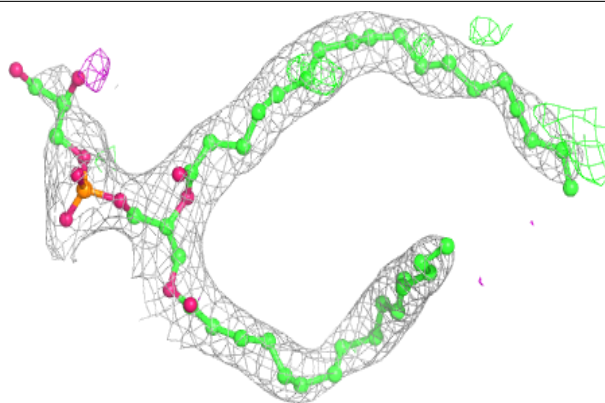
**Electron density around SOG B 413:**

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

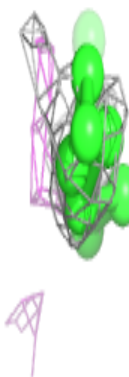
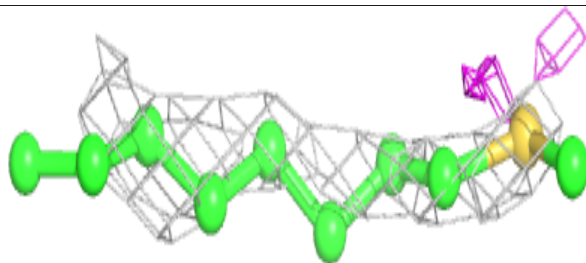
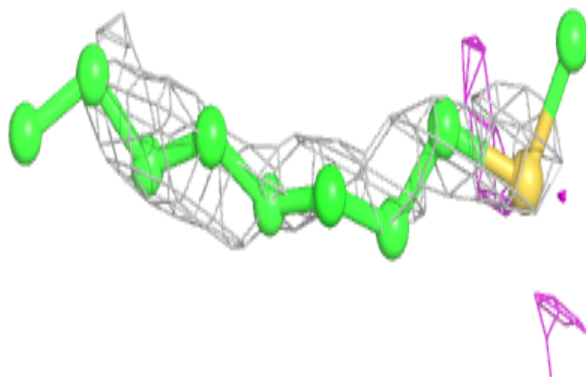


**Electron density around PGW B 404:**

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

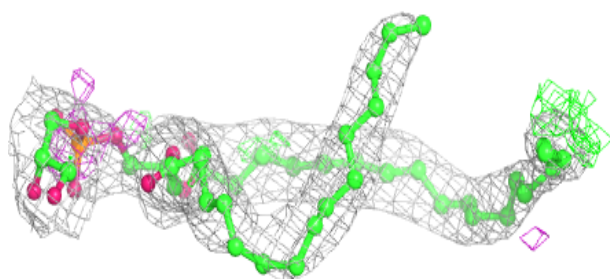
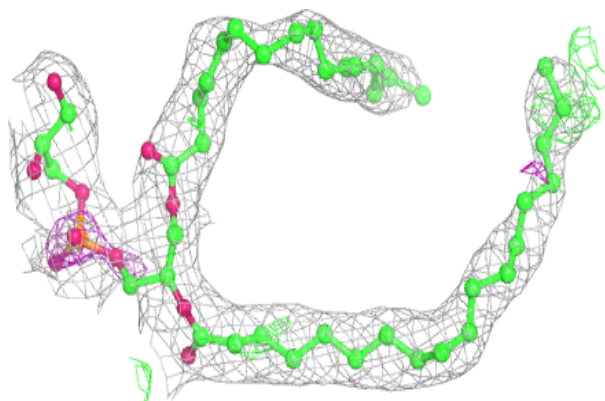
**Electron density around SOG B 410:**

