wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 08:25 PM BST

PDB ID	:	6TOD
Title	:	Crystal structure of the Orexin-1 receptor in complex with EMPA
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	:	2.11 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

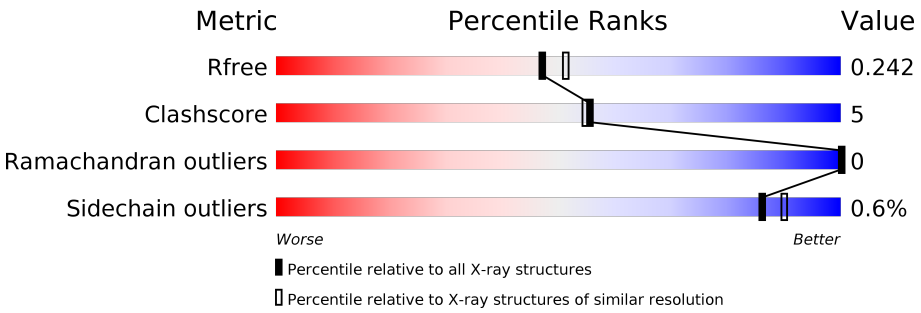
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	336	81% 8% 10%
1	B	336	85% 8% 7%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6001 atoms, of which 52 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
			Total	C	N	O	S			
1	A	301	2390	1584	399	390	17	0	0	0
1	B	311	2486	1652	411	406	17	0	0	0

There are 118 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	127	THR	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP O43613
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	127	THR	ALA	engineered mutation	UNP O43613
B	162	LEU	ARG	engineered mutation	UNP O43613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	ASN	engineered mutation	UNP O43613
B	198	ALA	LEU	engineered mutation	UNP O43613
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

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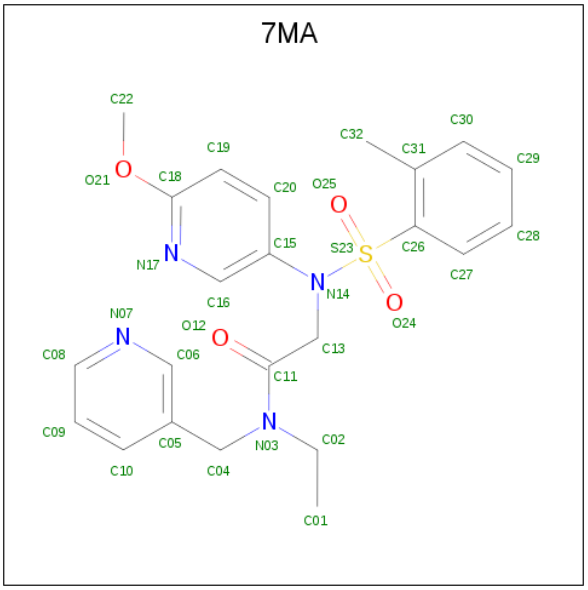
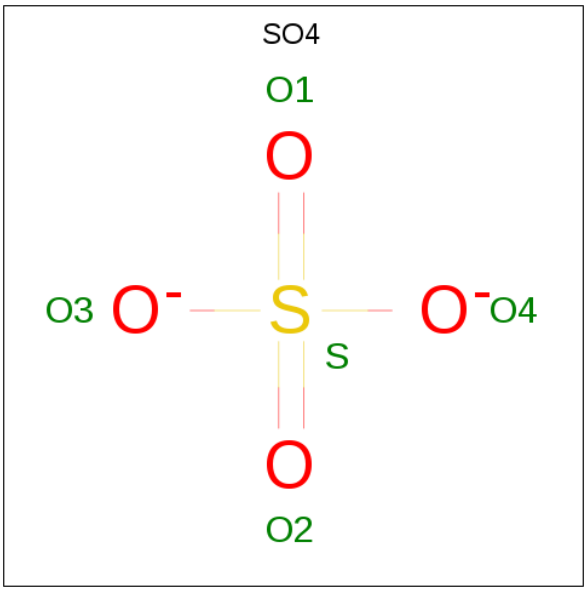
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is N-ethyl-2-[(6-methoxypyridin-3-yl)-(2-methylphenyl)sulfonyl-amino]-N-(pyridin-3-ylmethyl)ethanamide (three-letter code: 7MA) (formula: $C_{23}H_{26}N_4O_4S$) (labeled as "Ligand of Interest" by author).



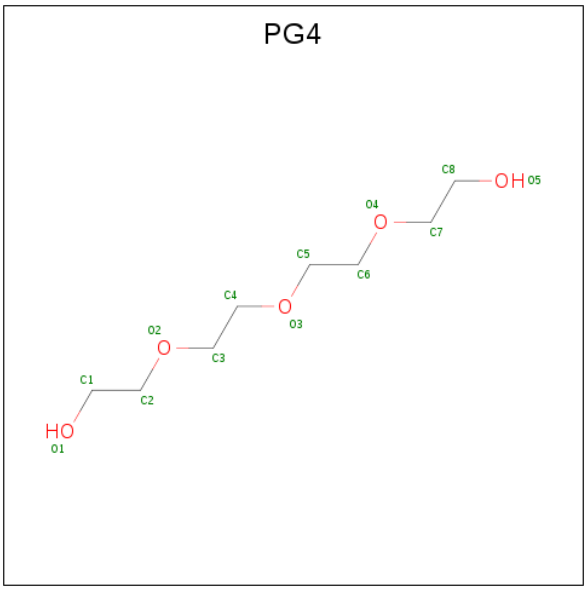
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	A	1	58	23	26	4	4	1	0	0
			Total	C	H	N	O	S		
2	B	1	58	23	26	4	4	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0

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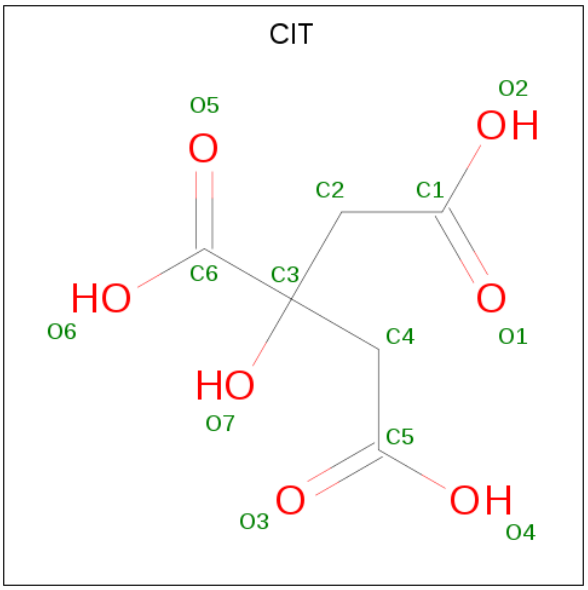
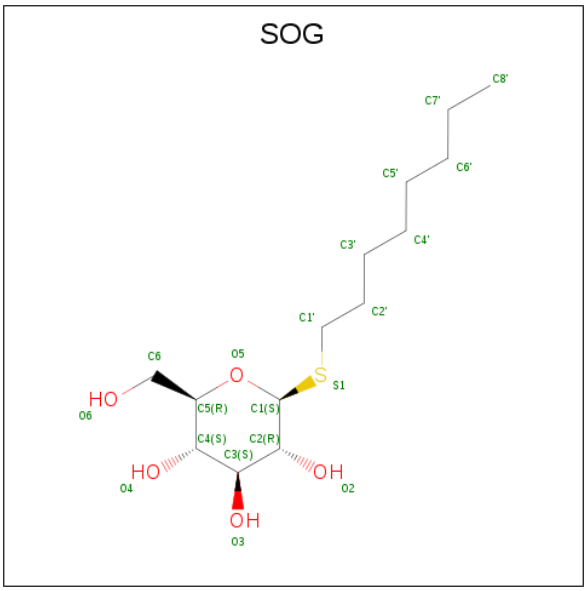
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- 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 17 11 5 1	0	0
6	A	1	Total C O S 16 10 5 1	0	0
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 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 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 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 20 14 5 1	0	0
6	A	1	Total C O S 20 14 5 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 1	0	0
6	A	1	Total C S 7 6 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
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 16 10 5 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 10 9 1	0	0
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C S 8 7 1	0	0

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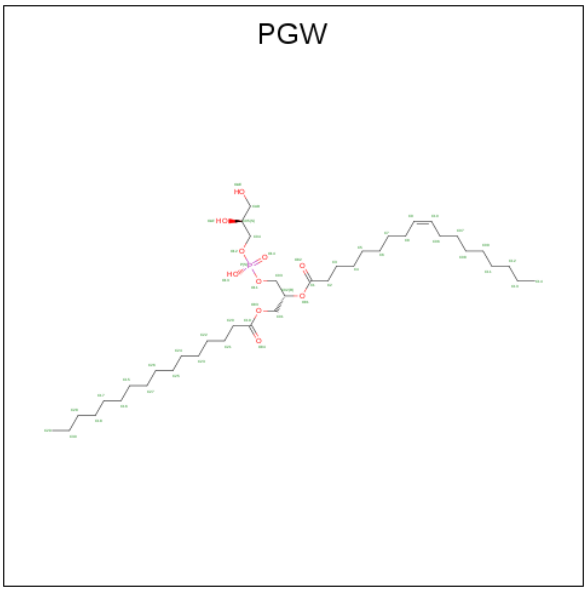
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C S 5 4 1	0	0
6	B	1	Total C O S 16 10 5 1	0	0
6	B	1	Total C S 8 7 1	0	0
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C S 6 5 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0

- Molecule 7 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: $C_{40}H_{77}O_{10}P$).



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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	B	1	1	1	0	0
			Total	Na		
8	A	1	1	1	0	0

- Molecule 9 is water.

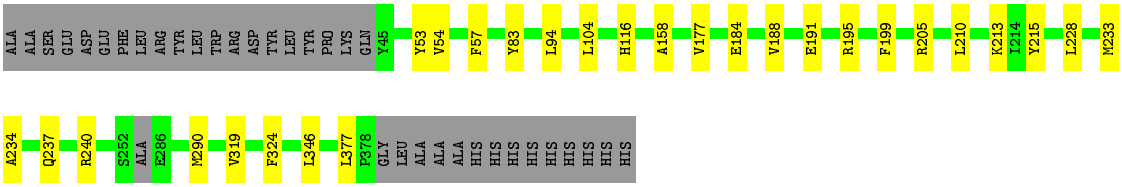
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	110	110	110	0	0
			Total	O		
9	B	101	101	101	0	0

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. 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. 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.

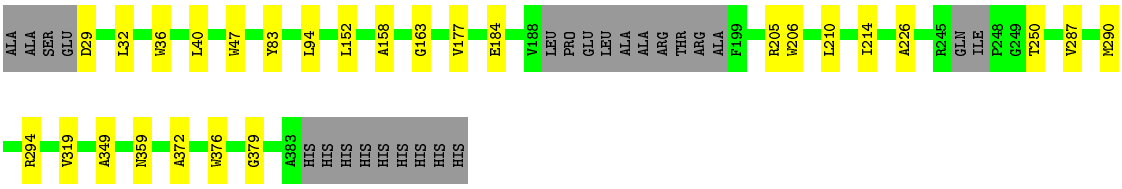
- Molecule 1: Orexin receptor type 1

Chain A:



- Molecule 1: Orexin receptor type 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	57.91Å 158.89Å 182.35Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	30.62 – 2.11 48.57 – 2.09	Depositor EDS
% Data completeness (in resolution range)	61.3 (30.62-2.11) 80.6 (48.57-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.32 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.188 , 0.208 0.224 , 0.242	Depositor DCC
R_{free} test set	4790 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6001	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PGW, PG4, SO4, CIT, 7MA

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	0/2456	0.61	0/3350
1	B	0.51	0/2557	0.60	0/3485
All	All	0.50	0/5013	0.60	0/6835

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	2390	0	2456	26	0
1	B	2486	0	2535	24	0
2	A	32	26	0	0	0
2	B	32	26	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	39	0	54	2	0
4	B	26	0	36	0	0
5	A	13	0	5	0	0
6	A	297	0	401	23	0
6	B	304	0	435	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	51	0	76	6	0
7	B	51	0	76	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	110	0	0	0	0
9	B	101	0	0	0	0
All	All	5949	52	6074	60	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 5.

The worst 5 of 60 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:290:MET:HE3	1:B:294:ARG:NH2	1.68	1.08
1:B:290:MET:HE3	1:B:294:ARG:HH21	0.98	1.05
6:A:410:SOG:H5	6:A:411:SOG:S1	2.00	1.01
1:A:213:LYS:HD3	6:A:411:SOG:H1'1	1.46	0.93
1:B:290:MET:CE	1:B:294:ARG:HH21	1.88	0.84

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	297/336 (88%)	292 (98%)	5 (2%)	0	100 100
1	B	305/336 (91%)	299 (98%)	6 (2%)	0	100 100
All	All	602/672 (90%)	591 (98%)	11 (2%)	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	252/280 (90%)	249 (99%)	3 (1%)	71	77
1	B	260/280 (93%)	260 (100%)	0	100	100
All	All	512/560 (91%)	509 (99%)	3 (1%)	86	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	ARG
1	A	290	MET
1	A	377	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	116	HIS
1	A	126	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 2 are monoatomic - leaving 60 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	421	-	16,16,20	1.12	1 (6%)	20,21,25	0.84	0
3	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.20	0
6	SOG	A	424	-	6,6,20	0.60	0	5,5,25	1.29	1 (20%)
6	SOG	B	414	-	20,20,20	0.99	1 (5%)	24,25,25	1.12	3 (12%)
6	SOG	B	426	-	6,6,20	0.51	0	5,5,25	0.84	0
4	PG4	B	405	-	12,12,12	0.50	0	11,11,11	0.34	0
6	SOG	A	416	-	20,20,20	1.03	2 (10%)	24,25,25	0.87	1 (4%)
6	SOG	B	427	-	6,6,20	0.52	0	5,5,25	0.68	0
4	PG4	B	404	-	12,12,12	0.41	0	11,11,11	0.59	0
6	SOG	A	428	-	6,6,20	0.53	0	5,5,25	0.50	0
3	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.13	0
6	SOG	B	417	-	8,8,20	0.48	0	7,7,25	0.69	0
6	SOG	B	415	-	5,5,20	0.25	0	4,4,25	0.37	0
6	SOG	A	407	-	17,17,20	1.05	2 (11%)	21,22,25	1.18	2 (9%)
6	SOG	B	430	-	6,6,20	0.49	0	5,5,25	0.82	0
6	SOG	B	418	-	7,7,20	0.51	0	6,6,25	0.91	0
6	SOG	A	418	-	20,20,20	0.99	1 (5%)	24,25,25	0.93	0
6	SOG	B	406	-	20,20,20	1.05	2 (10%)	24,25,25	1.17	1 (4%)
6	SOG	B	412	-	20,20,20	1.05	2 (10%)	24,25,25	0.74	0
2	7MA	A	401	-	34,34,34	5.53	11 (32%)	45,47,47	2.68	22 (48%)
6	SOG	A	408	-	16,16,20	1.15	2 (12%)	20,21,25	1.02	2 (10%)
5	CIT	A	406	-	3,12,12	0.49	0	3,17,17	1.03	0
6	SOG	B	420	-	4,4,20	0.69	0	3,3,25	0.71	0
7	PGW	B	431	-	50,50,50	0.97	2 (4%)	53,56,56	0.94	2 (3%)
6	SOG	A	410	-	20,20,20	0.85	1 (5%)	24,25,25	1.74	4 (16%)
6	SOG	A	420	-	6,6,20	0.50	0	5,5,25	0.75	0
6	SOG	A	411	-	20,20,20	0.76	1 (5%)	24,25,25	1.19	3 (12%)
6	SOG	B	429	-	6,6,20	0.52	0	5,5,25	0.80	0
6	SOG	A	413	-	20,20,20	0.95	1 (5%)	24,25,25	1.40	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	SOG	A	419	-	6,6,20	0.52	0	5,5,25	0.63	0
6	SOG	B	410	-	20,20,20	0.99	1 (5%)	24,25,25	0.82	0
6	SOG	A	412	-	20,20,20	1.10	2 (10%)	24,25,25	0.95	1 (4%)
6	SOG	B	407	-	20,20,20	1.12	2 (10%)	24,25,25	0.74	1 (4%)
6	SOG	A	415	-	14,14,20	0.91	1 (7%)	18,19,25	1.07	1 (5%)
6	SOG	A	409	-	20,20,20	0.98	1 (5%)	24,25,25	0.92	1 (4%)
6	SOG	B	428	-	6,6,20	0.52	0	5,5,25	0.80	0
6	SOG	B	408	-	20,20,20	1.01	2 (10%)	24,25,25	0.80	0
6	SOG	B	416	-	9,9,20	0.39	0	8,8,25	0.57	0
4	PG4	A	405	-	12,12,12	0.15	0	11,11,11	0.14	0
6	SOG	A	414	-	20,20,20	1.10	2 (10%)	24,25,25	0.80	0
6	SOG	B	409	-	20,20,20	1.12	2 (10%)	24,25,25	1.60	5 (20%)
6	SOG	B	425	-	6,6,20	0.54	0	5,5,25	0.88	0
6	SOG	A	425	-	6,6,20	0.53	0	5,5,25	0.71	0
7	PGW	A	429	-	50,50,50	0.94	2 (4%)	53,56,56	1.15	3 (5%)
6	SOG	A	417	-	20,20,20	1.11	2 (10%)	24,25,25	1.29	4 (16%)
6	SOG	A	421	-	6,6,20	0.56	0	5,5,25	1.01	0
6	SOG	A	426	-	6,6,20	0.52	0	5,5,25	0.63	0
3	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.13	0
6	SOG	A	427	-	6,6,20	0.51	0	5,5,25	0.55	0
6	SOG	B	424	-	5,5,20	0.52	0	4,4,25	0.45	0
6	SOG	A	422	-	6,6,20	0.48	0	5,5,25	0.54	0
4	PG4	A	403	-	12,12,12	0.48	0	11,11,11	0.33	0
4	PG4	A	404	-	12,12,12	0.58	0	11,11,11	0.18	0
6	SOG	B	423	-	8,8,20	0.45	0	7,7,25	0.69	0
6	SOG	B	411	-	20,20,20	0.98	2 (10%)	24,25,25	1.11	2 (8%)
6	SOG	A	423	-	6,6,20	0.52	0	5,5,25	0.80	0
6	SOG	B	419	-	8,8,20	0.49	0	7,7,25	0.64	0
2	7MA	B	401	-	34,34,34	5.65	11 (32%)	45,47,47	2.58	20 (44%)
6	SOG	B	422	-	7,7,20	0.52	0	6,6,25	0.72	0
6	SOG	B	413	-	16,16,20	1.20	1 (6%)	20,21,25	0.94	2 (10%)

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	421	-	-	4/7/27/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	B	417	-	-	4/6/6/31	-
6	SOG	A	424	-	-	2/4/4/31	-
6	SOG	B	414	-	-	4/11/31/31	0/1/1/1
6	SOG	B	426	-	-	1/4/4/31	-
4	PG4	B	405	-	-	8/10/10/10	-
6	SOG	A	416	-	-	7/11/31/31	0/1/1/1
6	SOG	B	427	-	-	1/4/4/31	-
4	PG4	B	404	-	-	4/10/10/10	-
6	SOG	A	428	-	-	1/4/4/31	-
6	SOG	B	415	-	-	2/3/3/31	-
6	SOG	A	407	-	-	5/8/28/31	0/1/1/1
6	SOG	B	430	-	-	3/4/4/31	-
6	SOG	B	418	-	-	3/5/5/31	-
6	SOG	A	418	-	-	6/11/31/31	0/1/1/1
6	SOG	B	406	-	-	6/11/31/31	0/1/1/1
6	SOG	B	412	-	-	5/11/31/31	0/1/1/1
2	7MA	A	401	-	-	7/32/32/32	0/3/3/3
6	SOG	A	408	-	-	4/7/27/31	0/1/1/1
5	CIT	A	406	-	-	2/6/16/16	-
6	SOG	B	420	-	-	2/2/2/31	-
7	PGW	B	431	-	-	28/55/55/55	-
6	SOG	A	410	-	-	5/11/31/31	0/1/1/1
6	SOG	A	420	-	-	1/4/4/31	-
6	SOG	A	411	-	-	2/11/31/31	0/1/1/1
6	SOG	B	429	-	-	1/4/4/31	-
6	SOG	A	413	-	-	4/11/31/31	0/1/1/1
6	SOG	A	419	-	-	1/4/4/31	-
6	SOG	B	410	-	-	9/11/31/31	0/1/1/1
6	SOG	A	412	-	-	5/11/31/31	0/1/1/1
6	SOG	B	407	-	-	6/11/31/31	0/1/1/1
6	SOG	A	415	-	-	1/5/25/31	0/1/1/1
6	SOG	A	409	-	-	6/11/31/31	0/1/1/1
6	SOG	B	428	-	-	1/4/4/31	-
6	SOG	B	408	-	-	7/11/31/31	0/1/1/1
6	SOG	B	416	-	-	1/7/7/31	-
4	PG4	A	405	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	A	414	-	-	6/11/31/31	0/1/1/1
6	SOG	B	409	-	-	4/11/31/31	0/1/1/1
6	SOG	B	425	-	-	2/4/4/31	-
6	SOG	A	425	-	-	2/4/4/31	-
7	PGW	A	429	-	-	26/55/55/55	-
6	SOG	A	417	-	-	7/11/31/31	0/1/1/1
6	SOG	A	421	-	-	1/4/4/31	-
6	SOG	A	426	-	-	1/4/4/31	-
6	SOG	A	427	-	-	3/4/4/31	-
6	SOG	B	424	-	-	2/3/3/31	-
6	SOG	A	422	-	-	3/4/4/31	-
4	PG4	A	403	-	-	3/10/10/10	-
4	PG4	A	404	-	-	5/10/10/10	-
6	SOG	B	423	-	-	3/6/6/31	-
6	SOG	B	411	-	-	7/11/31/31	0/1/1/1
6	SOG	A	423	-	-	3/4/4/31	-
6	SOG	B	419	-	-	5/6/6/31	-
2	7MA	B	401	-	-	6/32/32/32	0/3/3/3
6	SOG	B	422	-	-	2/5/5/31	-
6	SOG	B	413	-	-	3/7/27/31	0/1/1/1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7MA	O24-S23	20.06	1.65	1.43
2	A	401	7MA	O24-S23	19.73	1.65	1.43
2	B	401	7MA	O25-S23	17.26	1.62	1.43
2	A	401	7MA	O25-S23	17.07	1.62	1.43
2	B	401	7MA	S23-N14	13.63	1.84	1.65

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	7MA	C16-N17-C18	6.51	122.36	116.63
2	A	401	7MA	C16-N17-C18	6.01	121.92	116.63
2	A	401	7MA	O25-S23-O24	-5.79	110.13	119.52
6	A	410	SOG	C1-O5-C5	5.75	123.19	112.58
7	A	429	PGW	O01-C1-C2	5.61	123.59	111.50

There are no chirality outliers.