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

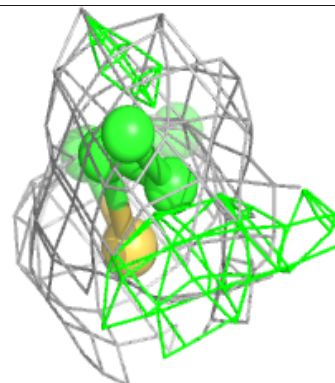
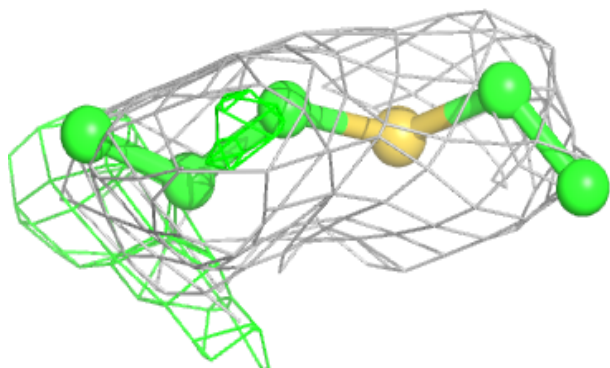
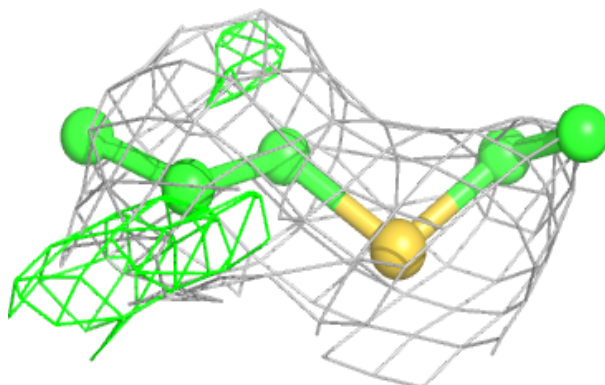


**Electron density around PGW B 405:**

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

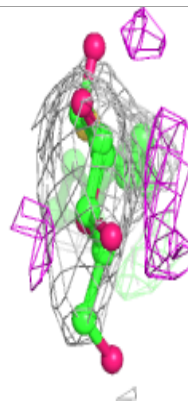
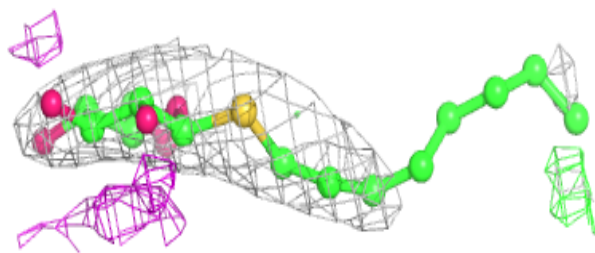
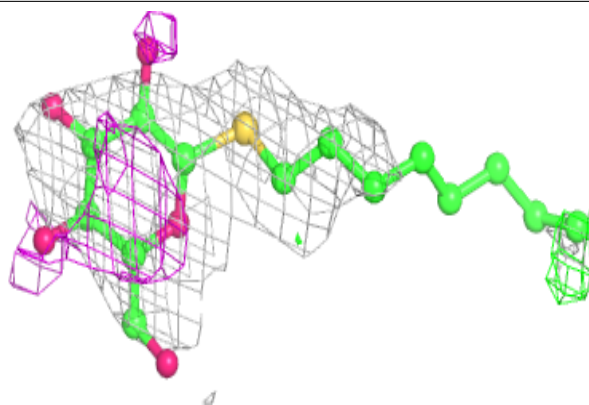
**Electron density around SOG B 414:**

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

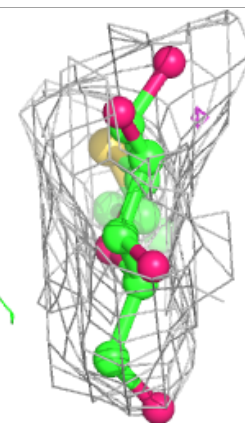
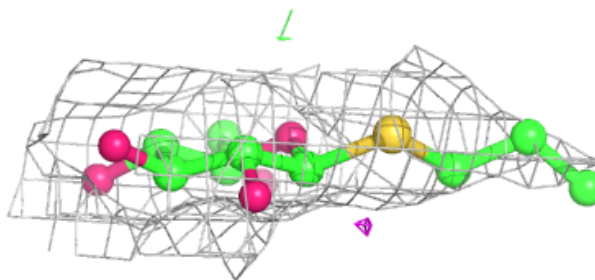
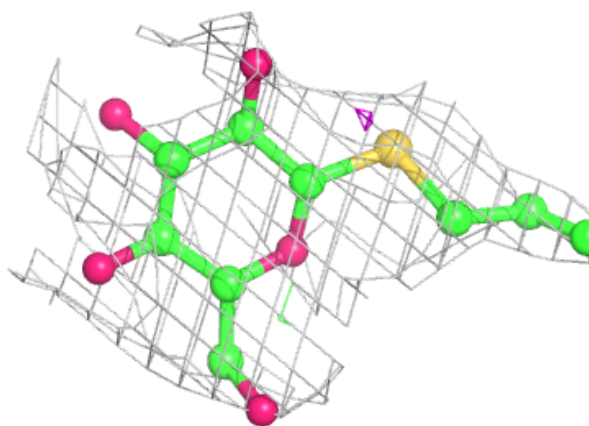


**Electron density around SOG A 411:**

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

**Electron density around SOG B 415:**

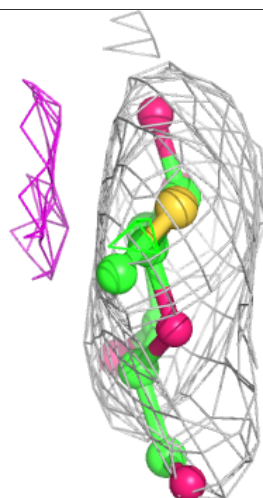
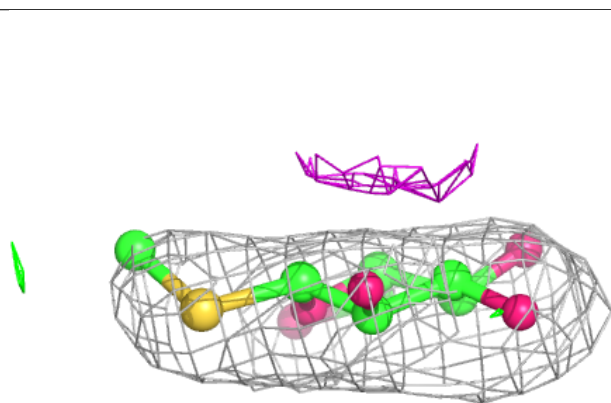
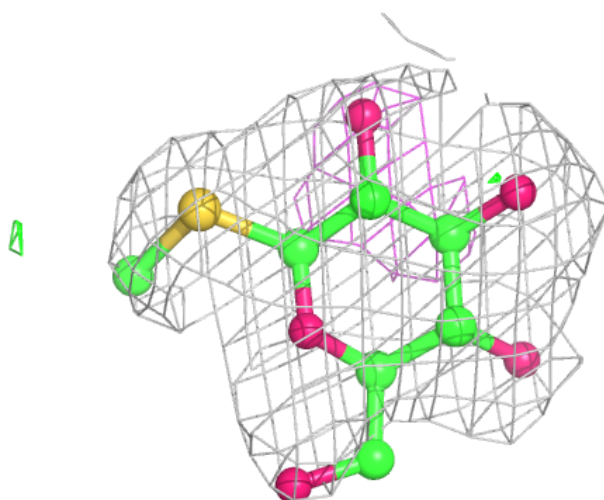
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





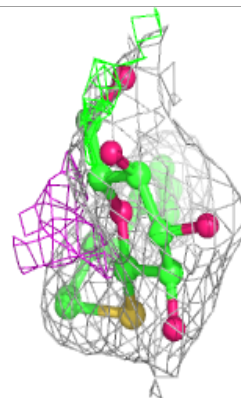
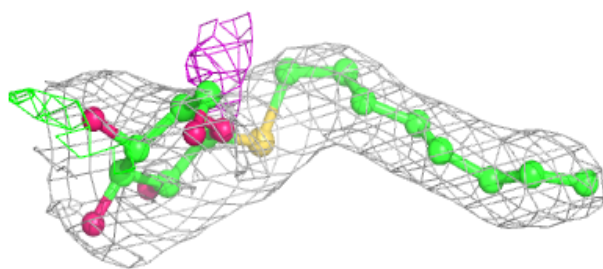
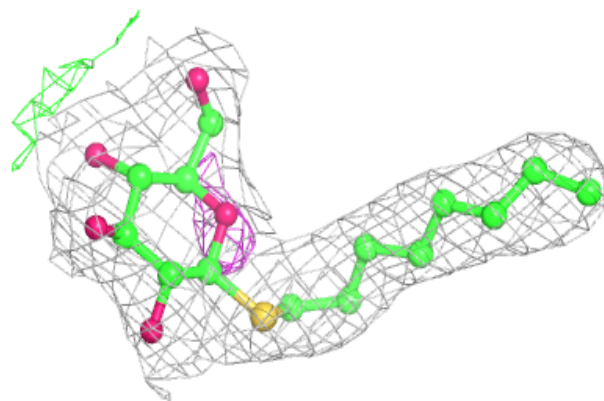
**Electron density around SOG B 407:**