5 of 256 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	414	SOG	O5-C1-S1-C1'
6	B	418	SOG	S1-C1'-C2'-C3'
6	B	420	SOG	S1-C1'-C2'-C3'
7	B	431	PGW	OAF-C05-CAD-OAE
7	B	431	PGW	C04-C05-CAD-OAE

There are no ring outliers.

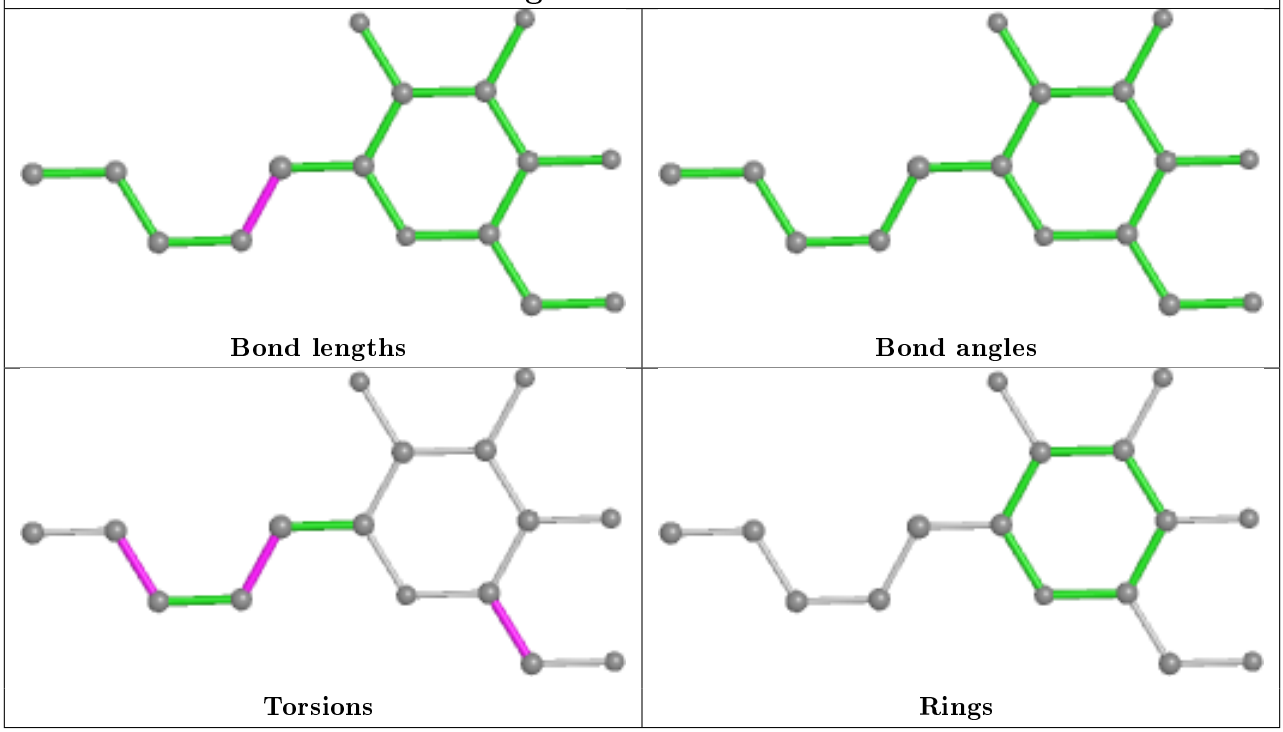
25 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	421	SOG	2	0
6	B	414	SOG	3	0
6	A	416	SOG	1	0
6	B	418	SOG	1	0
7	B	431	PGW	3	0
6	A	410	SOG	7	0
6	A	411	SOG	7	0
6	A	413	SOG	1	0
6	A	412	SOG	1	0
6	B	407	SOG	1	0
6	A	415	SOG	2	0
6	A	409	SOG	1	0
6	B	428	SOG	1	0
6	B	408	SOG	2	0
6	B	416	SOG	1	0
4	A	405	PG4	1	0
6	A	414	SOG	1	0
6	B	409	SOG	4	0
7	A	429	PGW	6	0
6	A	417	SOG	4	0
6	A	426	SOG	1	0
6	A	427	SOG	1	0
6	B	424	SOG	1	0
4	A	404	PG4	1	0
6	B	413	SOG	1	0

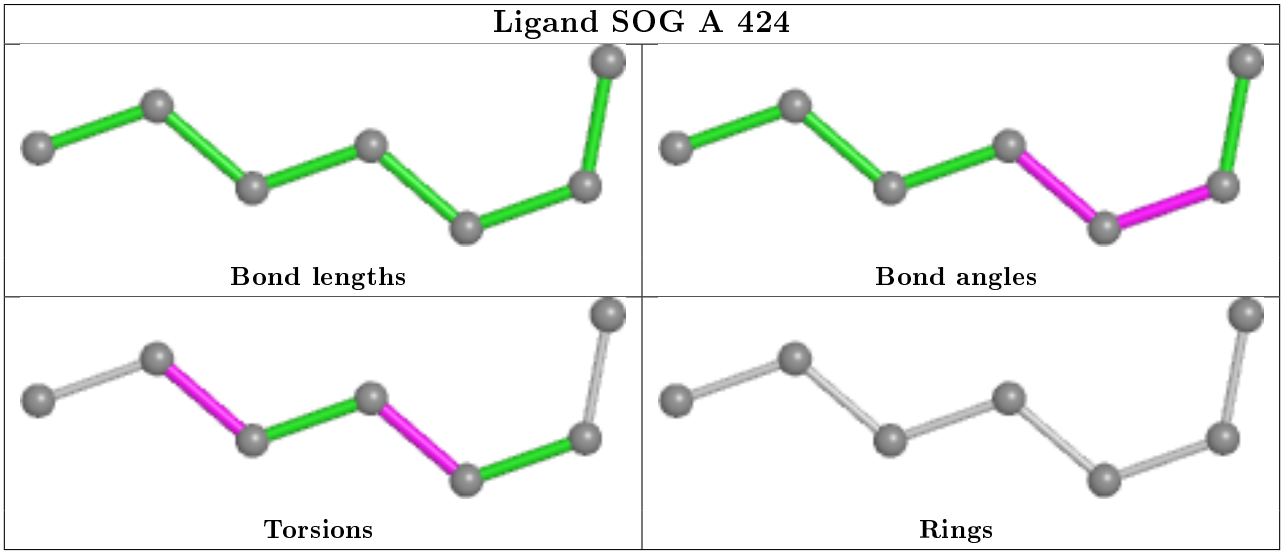
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

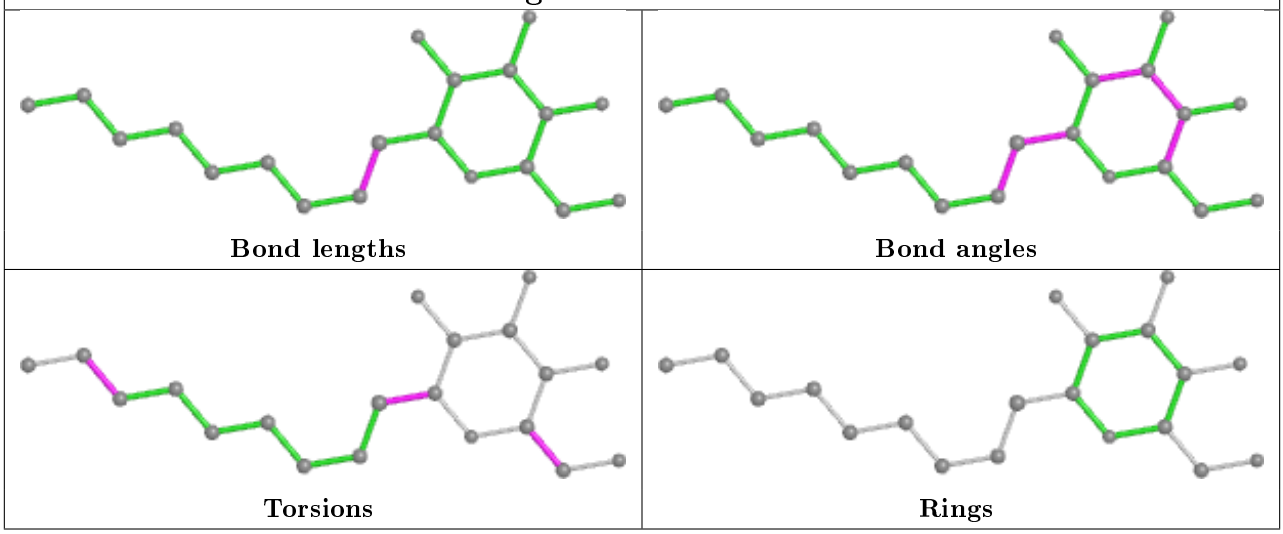
Ligand SOG B 421



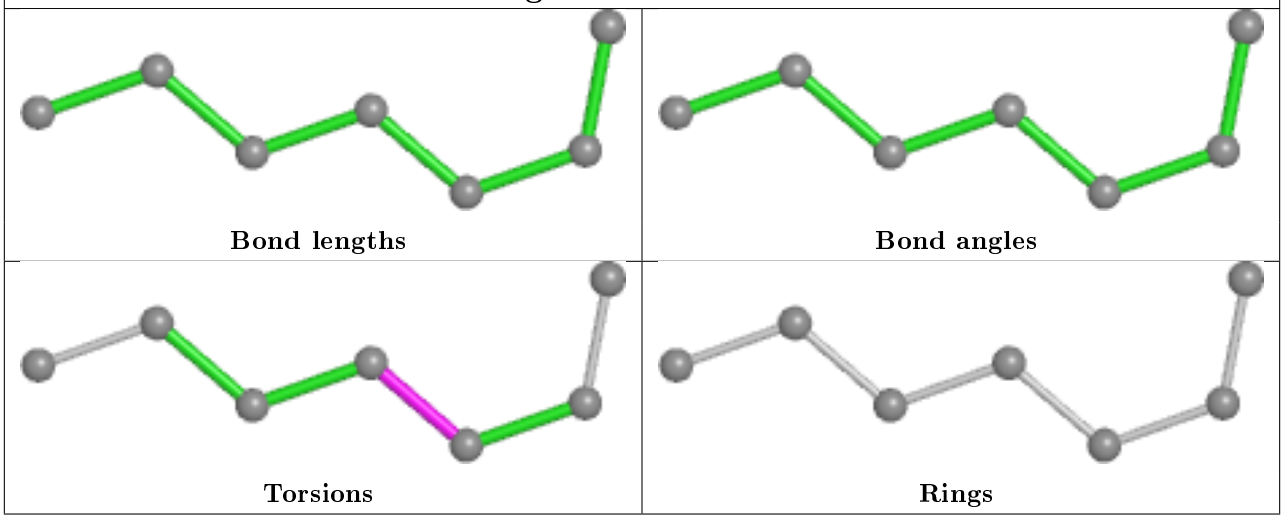
Ligand SOG A 424



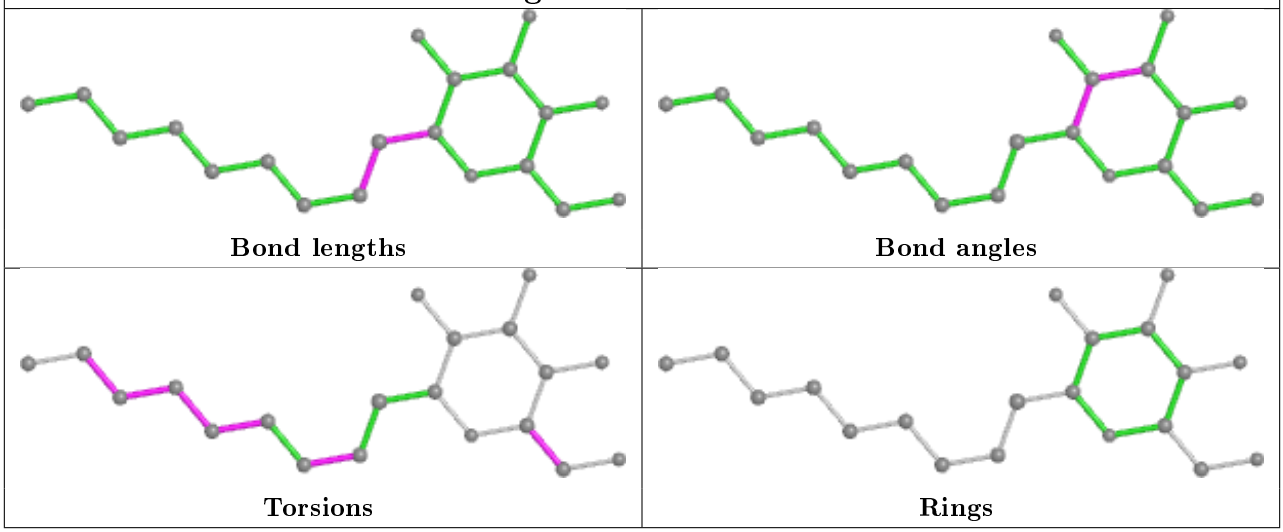
Ligand SOG B 414



Ligand SOG B 426



Ligand SOG A 416



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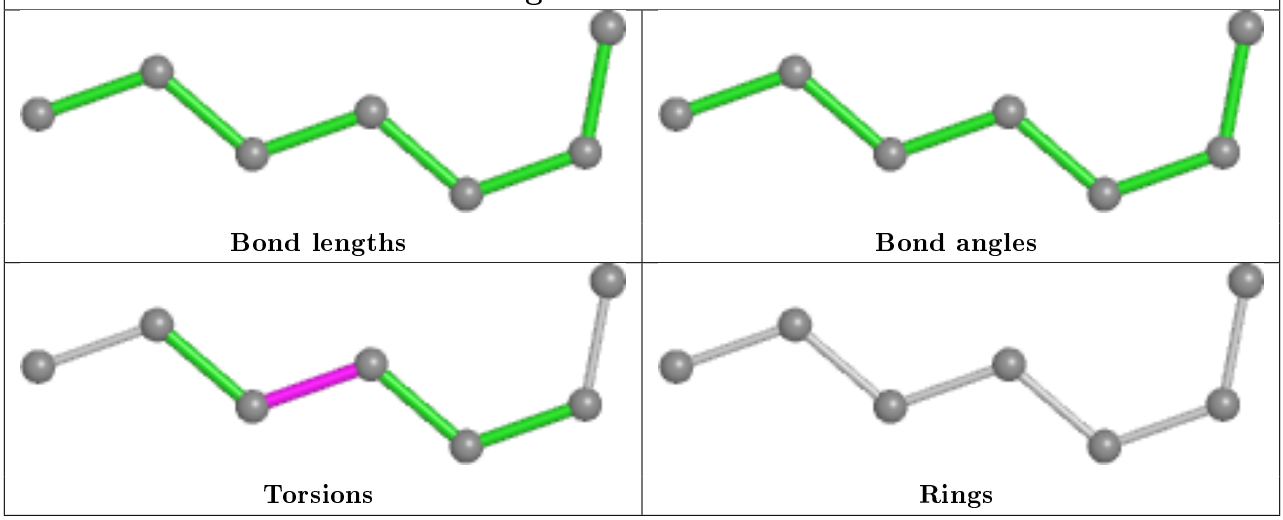
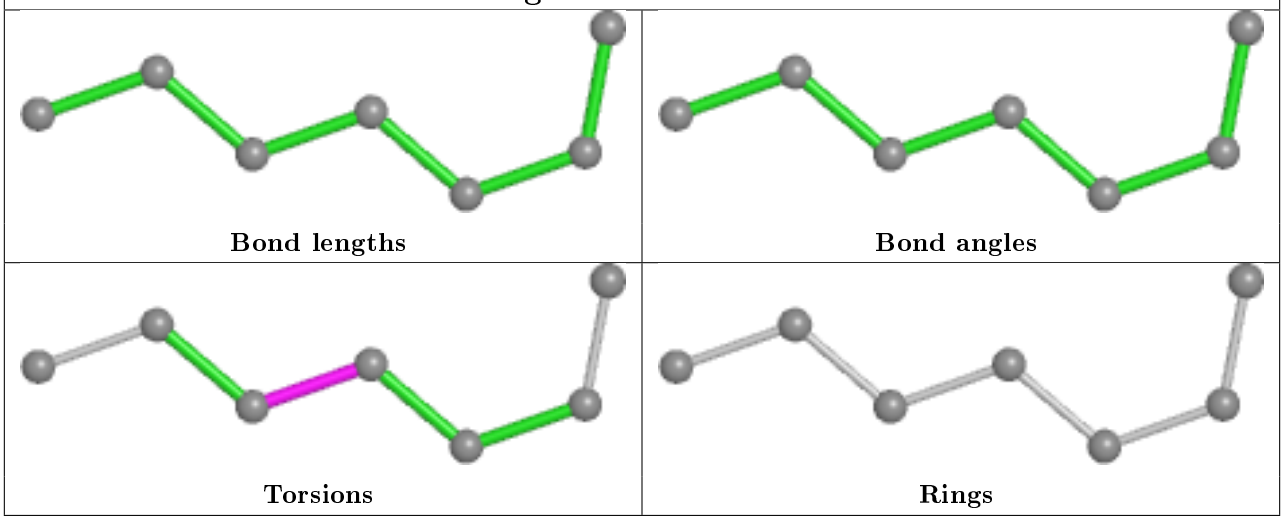


Ligand SOG A 428



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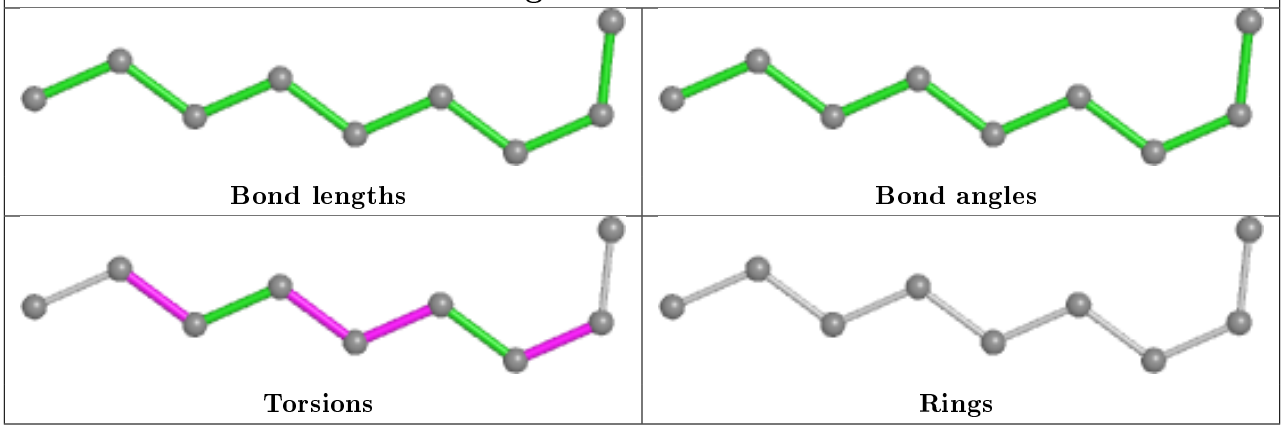

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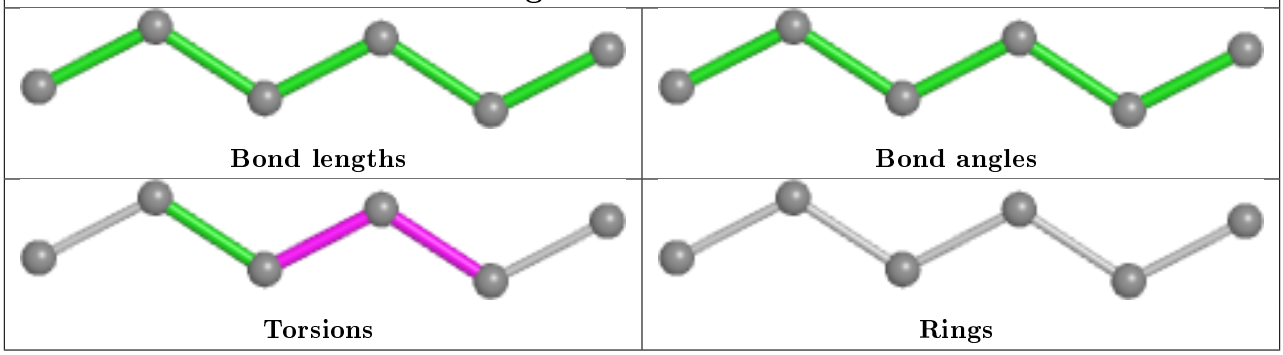