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

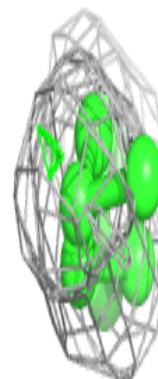
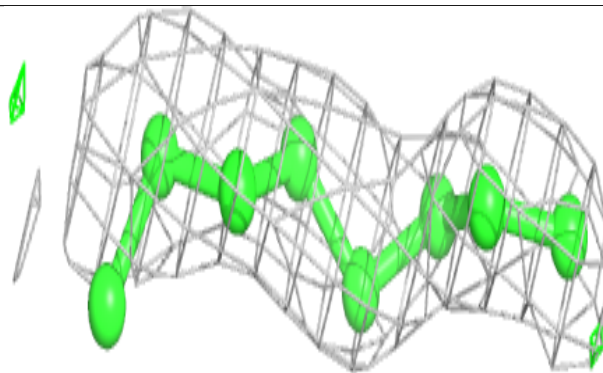
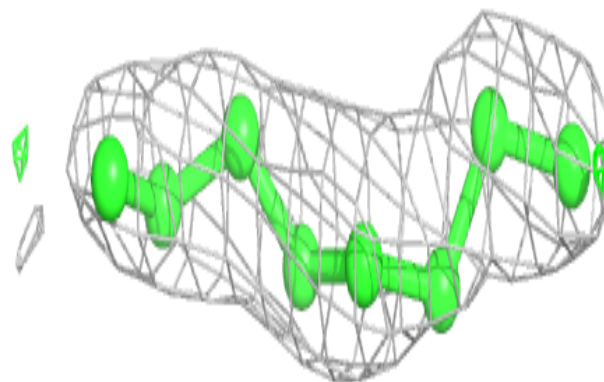


**Electron density around SOG B 408:**

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

**Electron density around SOG A 410:**

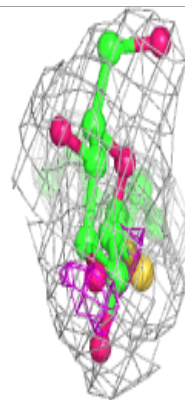
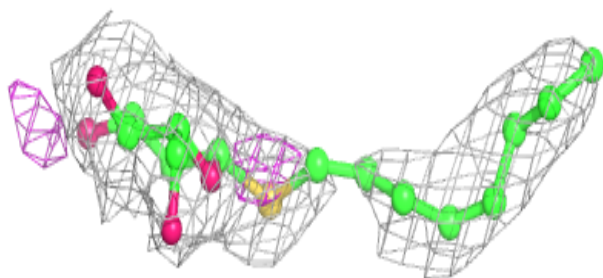
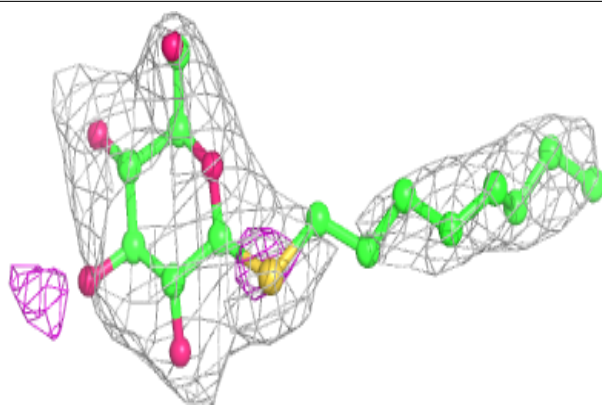
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



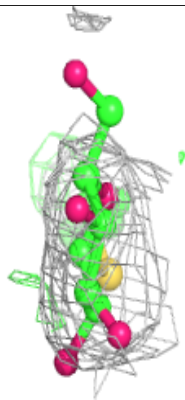
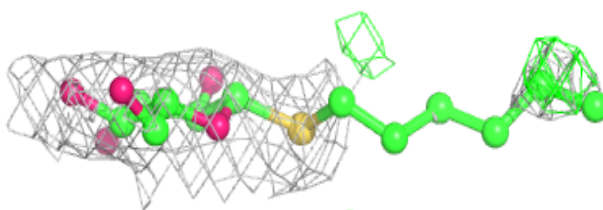
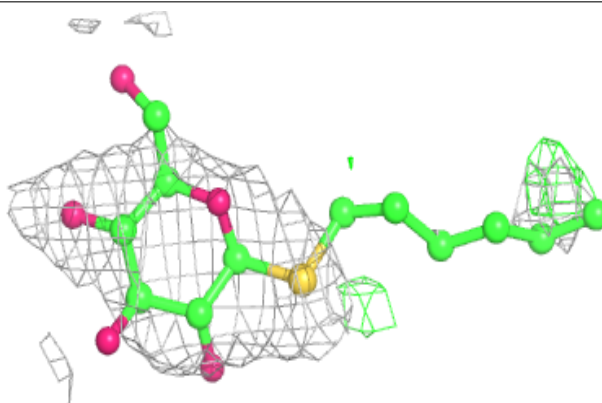