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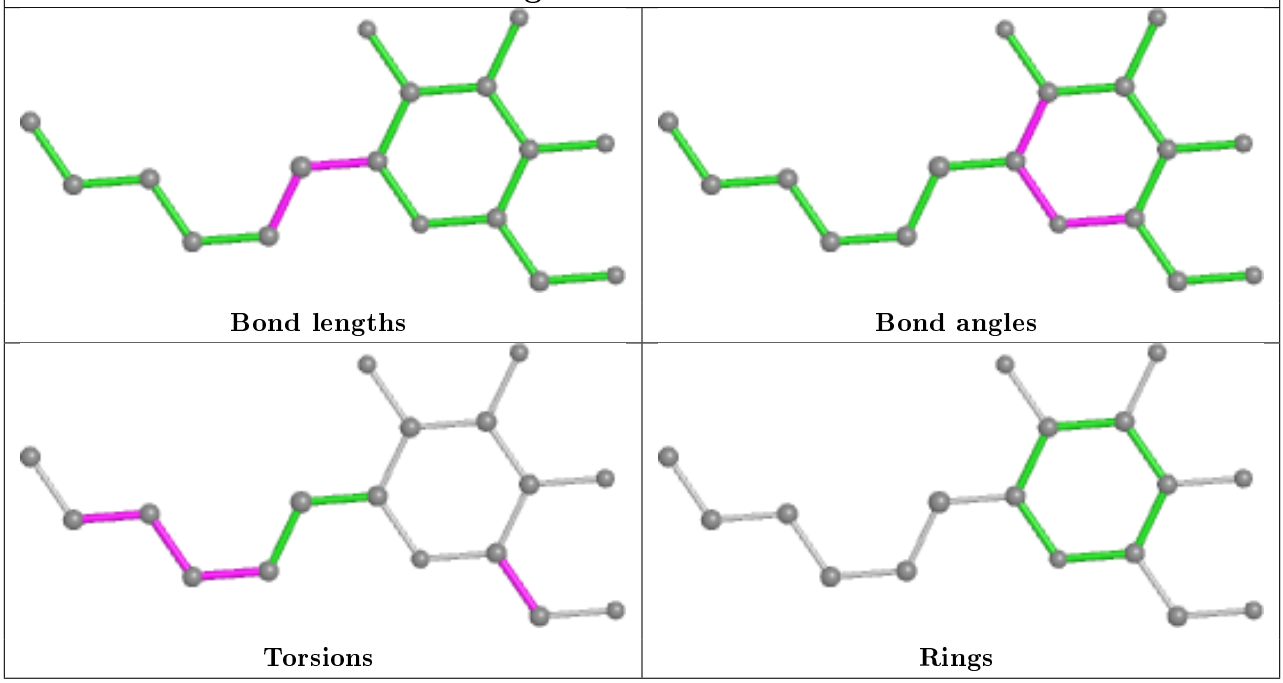
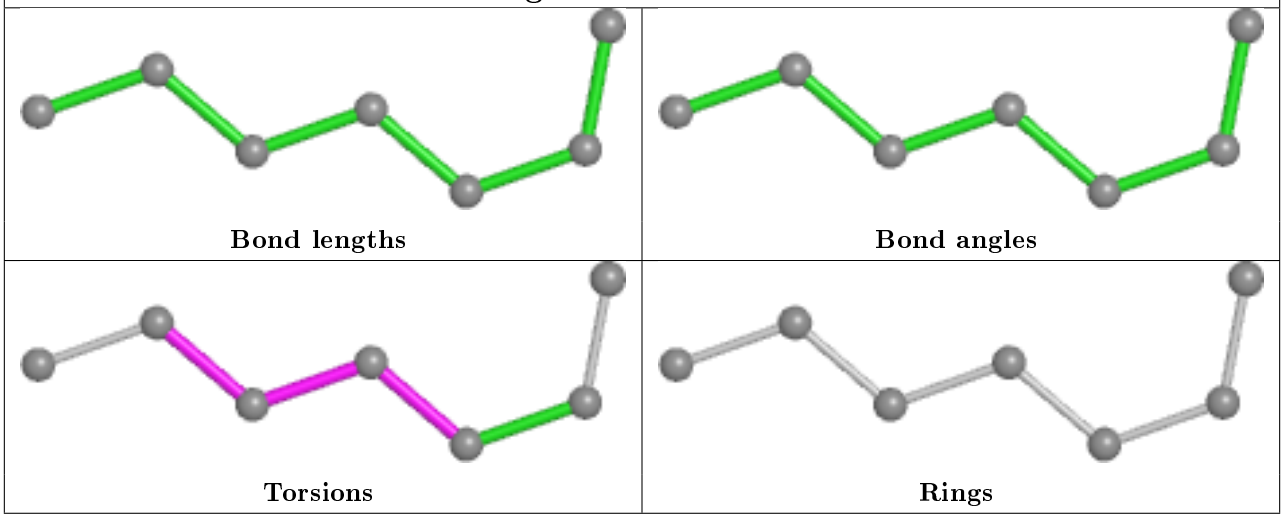
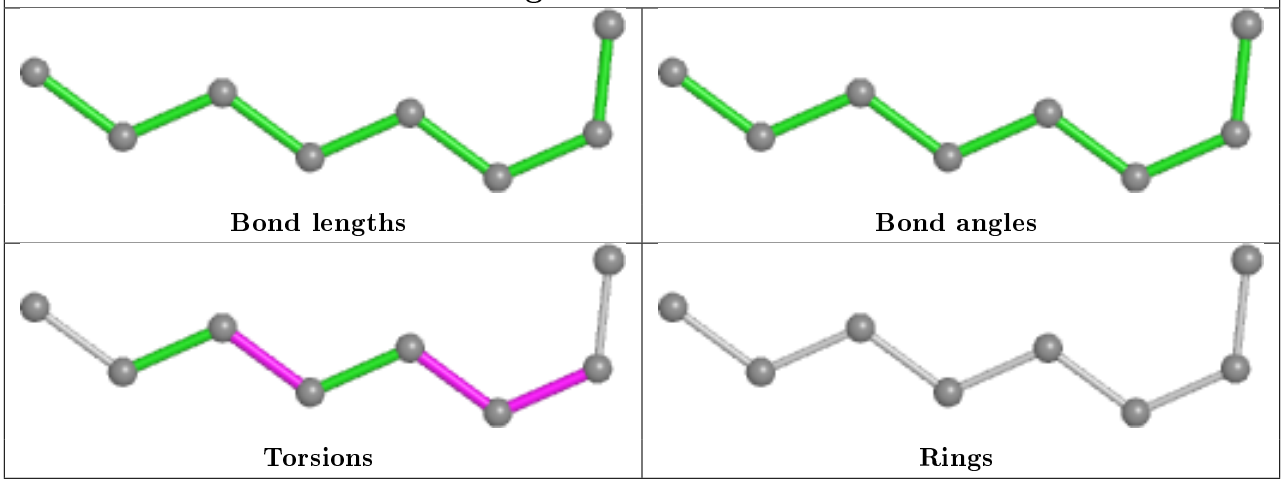


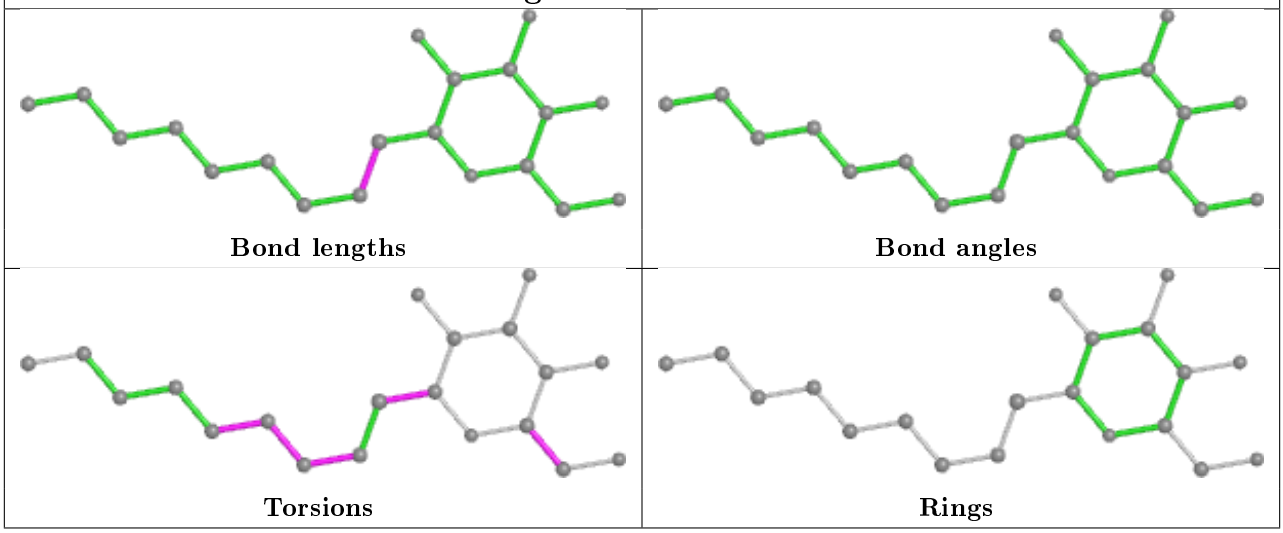
Ligand SOG B 430



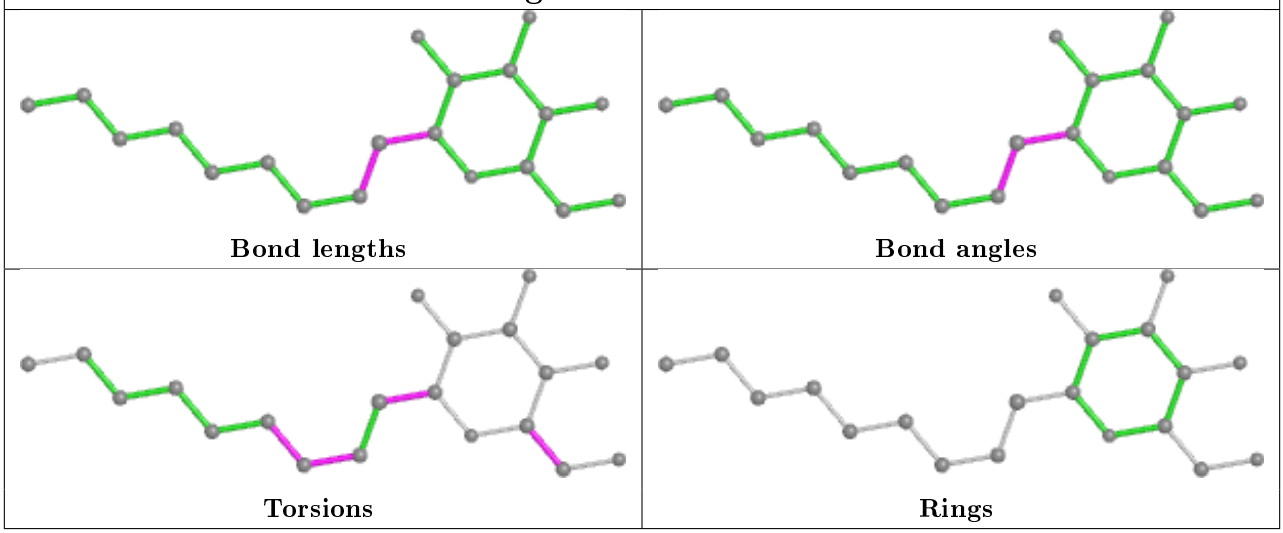
Ligand SOG B 418



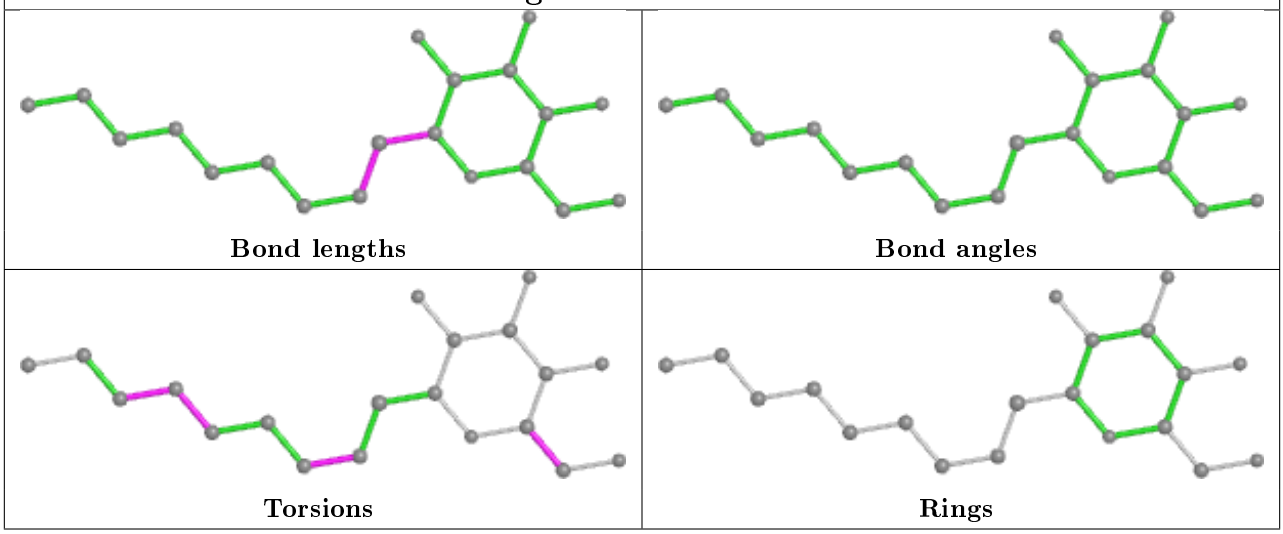
Ligand SOG A 418



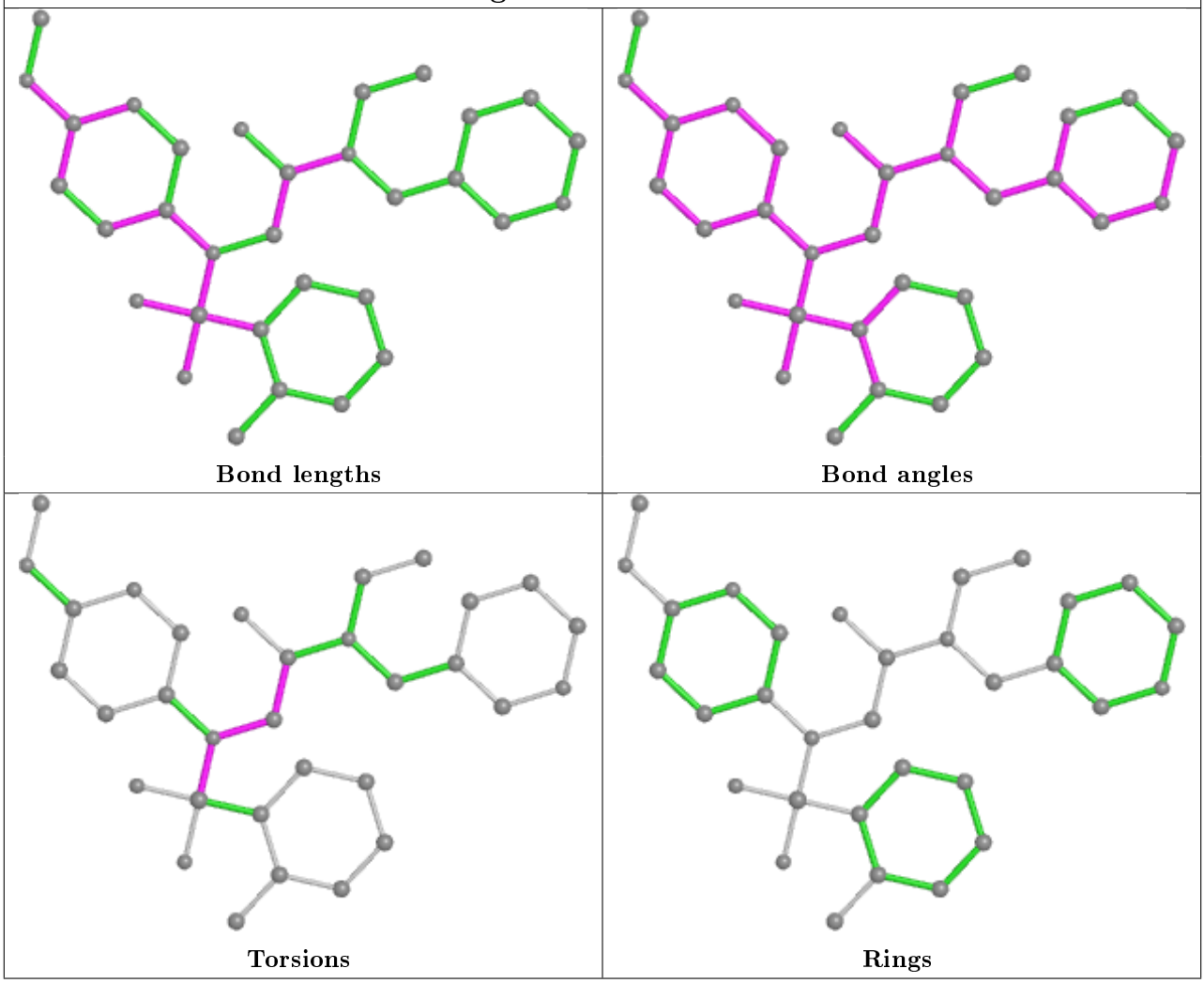
Ligand SOG B 406



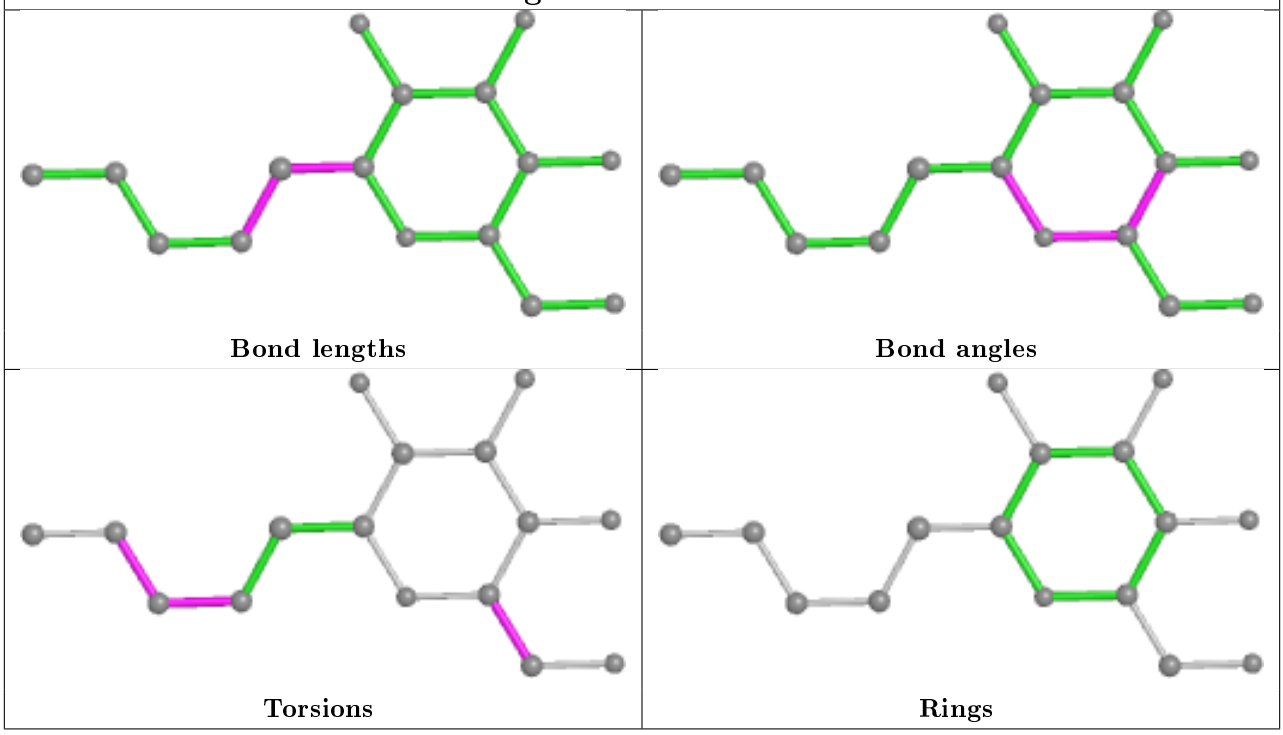
Ligand SOG B 412



Ligand 7MA A 401



Ligand SOG A 408



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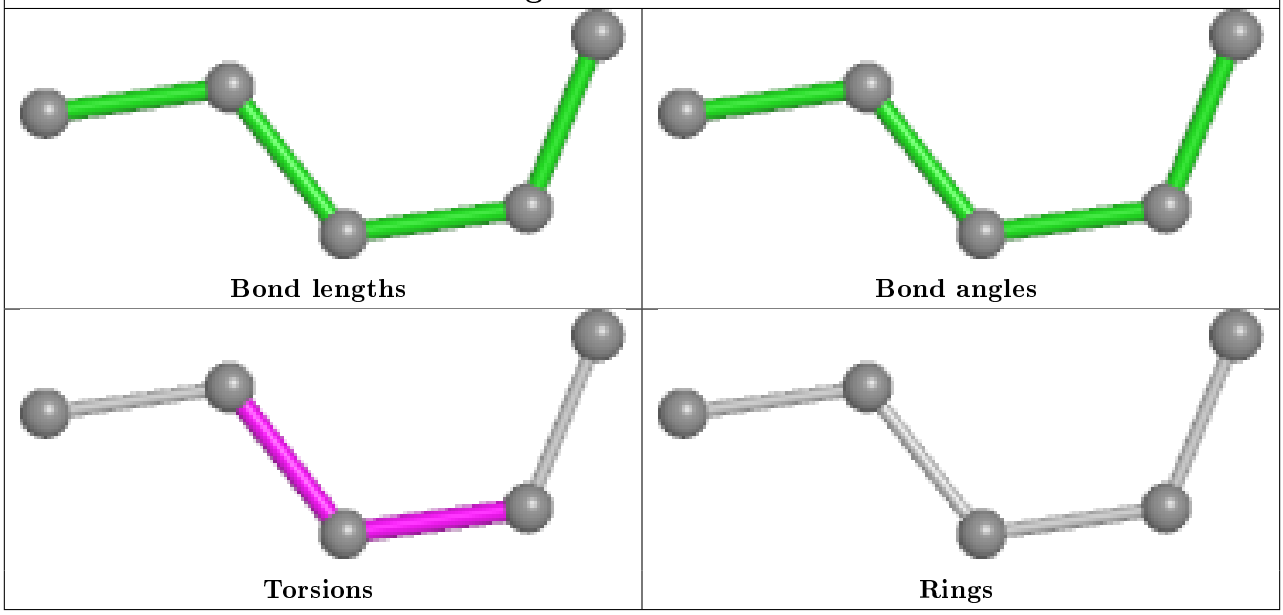
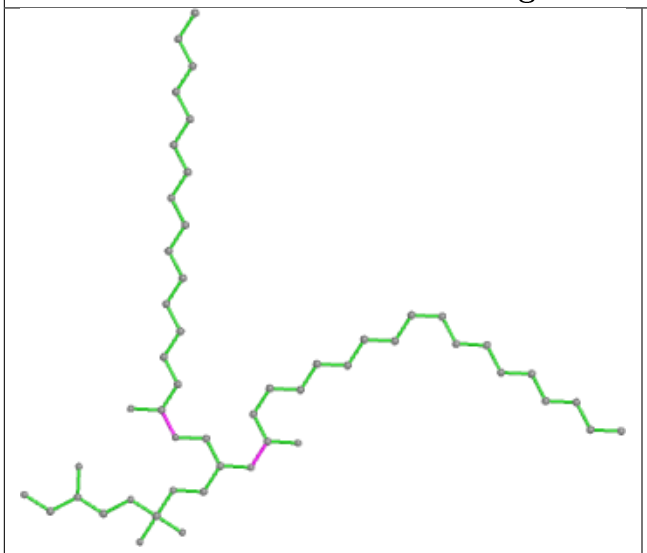
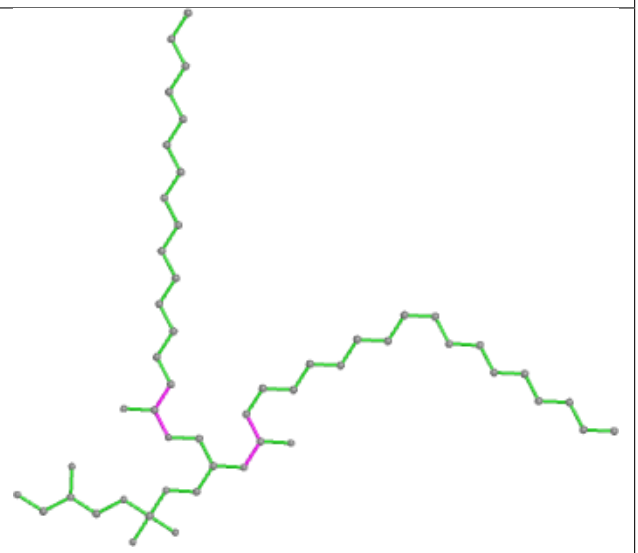


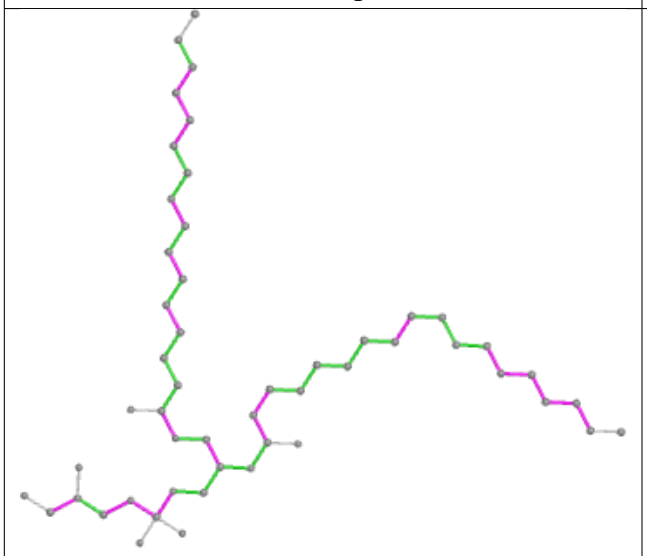
Ligand PGW B 431



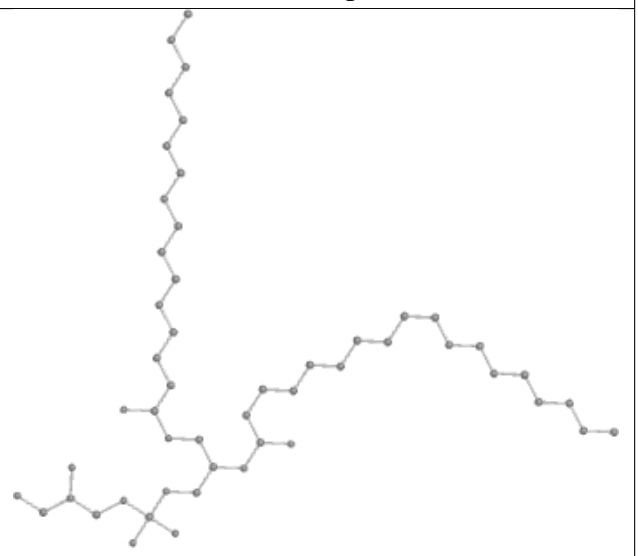
Bond lengths



Bond angles

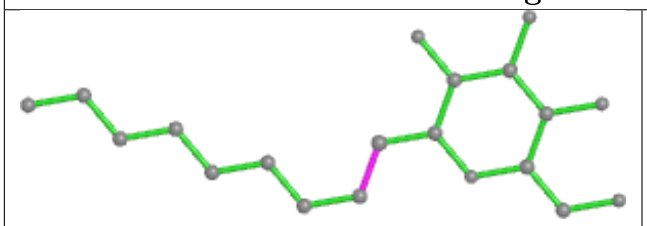


Torsions

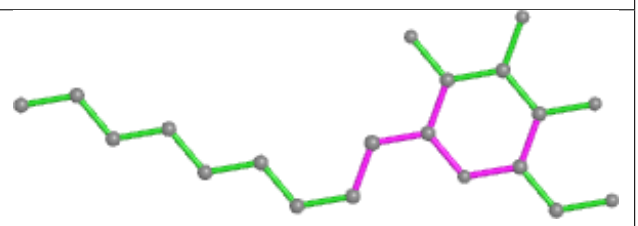


Rings

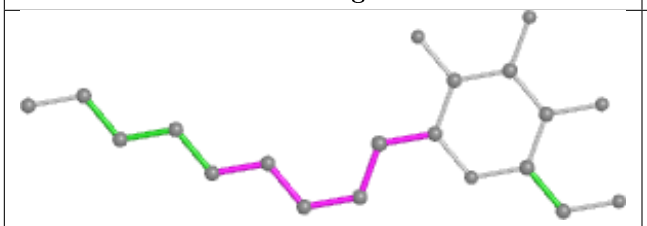
Ligand SOG A 410



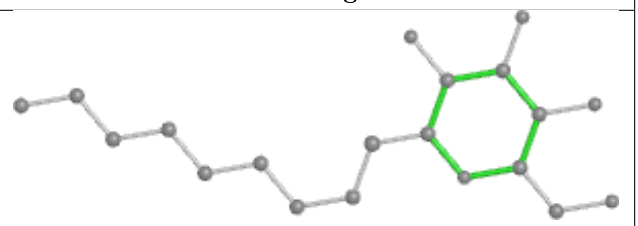
Bond lengths



Bond angles

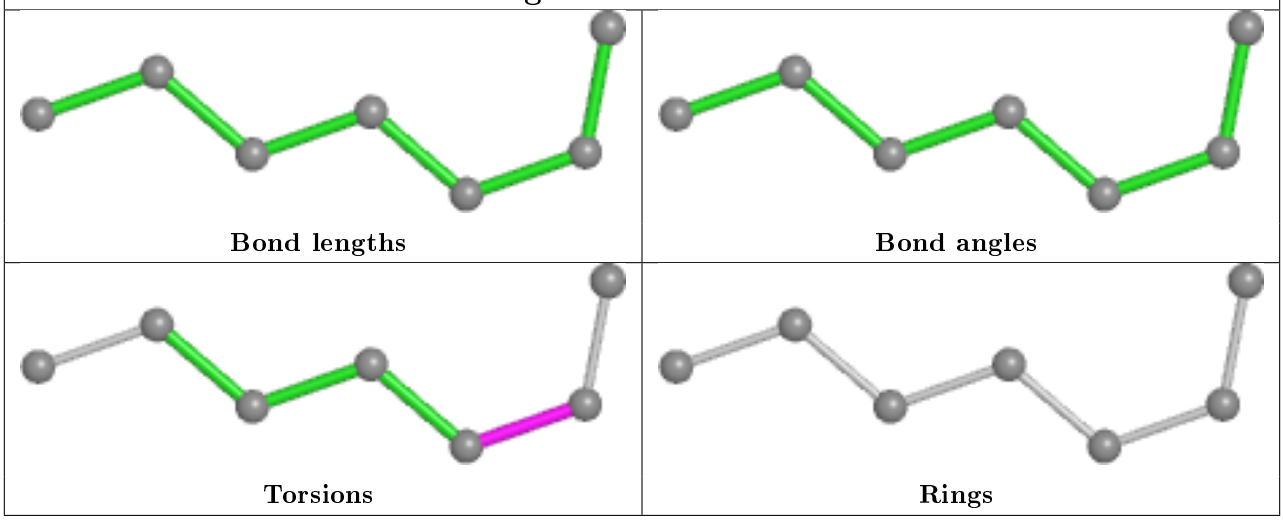


Torsions

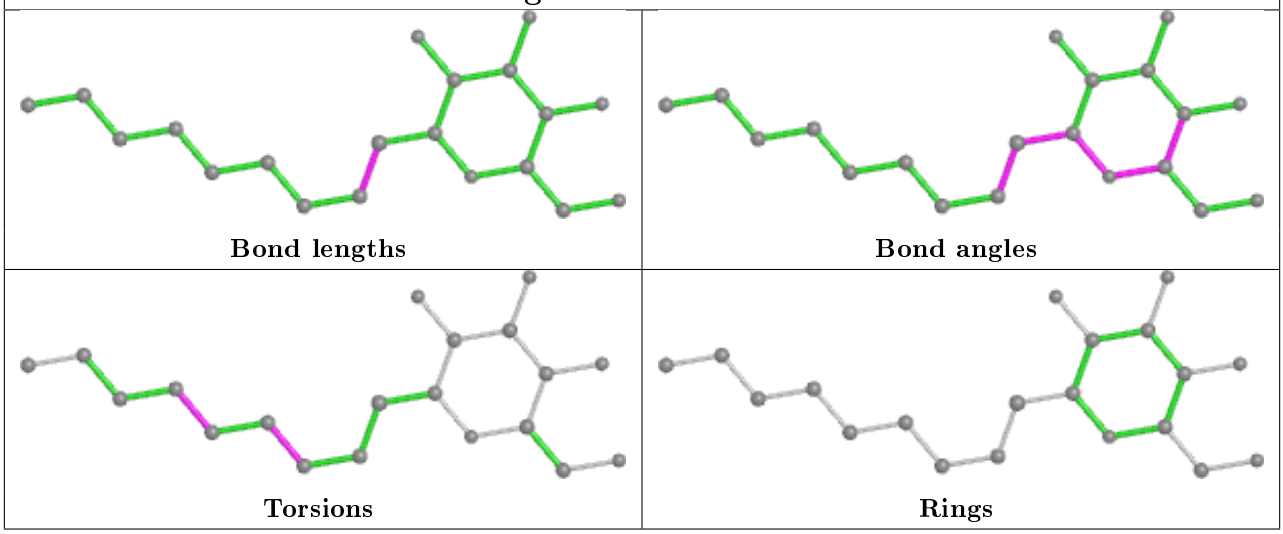


Rings

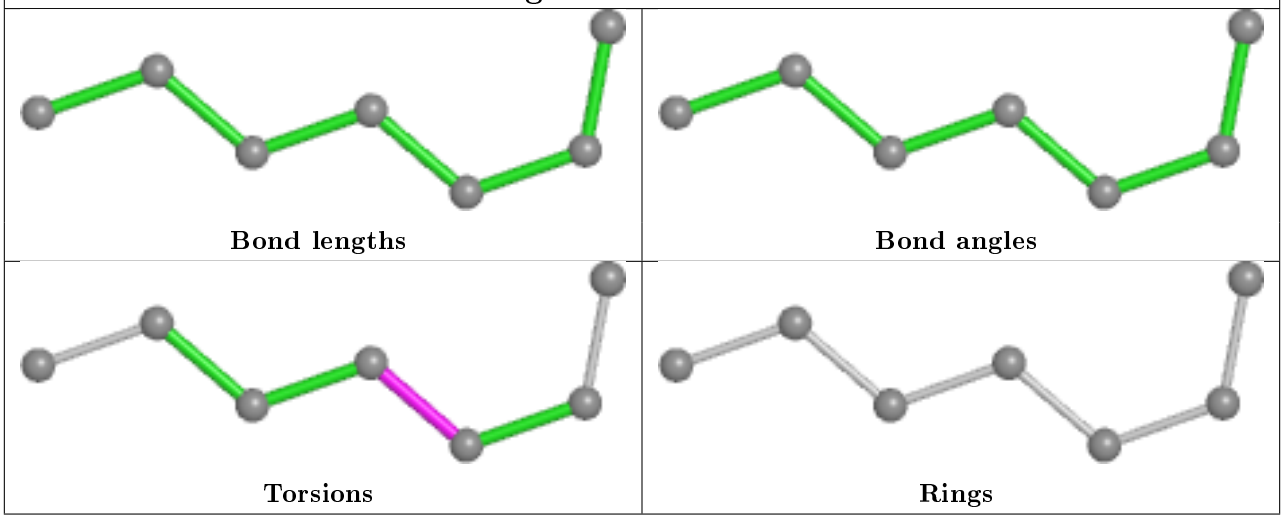
Ligand SOG A 420



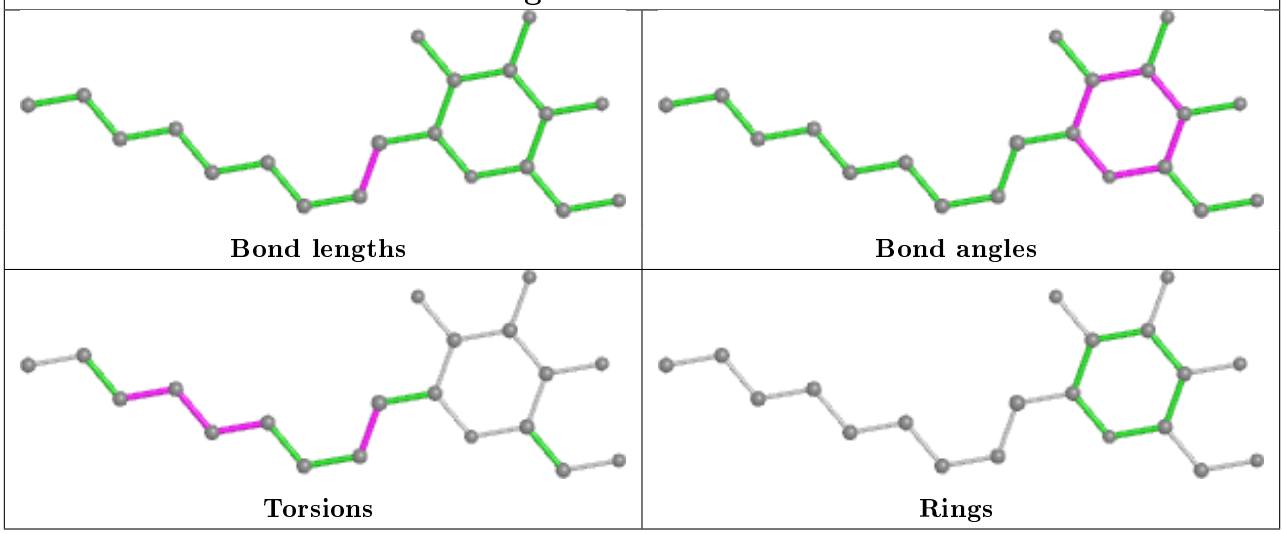
Ligand SOG A 411



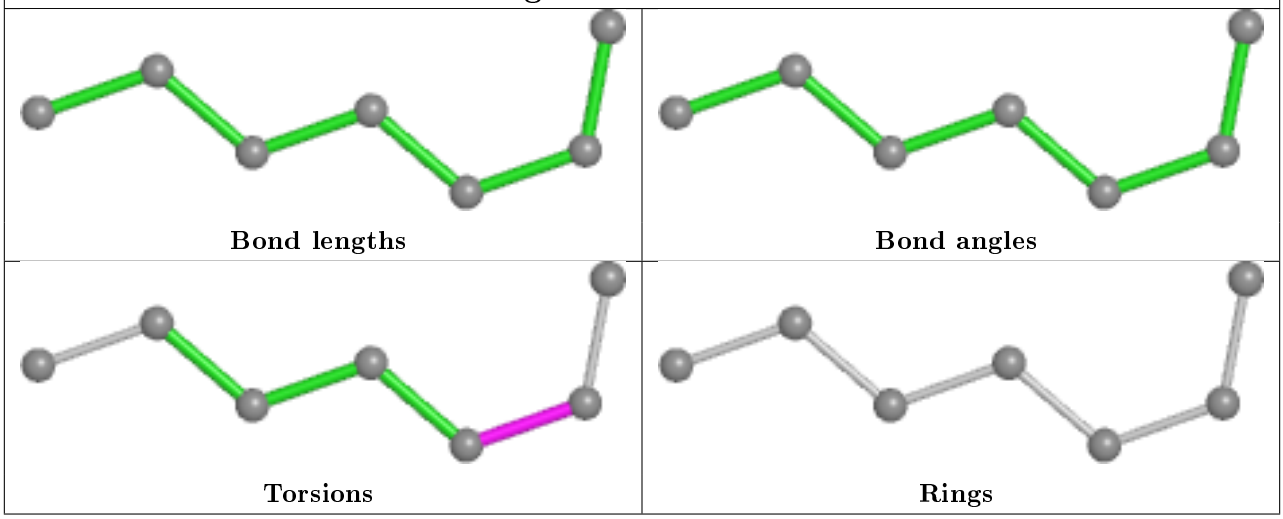
Ligand SOG B 429



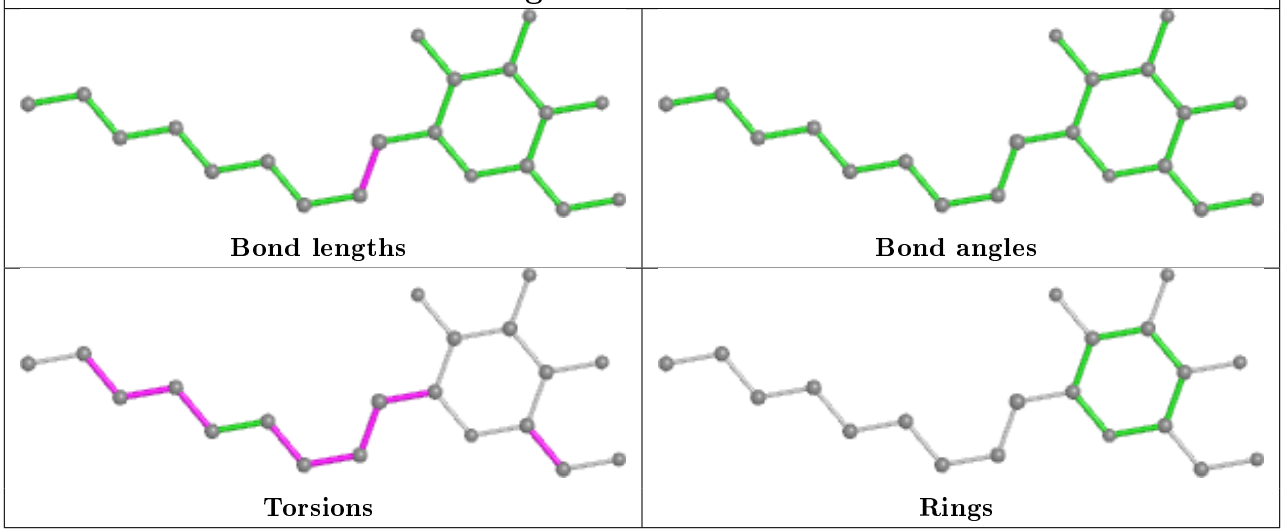
Ligand SOG A 413