**Electron density around SOG A 407:**

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

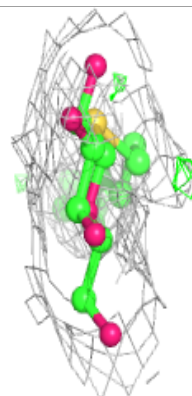
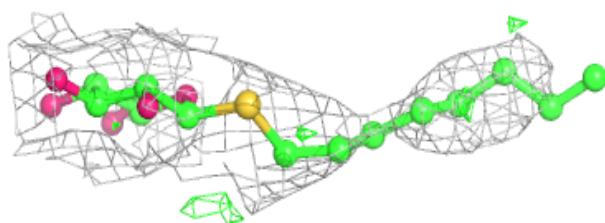
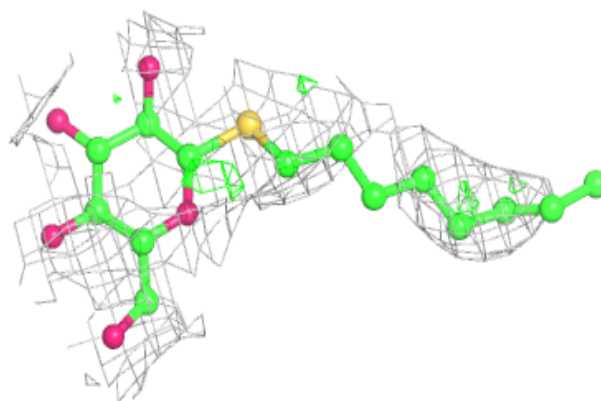
**Electron density around SOG A 416:**

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

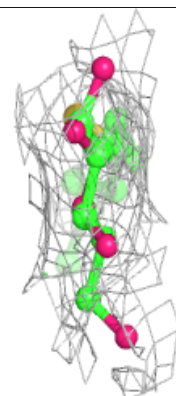
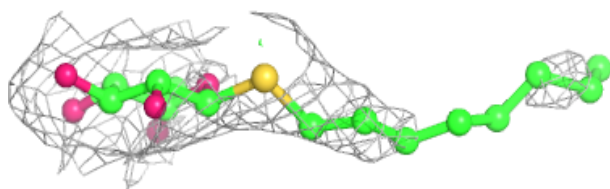
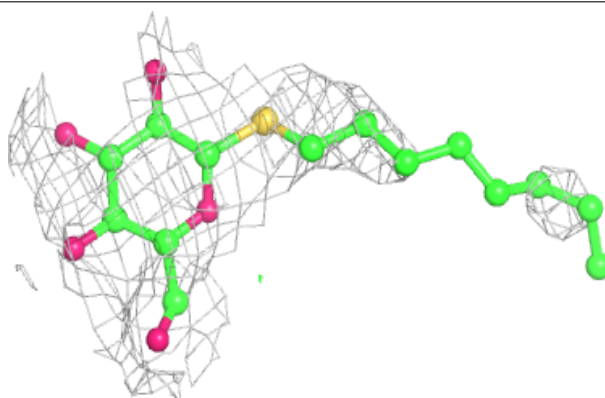