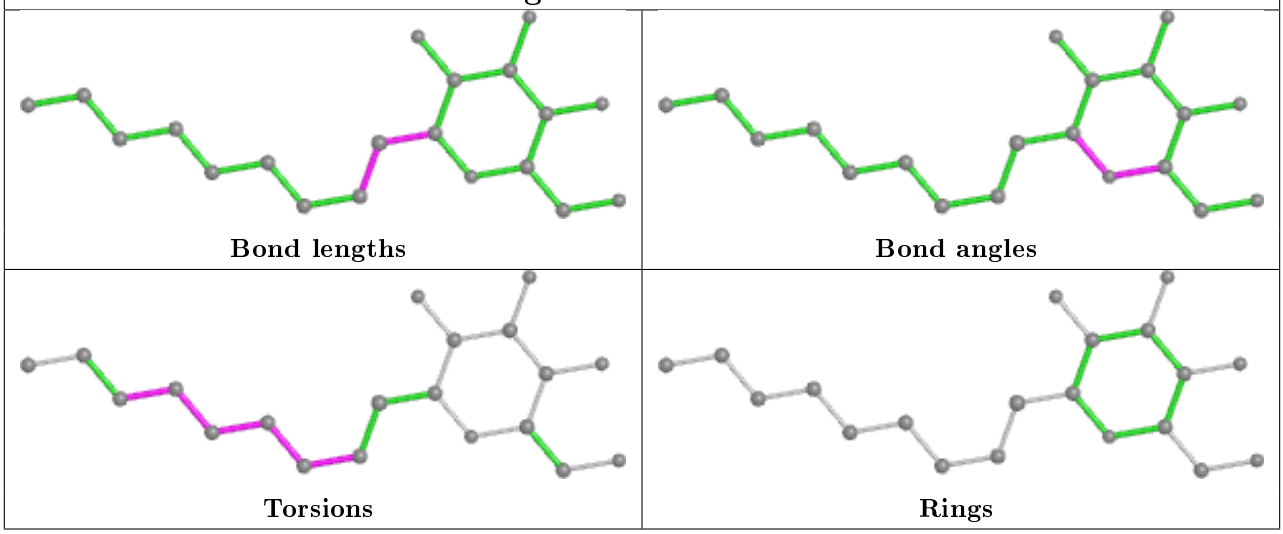
Ligand SOG A 419



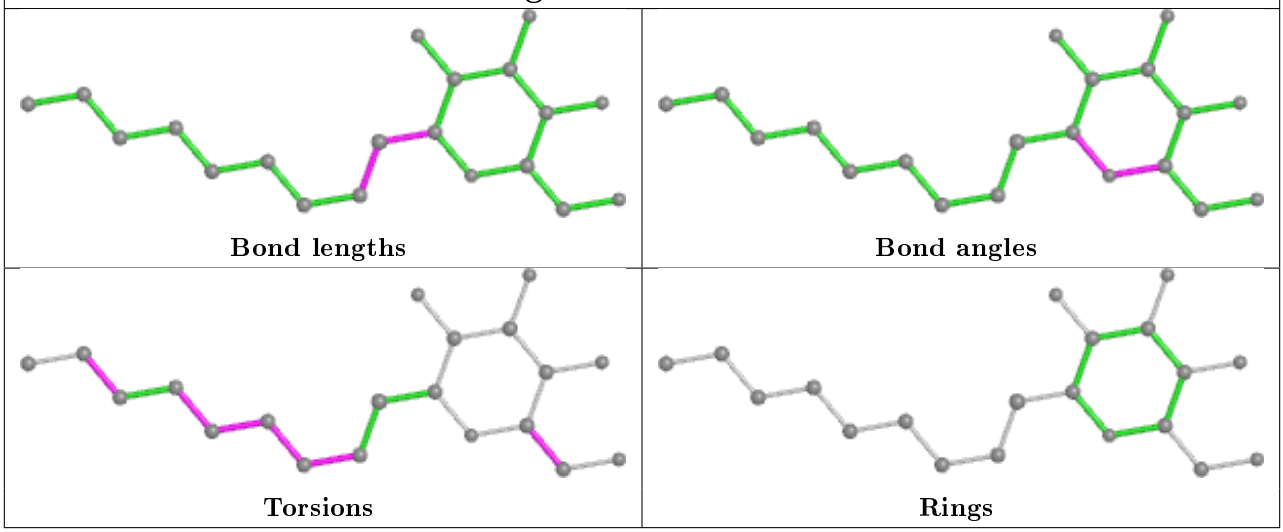
Ligand SOG B 410



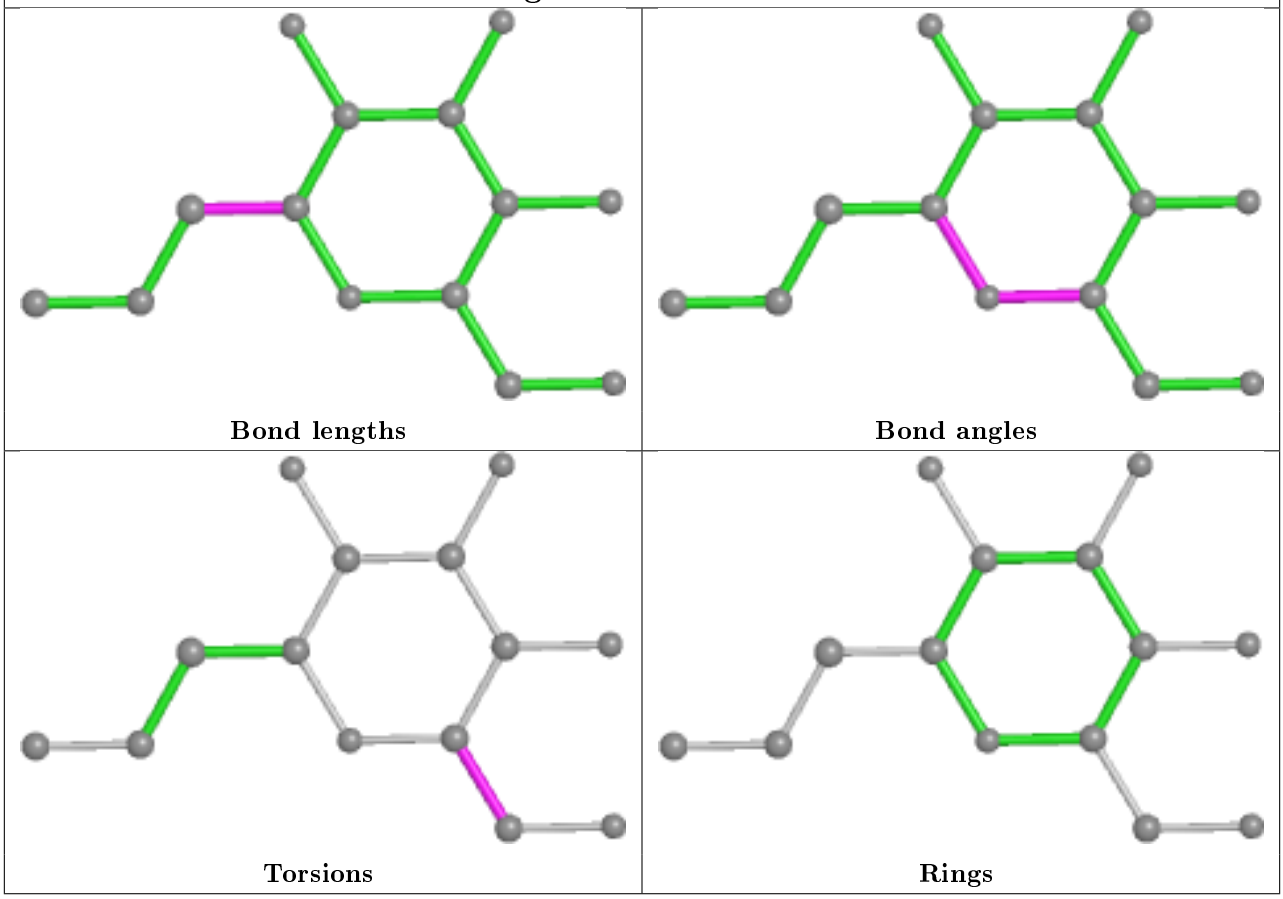
Ligand SOG A 412



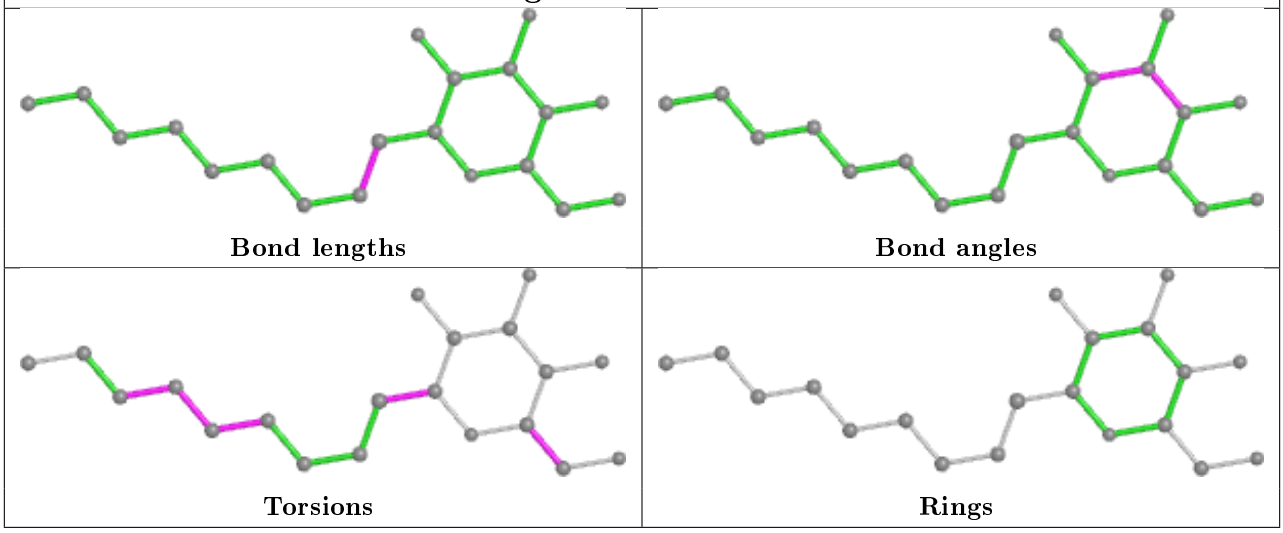
Ligand SOG B 407



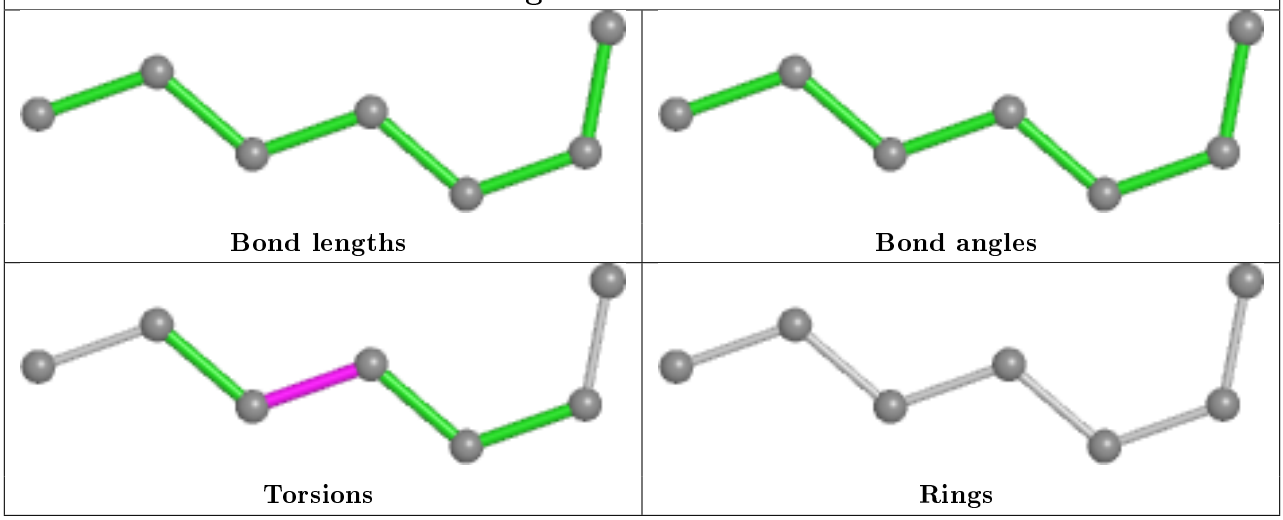
Ligand SOG A 415



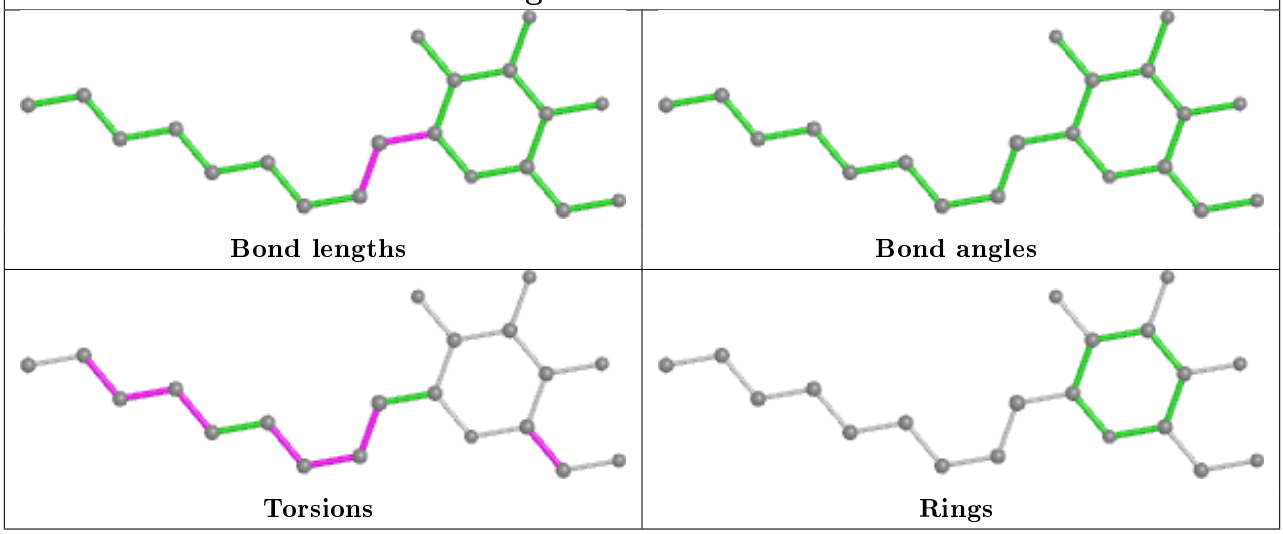
Ligand SOG A 409



Ligand SOG B 428



Ligand SOG B 408



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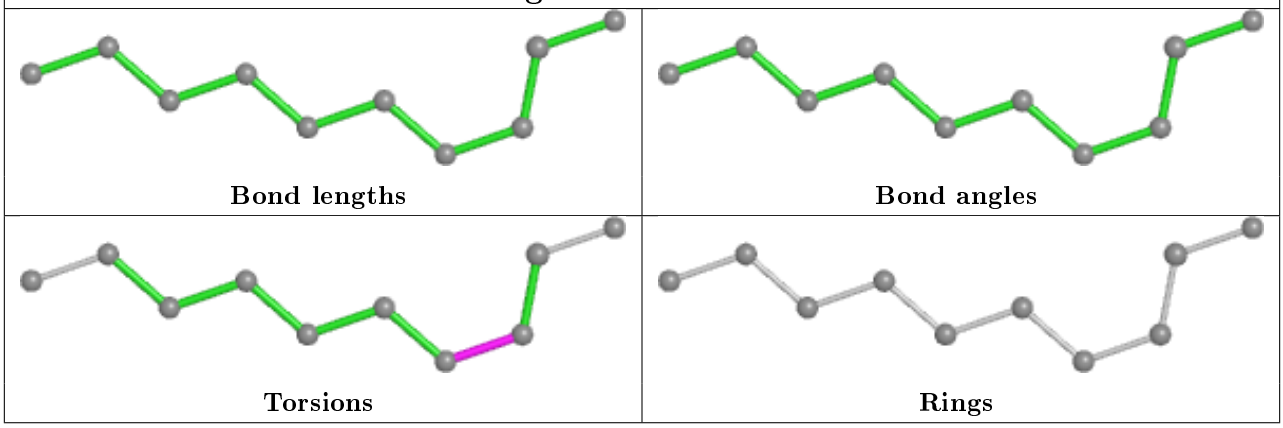
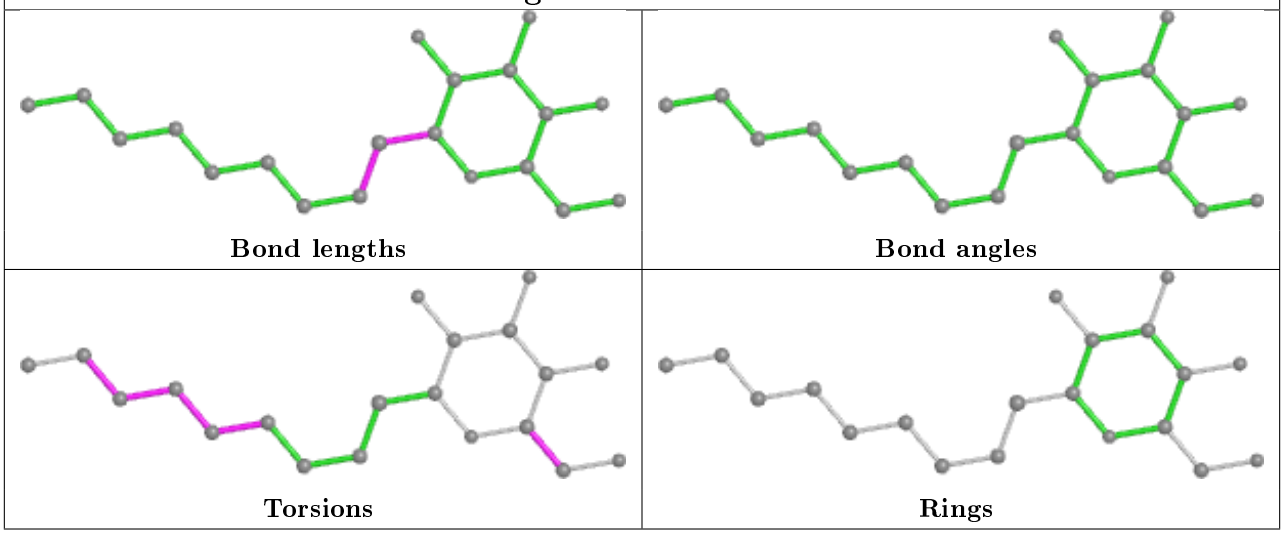


Ligand SOG A 414



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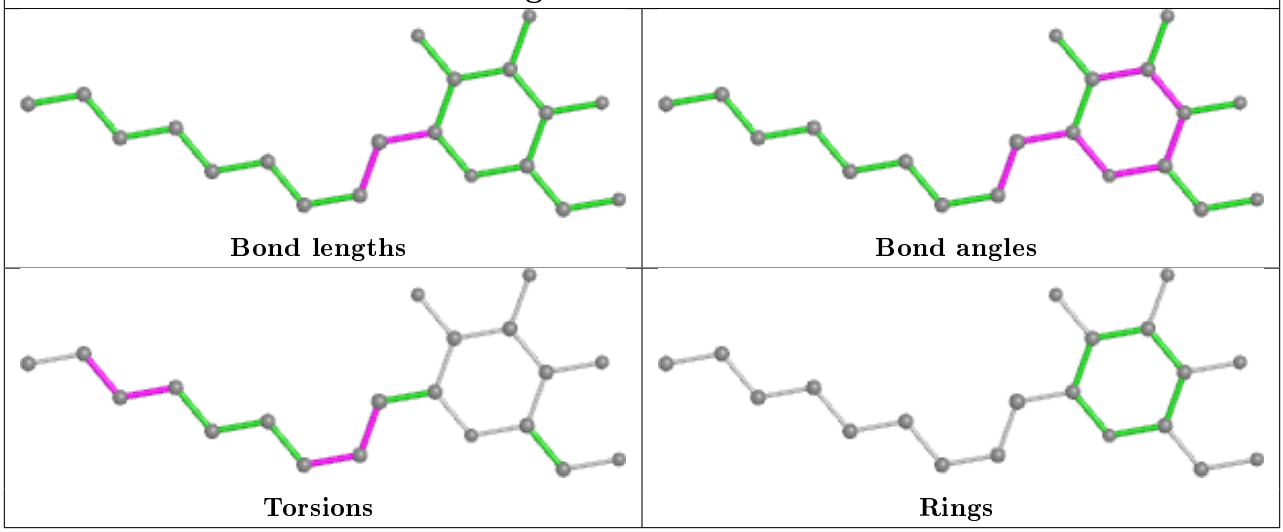
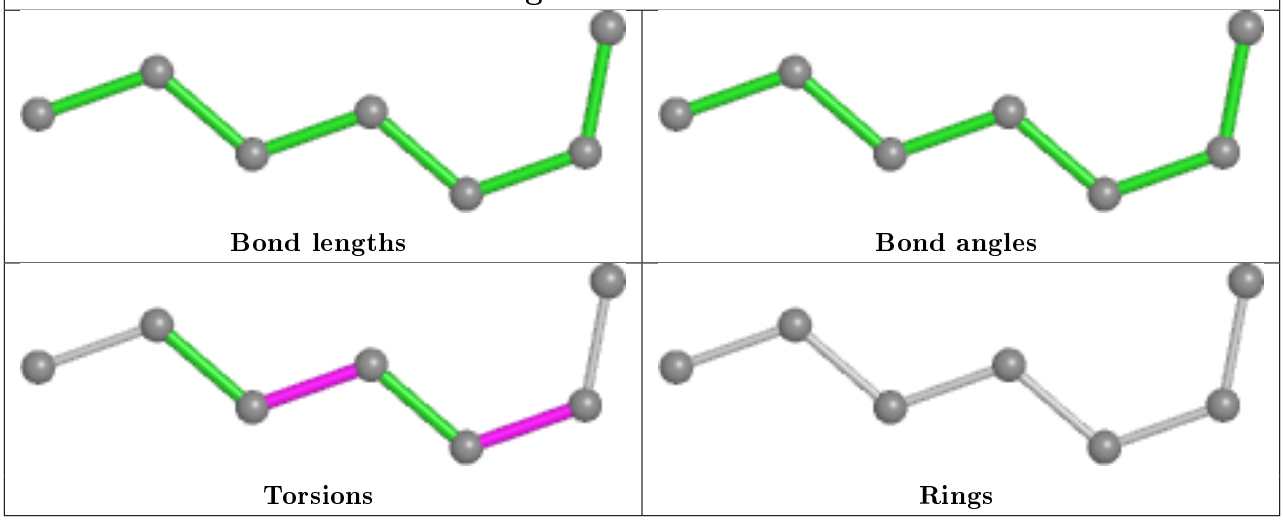
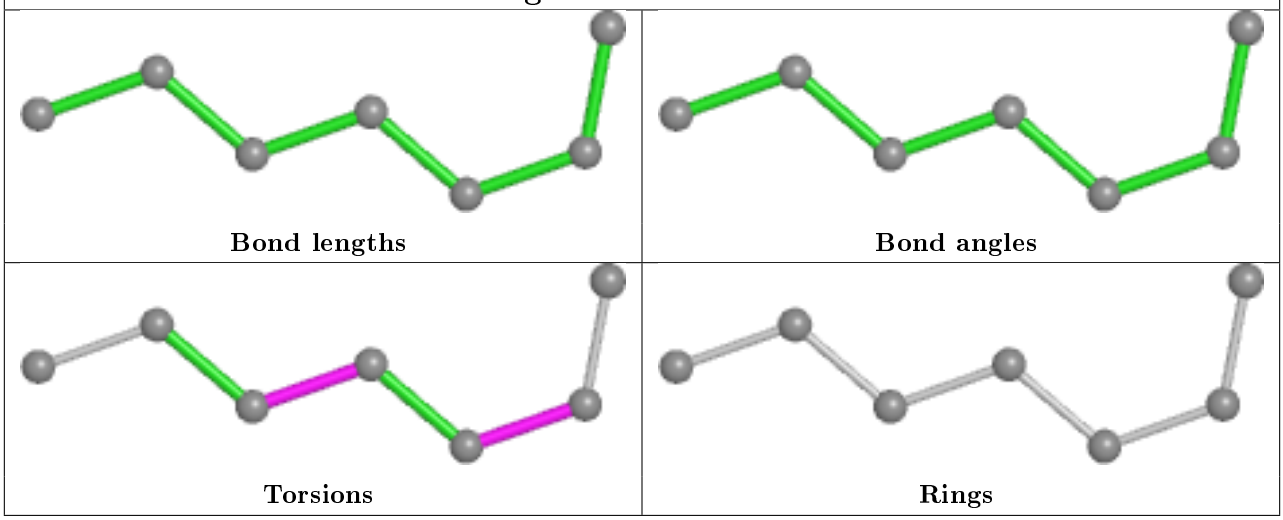


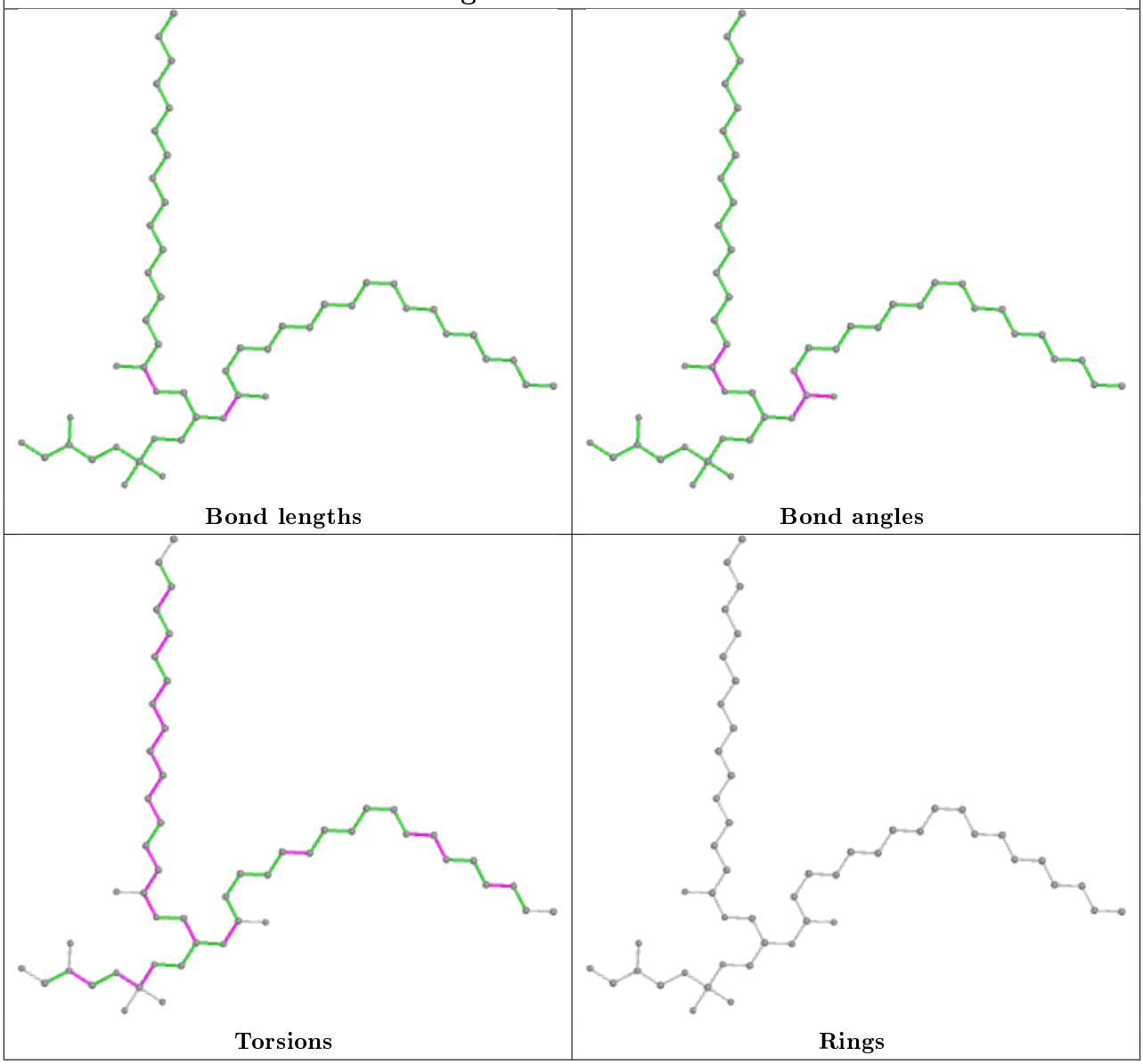
Ligand SOG B 425



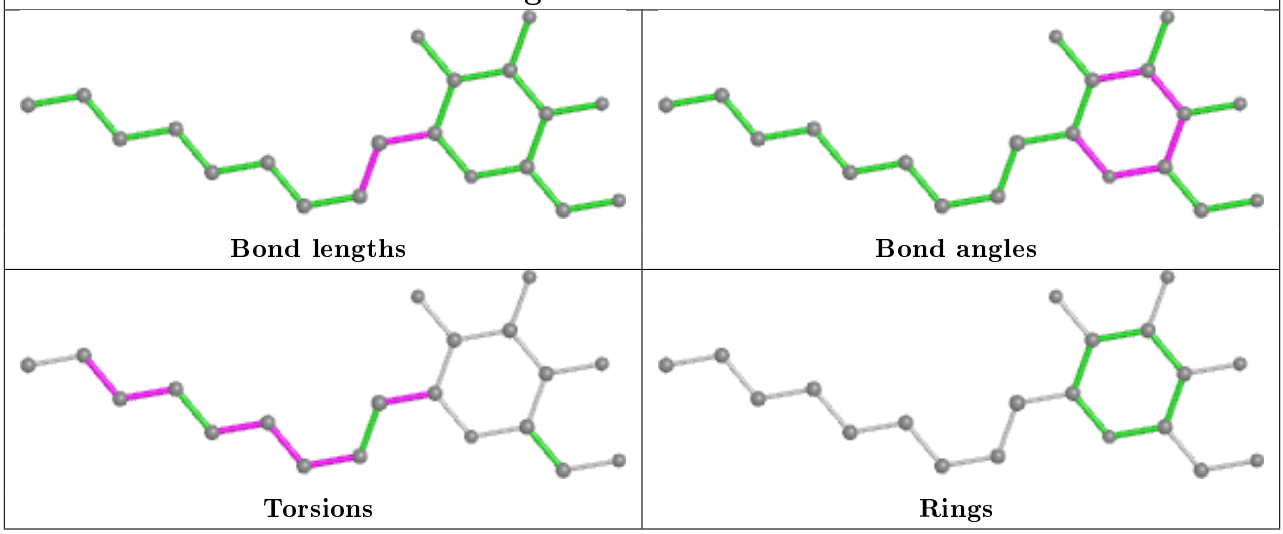
Ligand SOG A 425



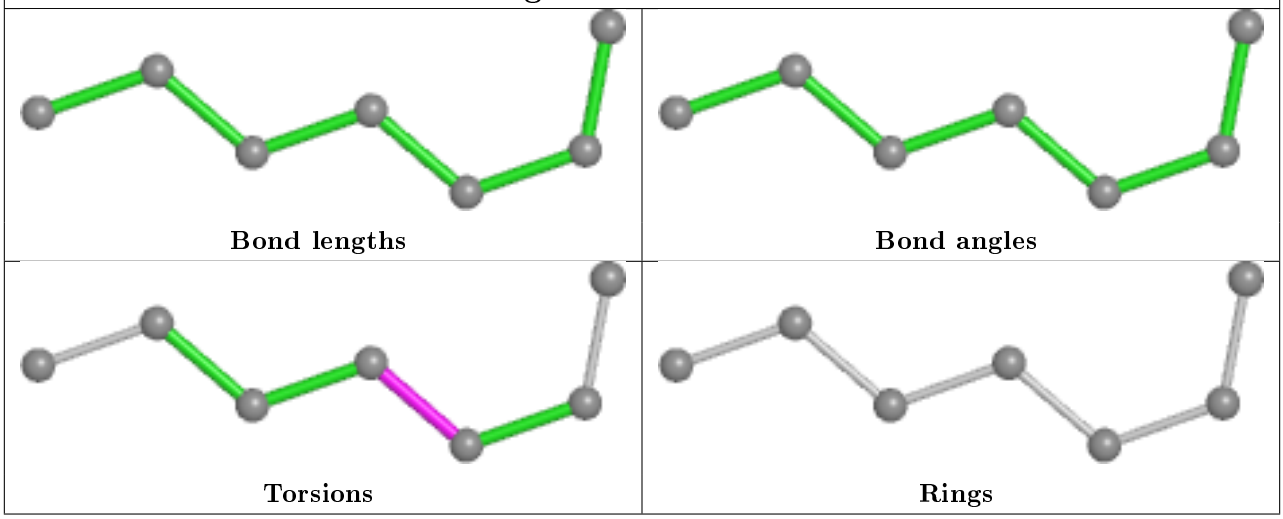
Ligand PGW A 429



Ligand SOG A 417



Ligand SOG A 421



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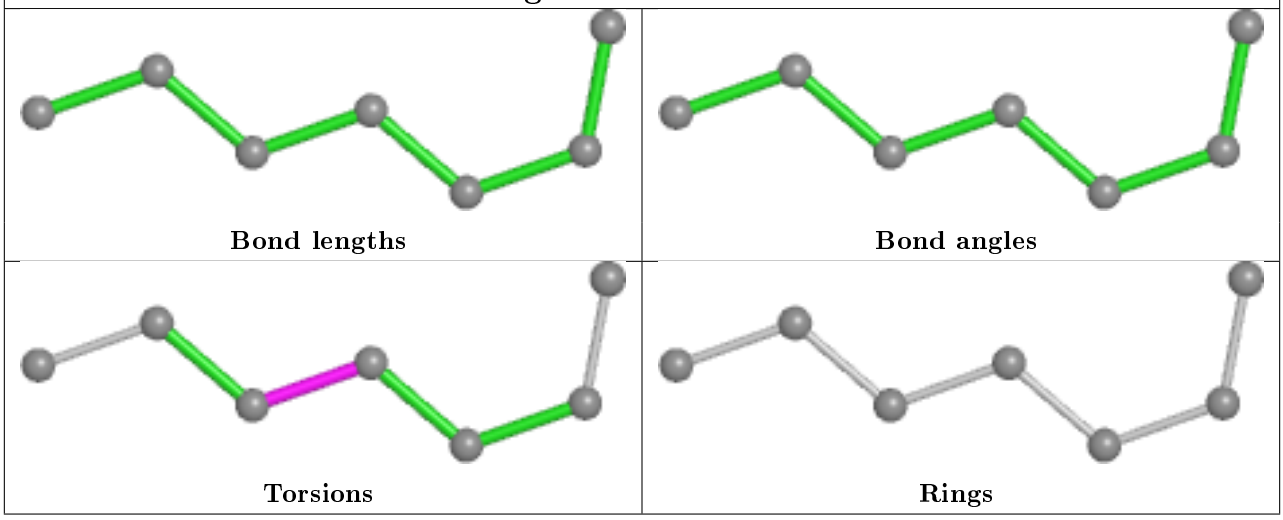
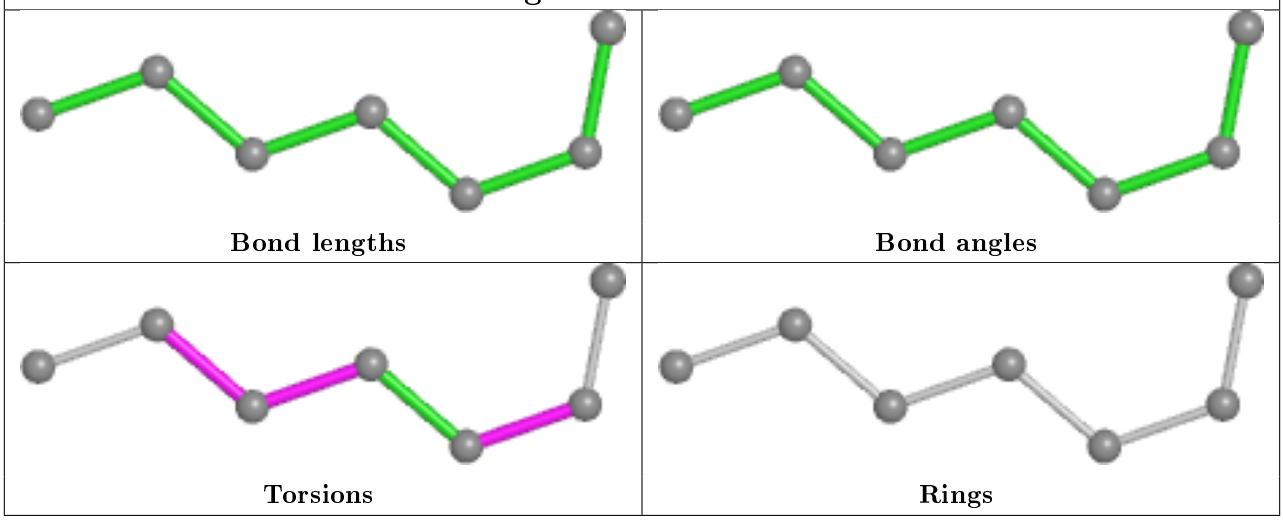
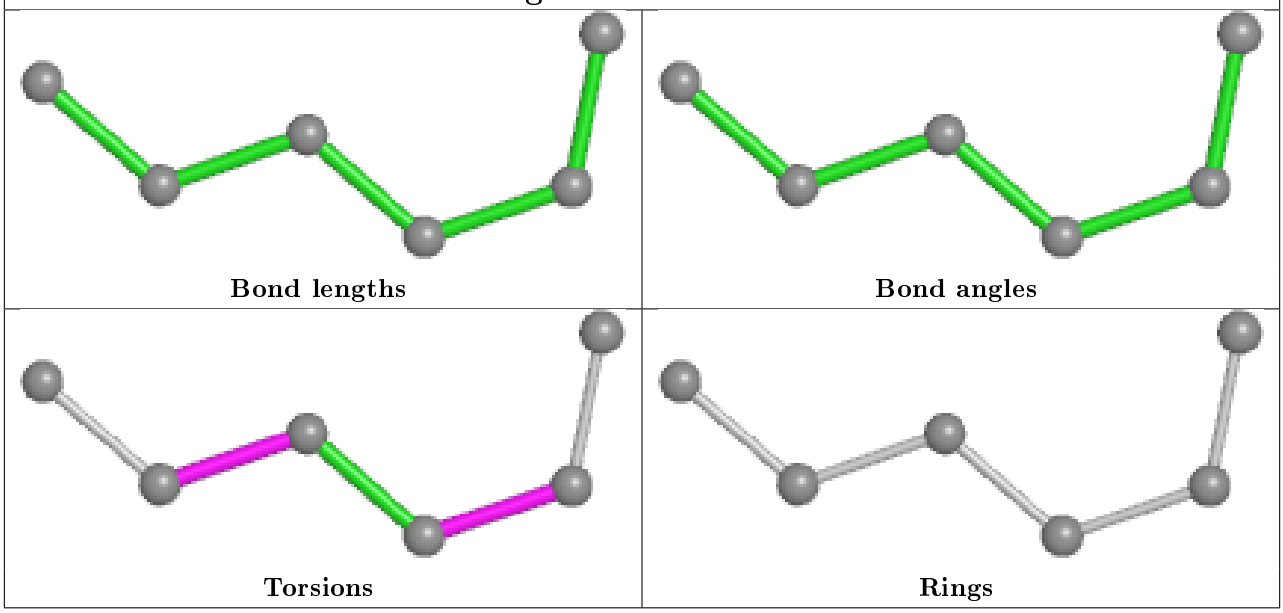


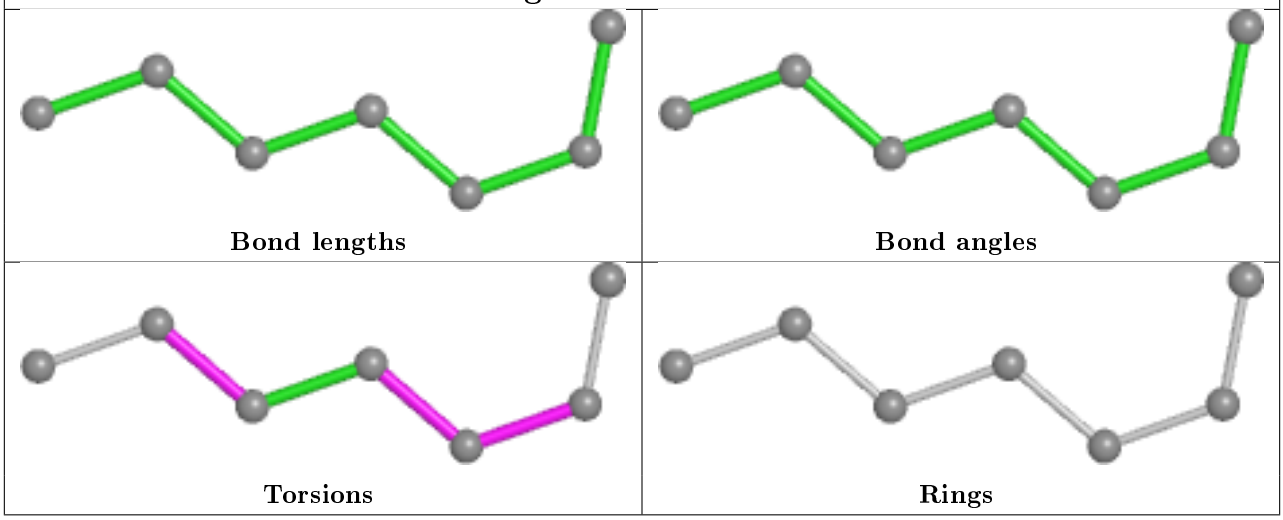
Ligand SOG A 427



Ligand SOG B 424



Ligand SOG A 422



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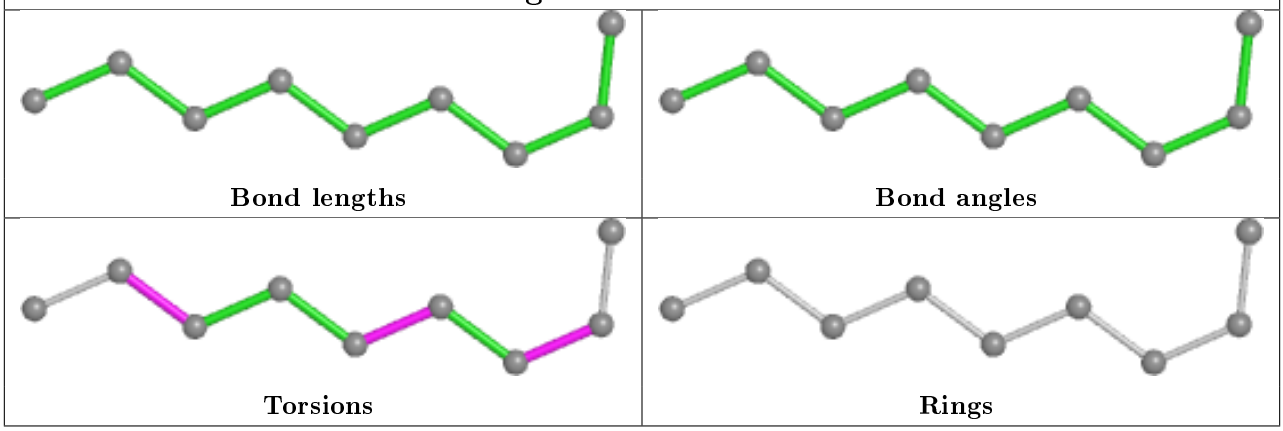
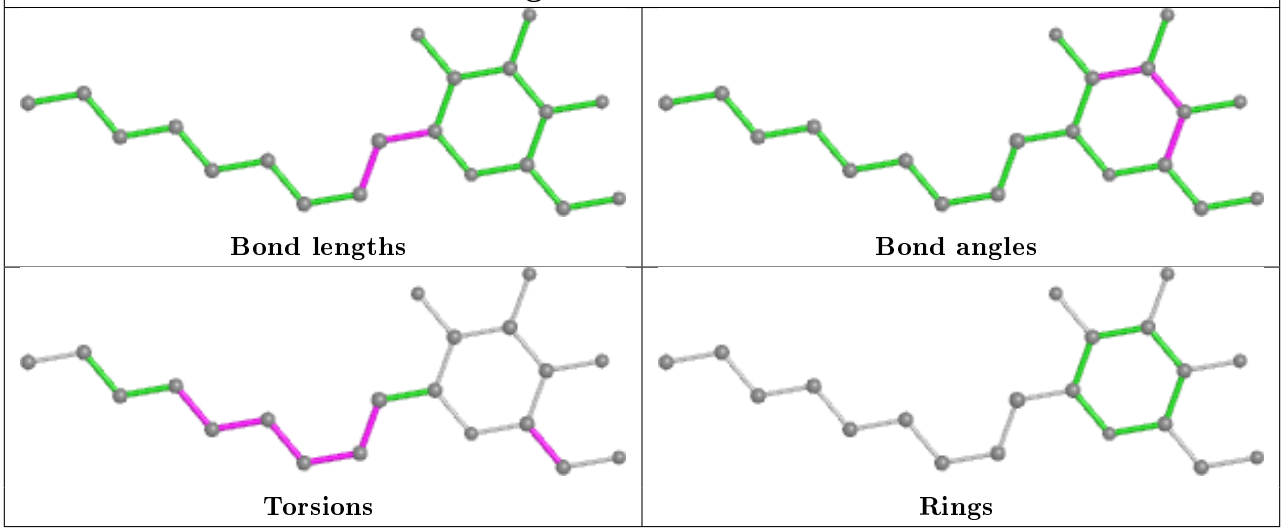
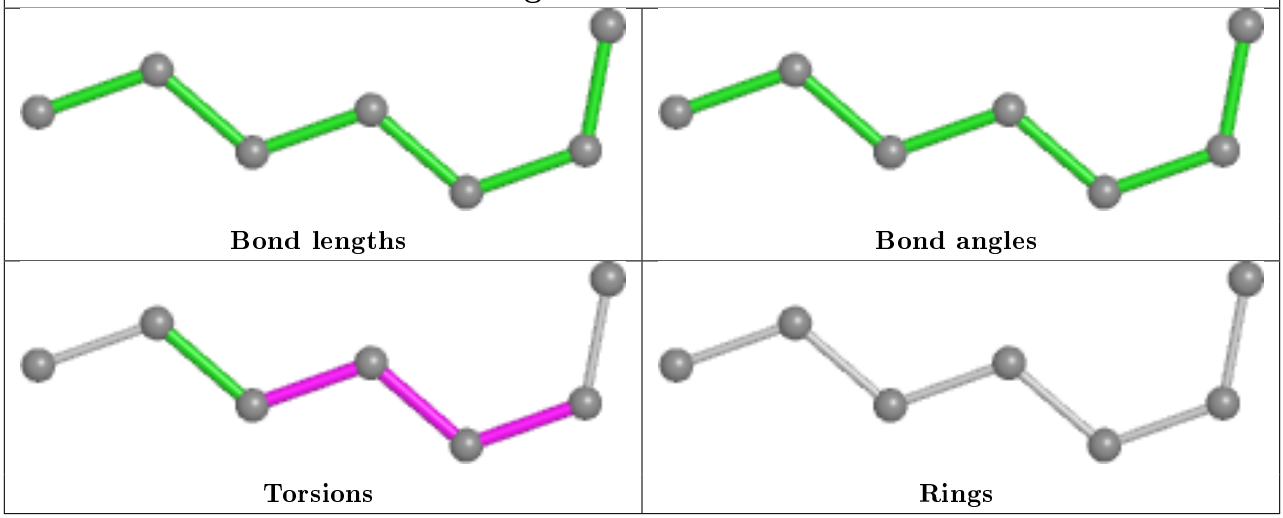