**Electron density around SOG A 408:**

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

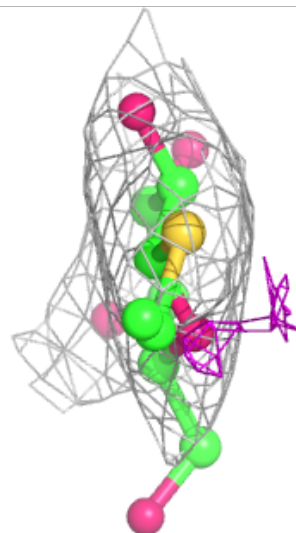
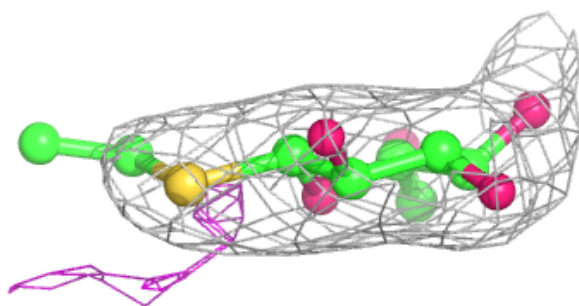
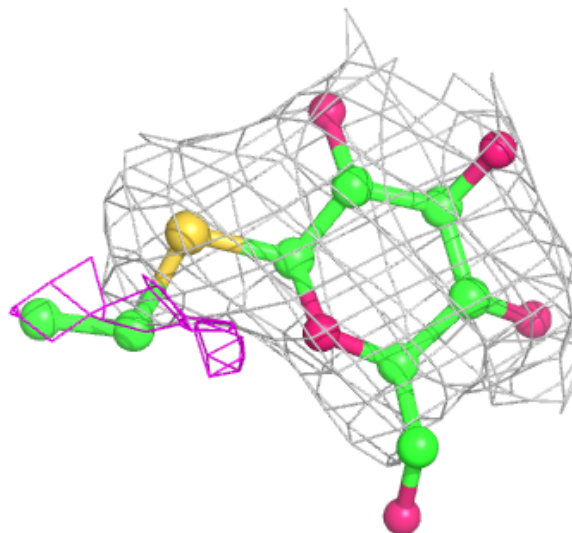
**Electron density around SOG B 420:**

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



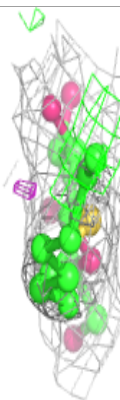
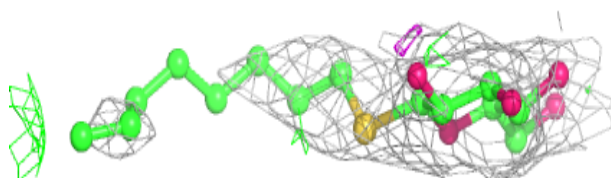
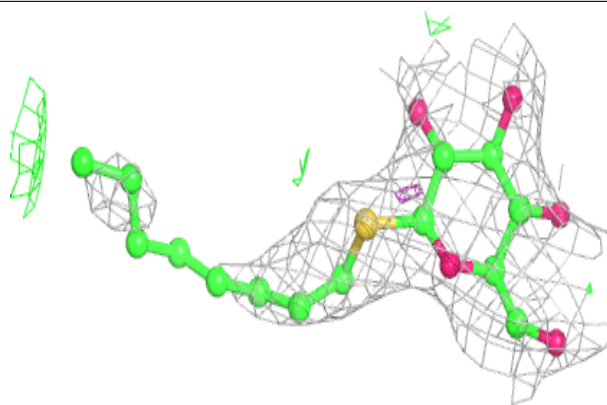
**Electron density around SOG A 412:**

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

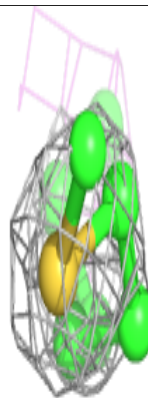
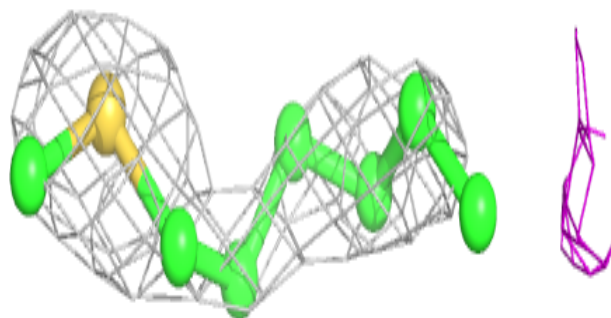
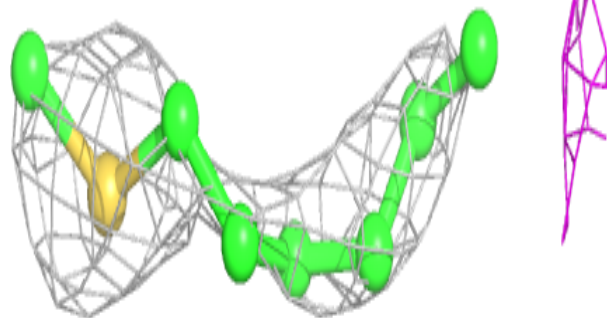


**Electron density around SOG B 412:**

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

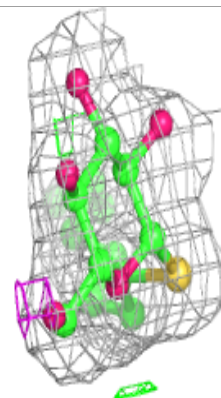
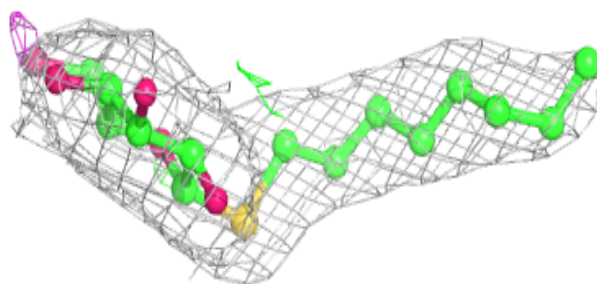
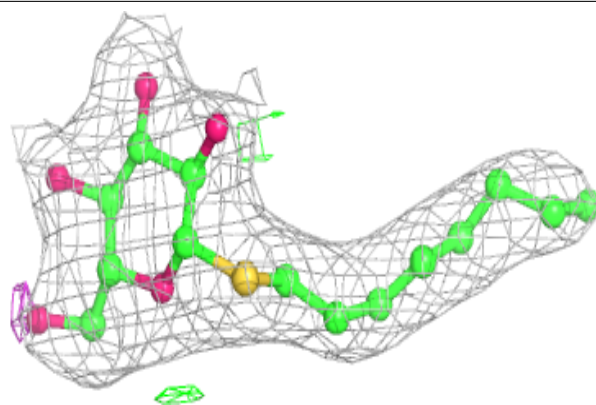
**Electron density around SOG A 415:**

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

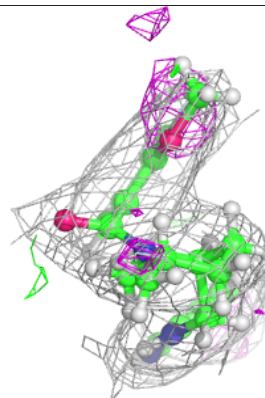
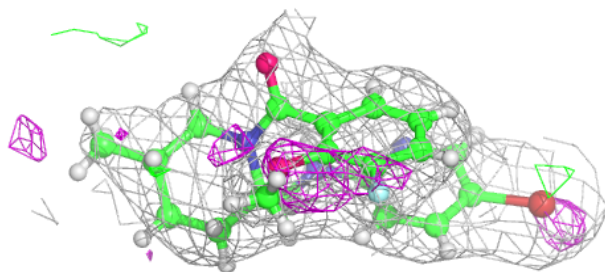
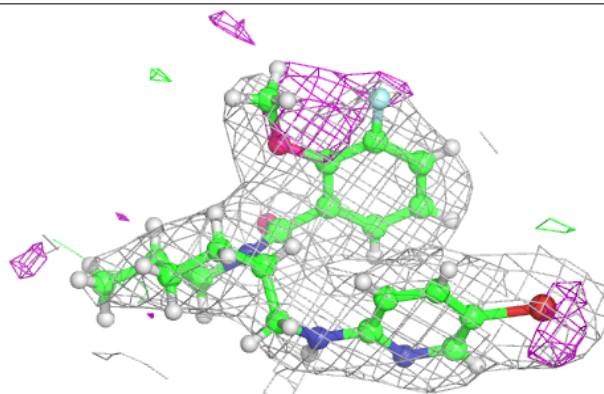


**Electron density around SOG B 406:**

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

**Electron density around NRE B 401:**

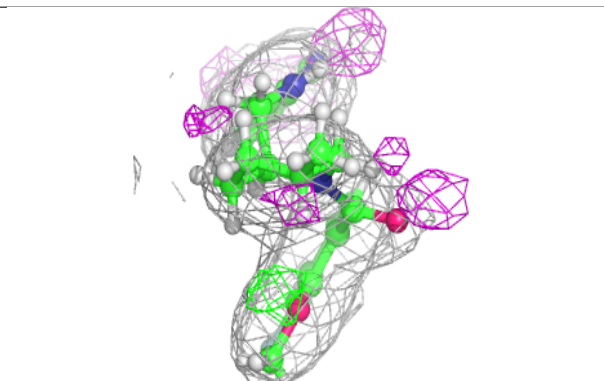
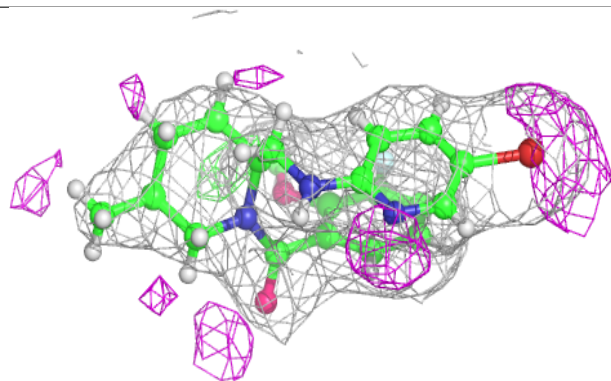
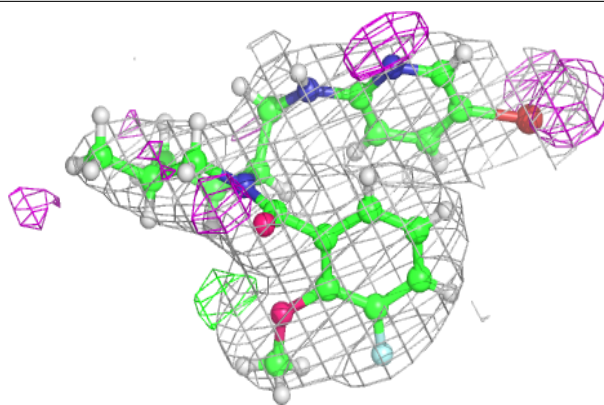
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



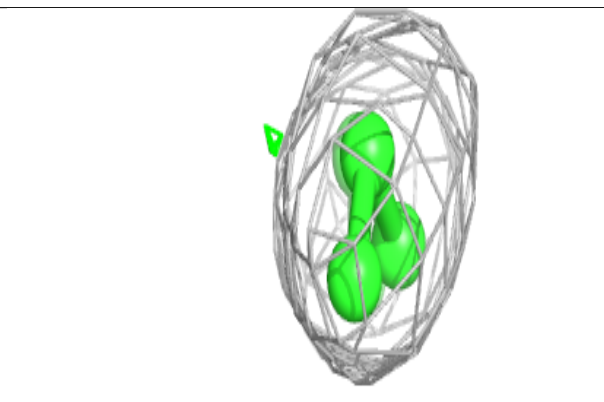
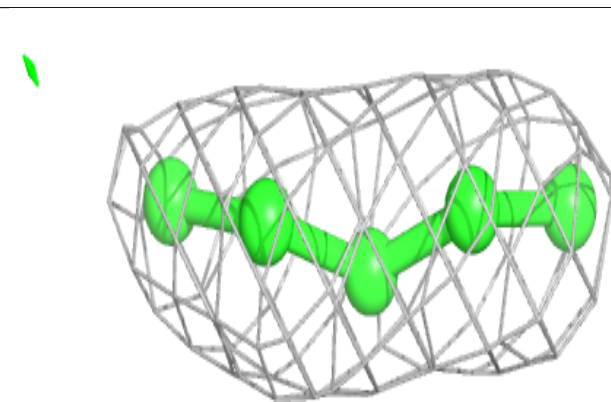
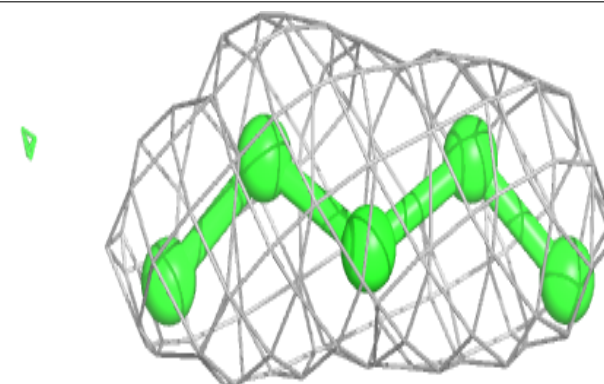


**Electron density around NRE A 401:**

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

**Electron density around SOG A 409:**

$2mF_o-DF_c$  (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.