Ligand SOG B 411



Ligand SOG A 423



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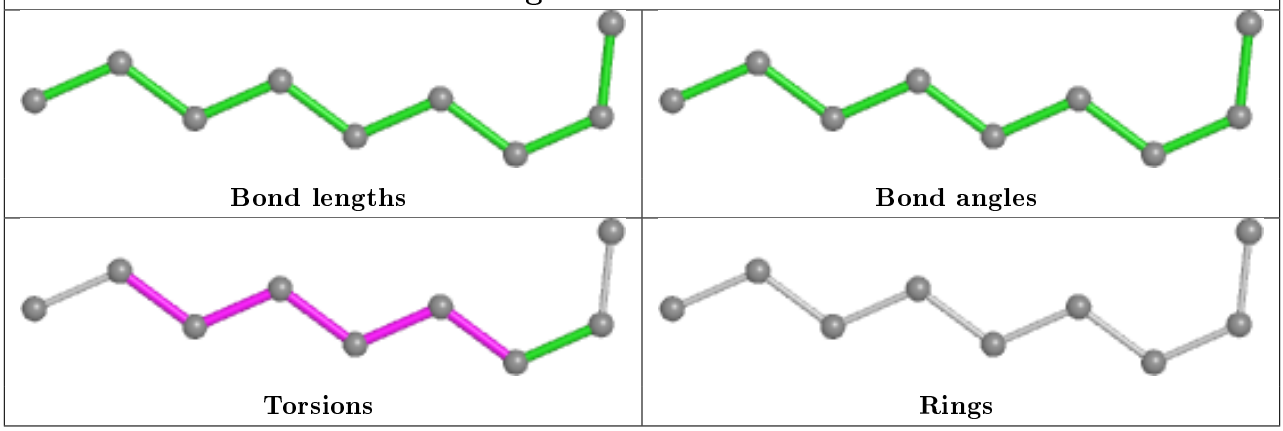
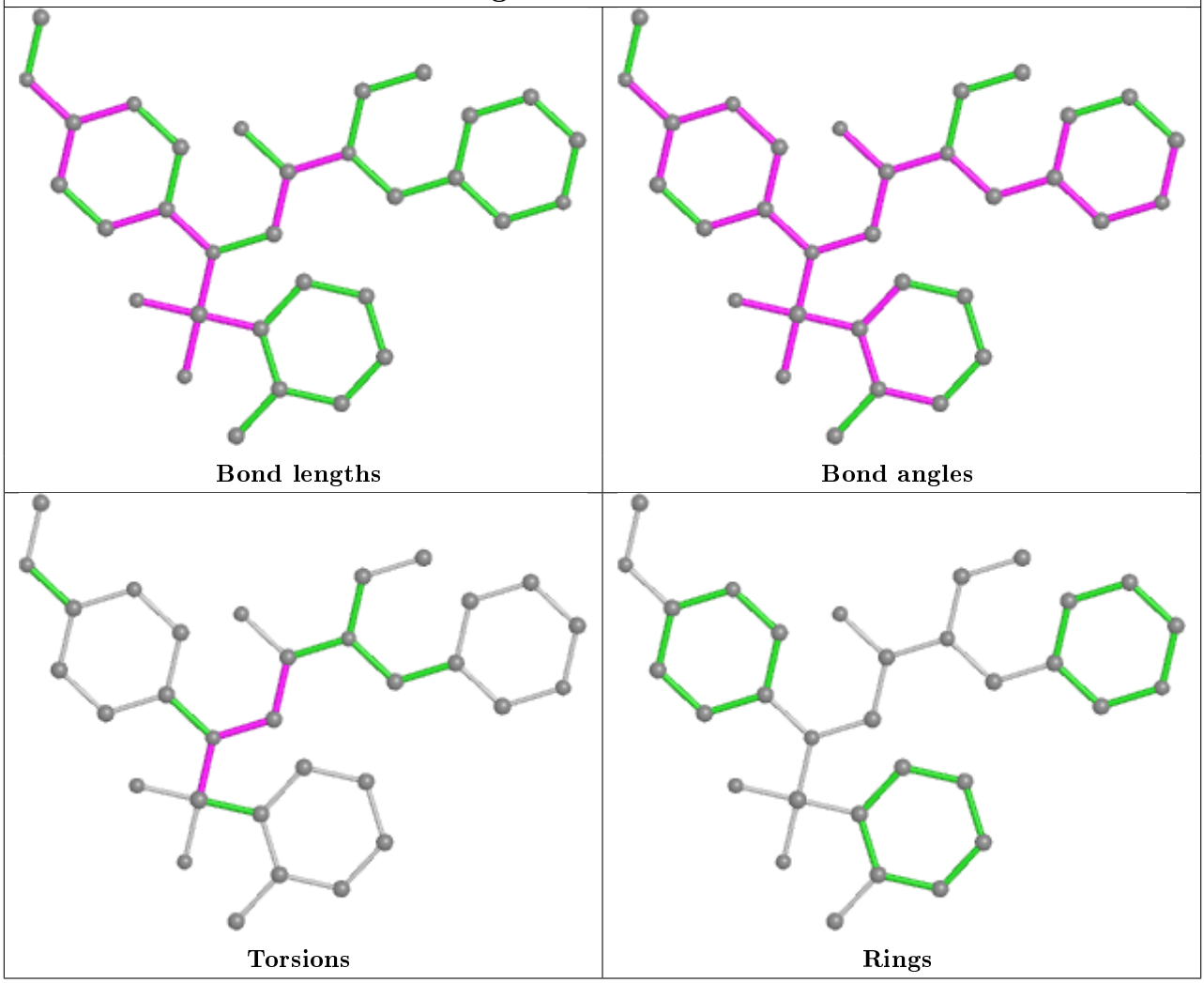
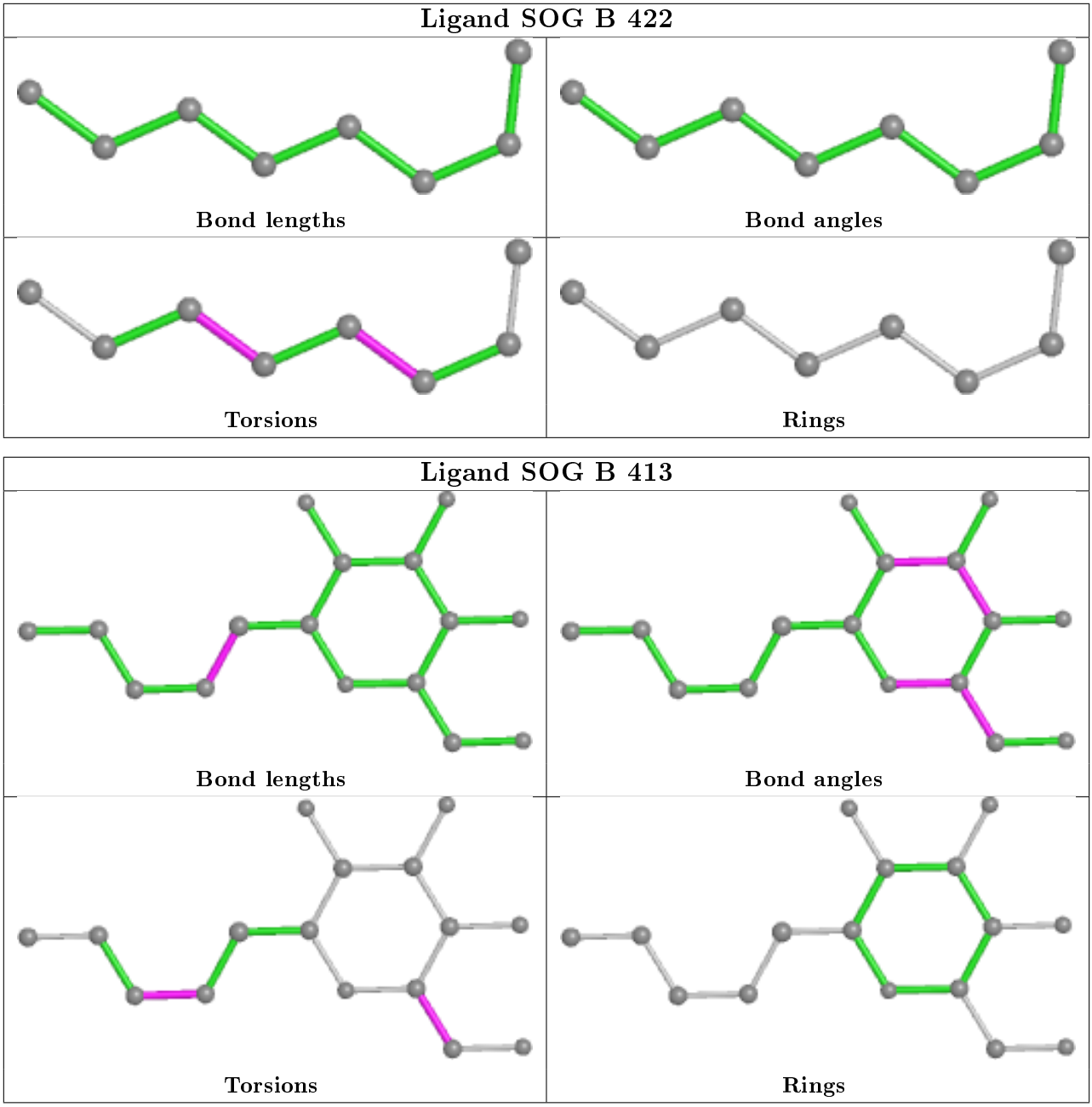


Ligand 7MA B 401





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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

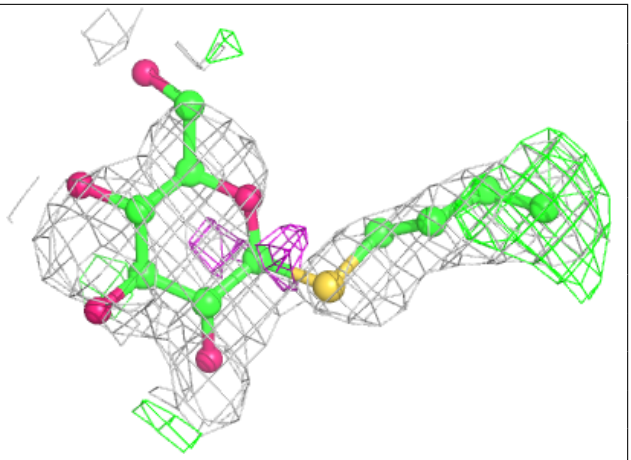
6.4 Ligands (i)

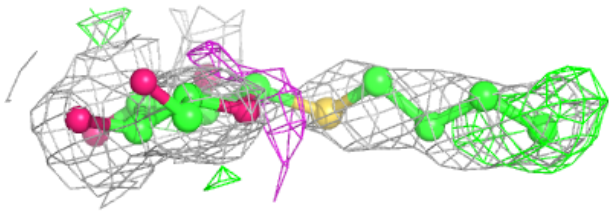
Unable to reproduce the depositors R factor - this section is therefore empty.

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 421:

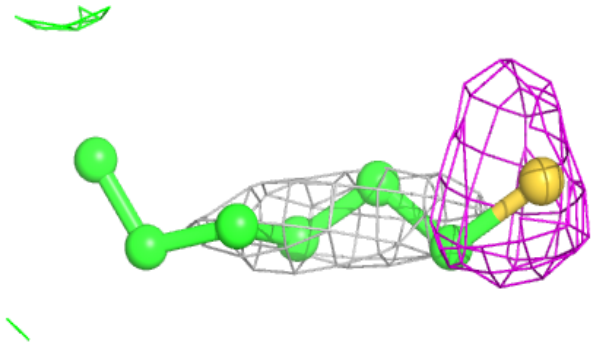
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

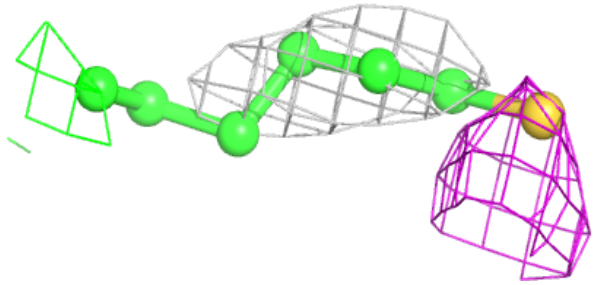


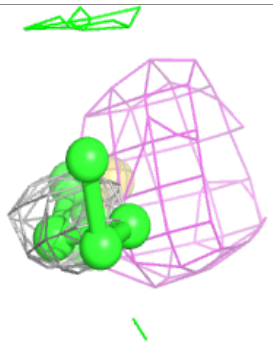


Electron density around SOG A 424:

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

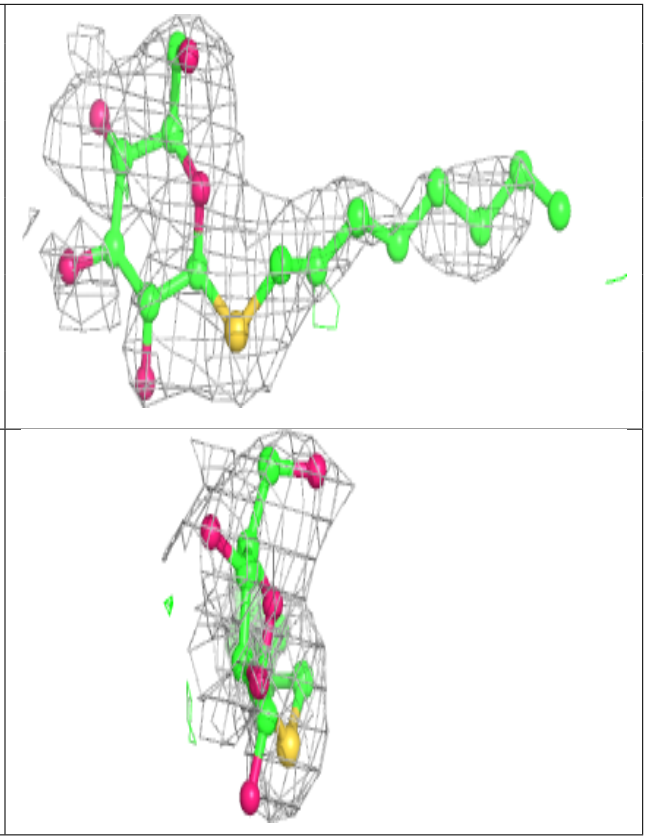






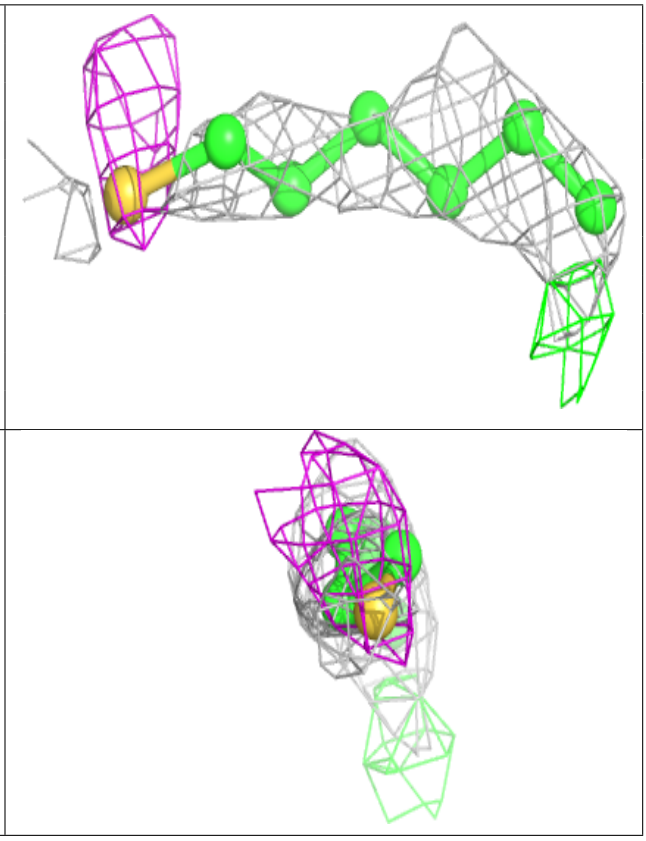
Electron density around SOG B 414:

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



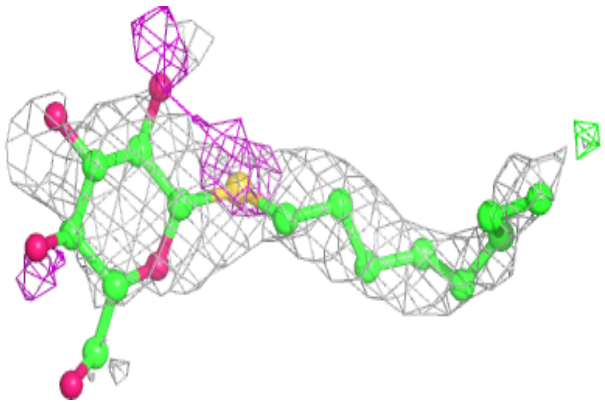
Electron density around SOG B 426:

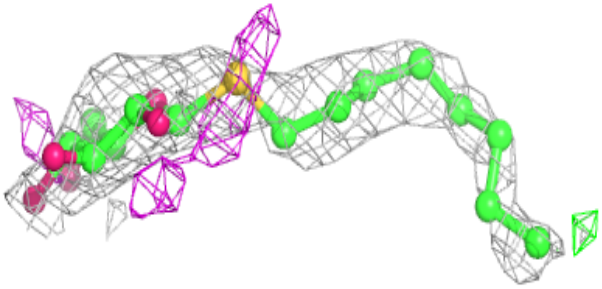
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

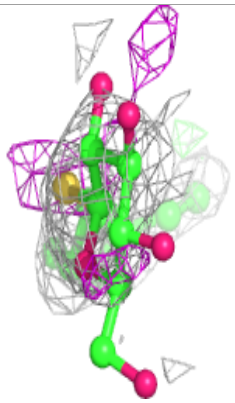


Electron density around SOG A 416:

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

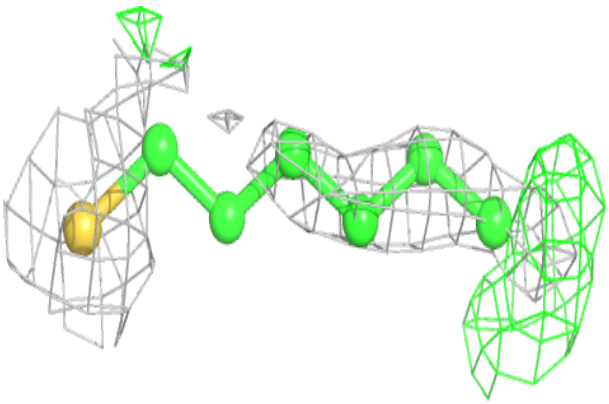


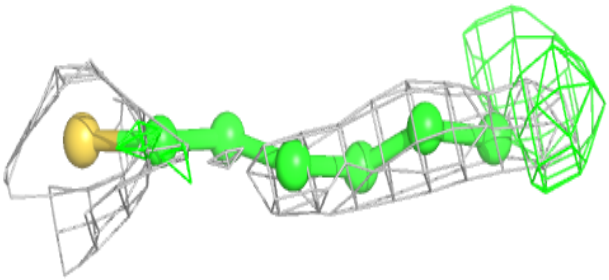


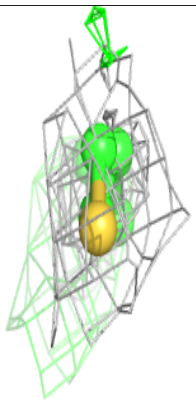


Electron density around SOG B 427:

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

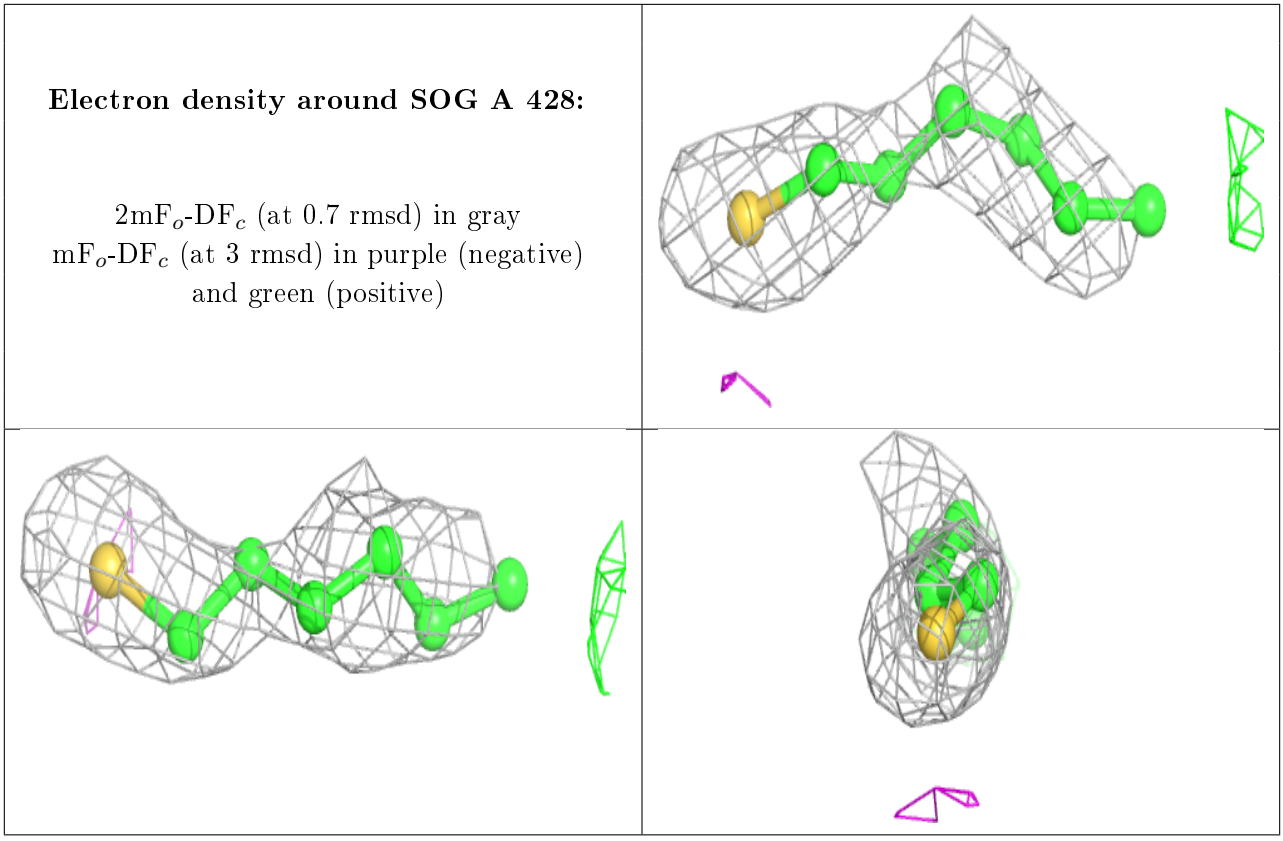






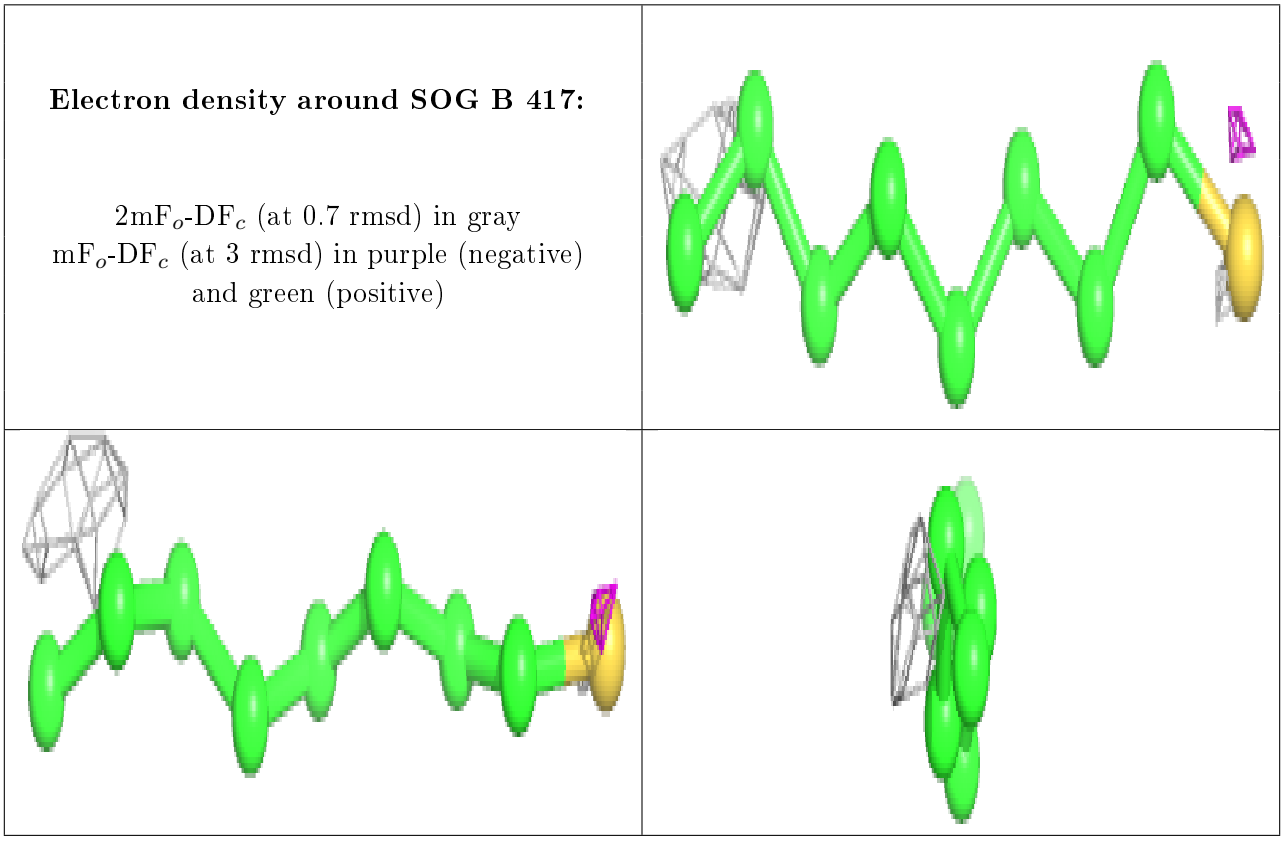
Electron density around SOG A 428:

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



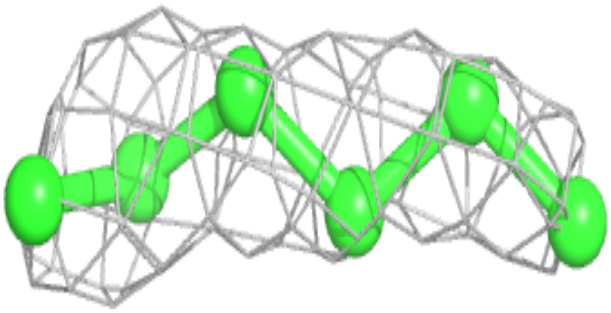
Electron density around SOG B 417:

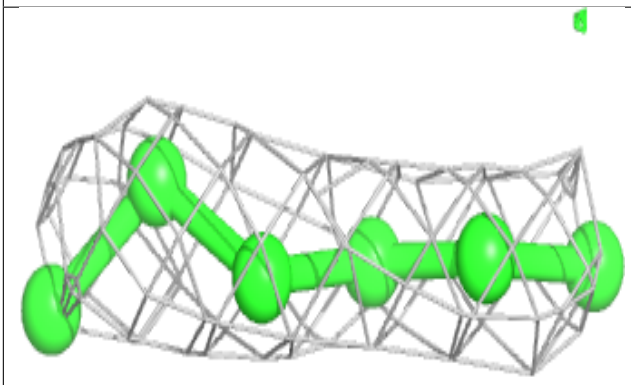
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

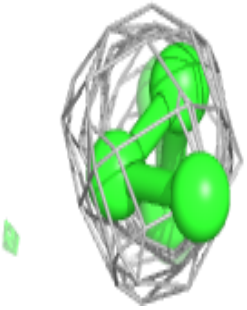


Electron density around SOG B 415:

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

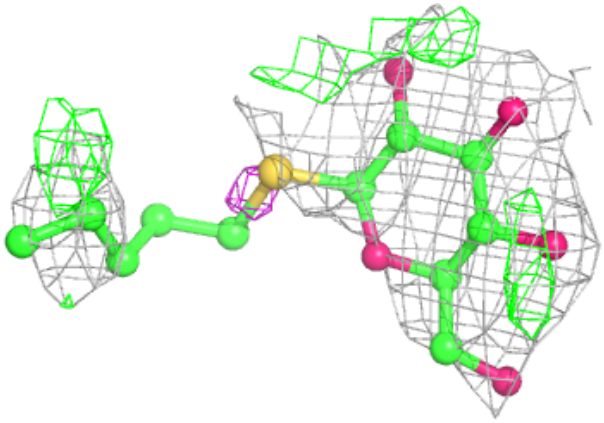


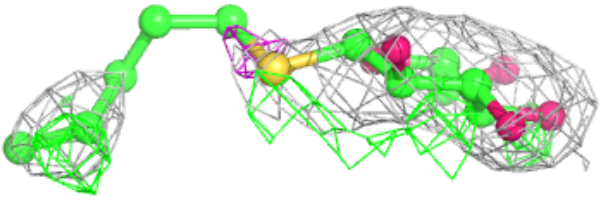


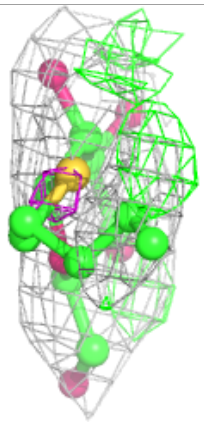


Electron density around SOG A 407:

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

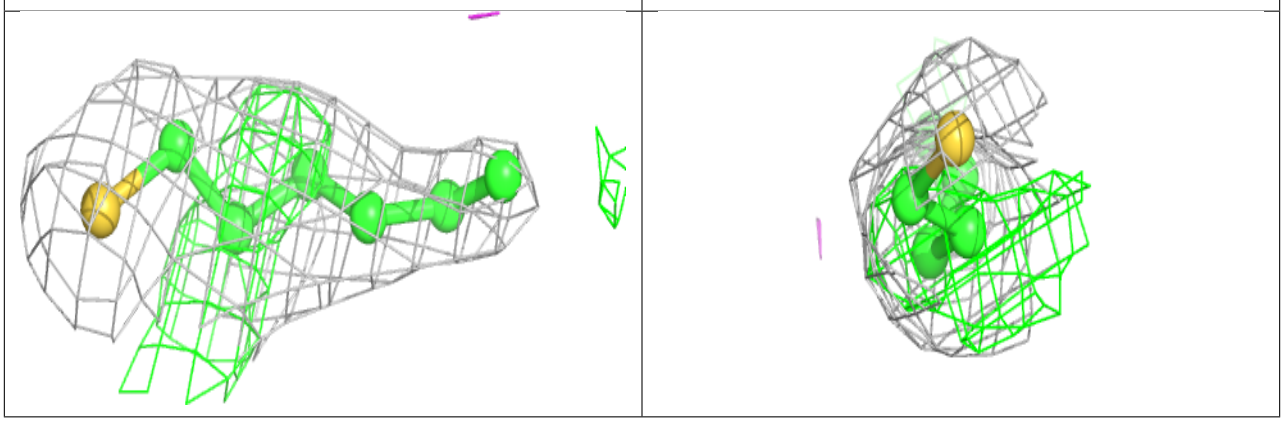






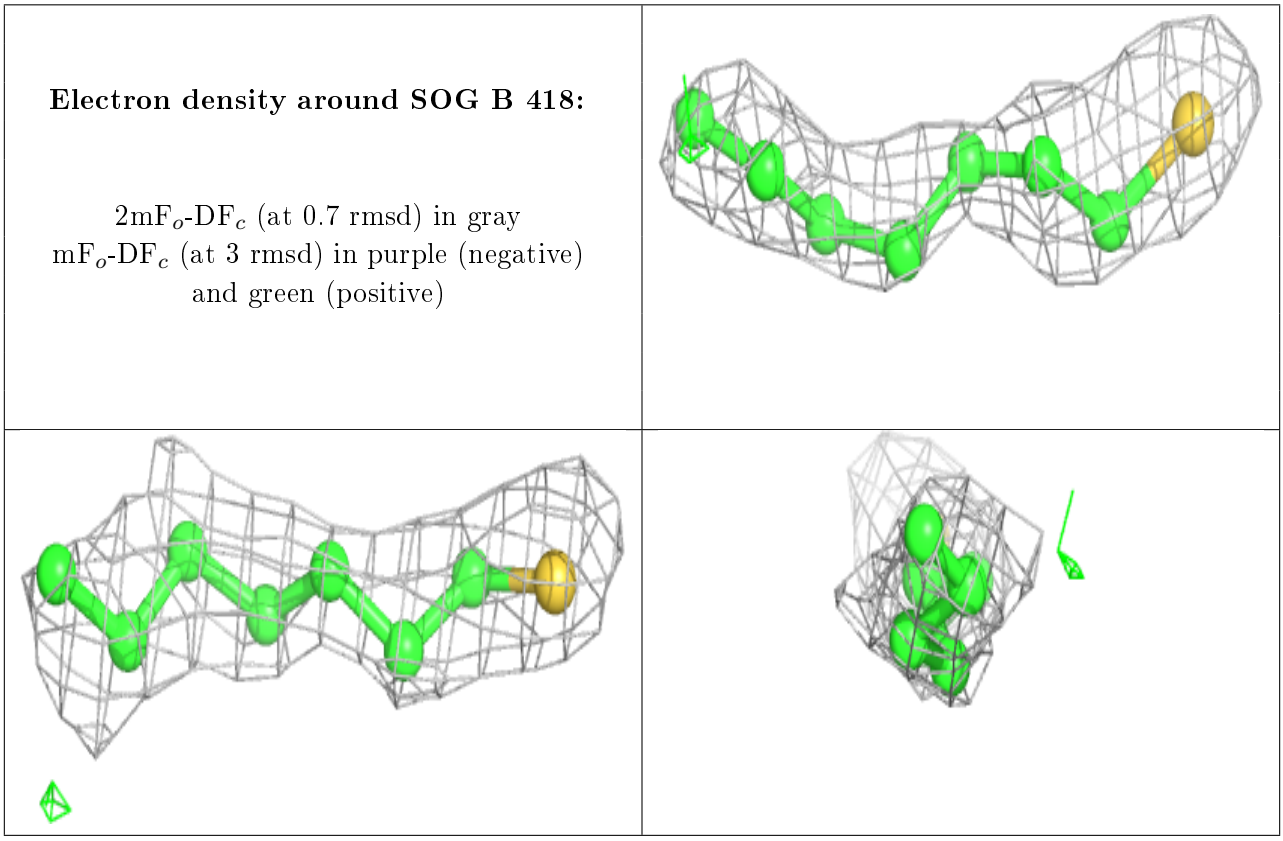
Electron density around SOG B 430:

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



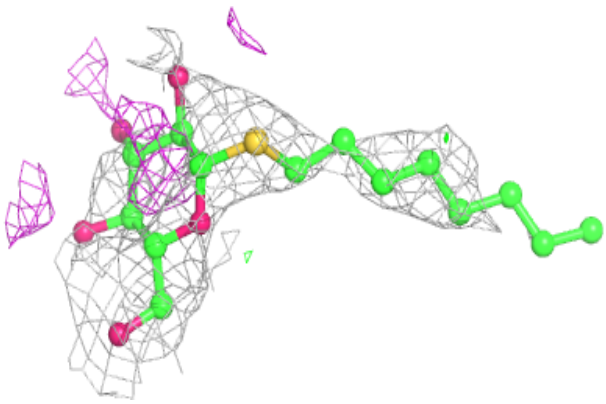
Electron density around SOG B 418:

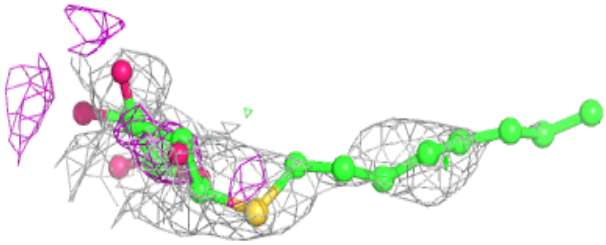
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

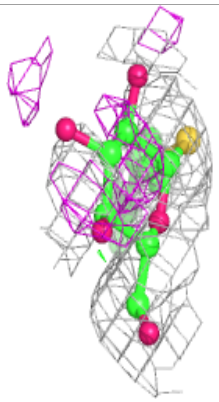


Electron density around SOG A 418:

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

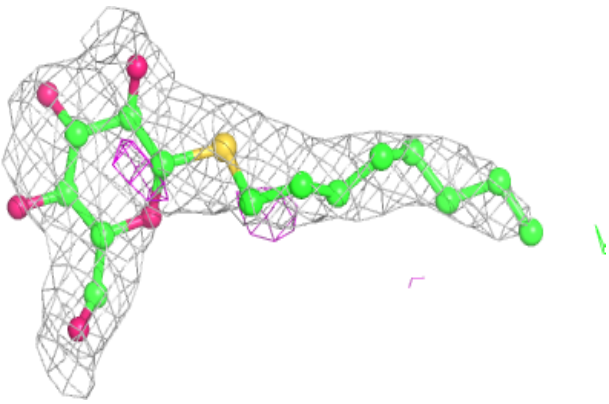


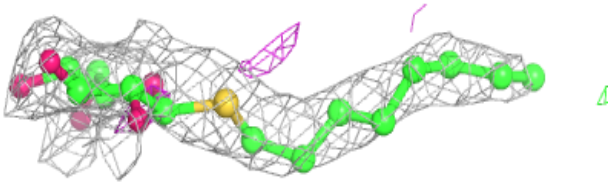


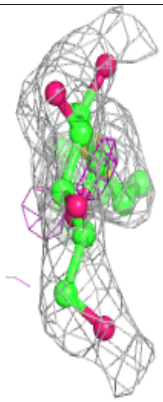


Electron density around SOG B 412:

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

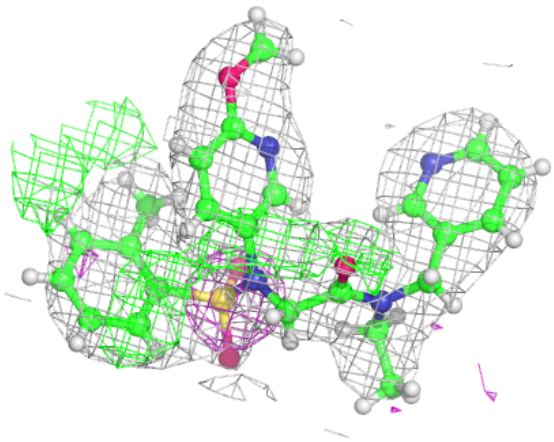


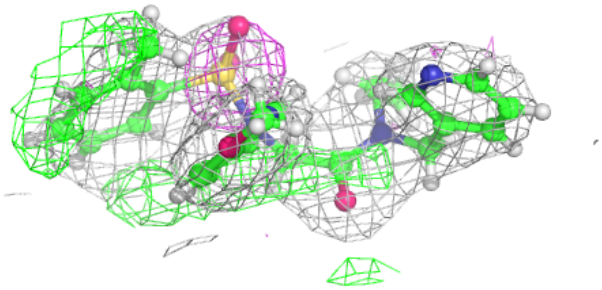


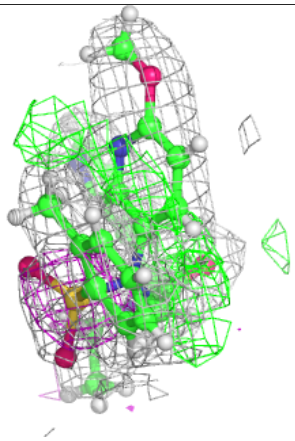


Electron density around 7MA A 401:

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

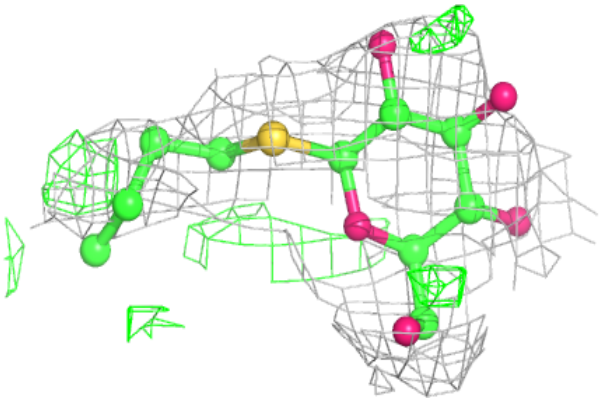


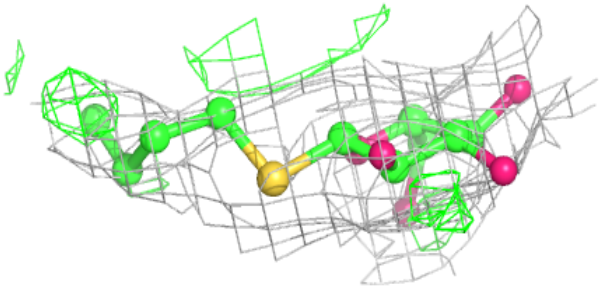


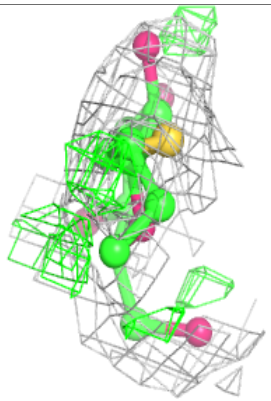


Electron density around SOG A 408:

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

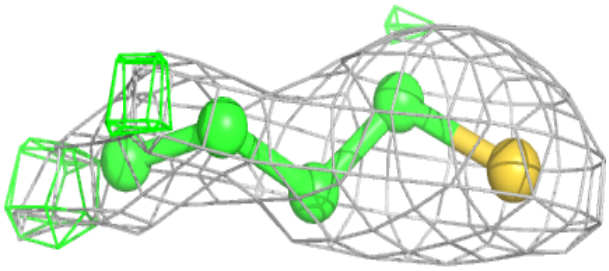


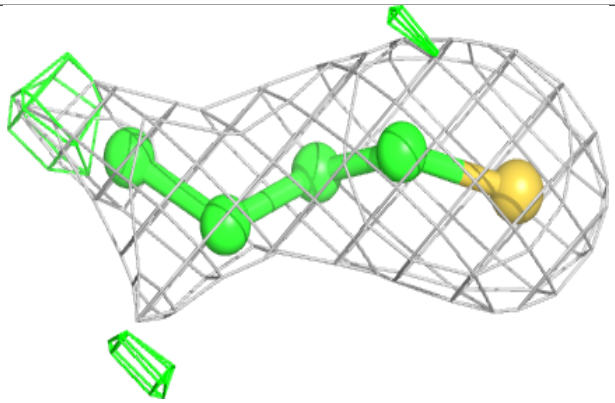


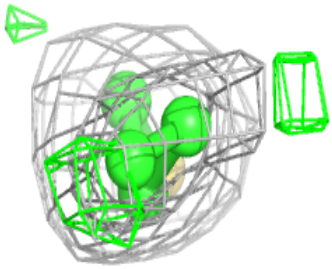


Electron density around SOG B 420:

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

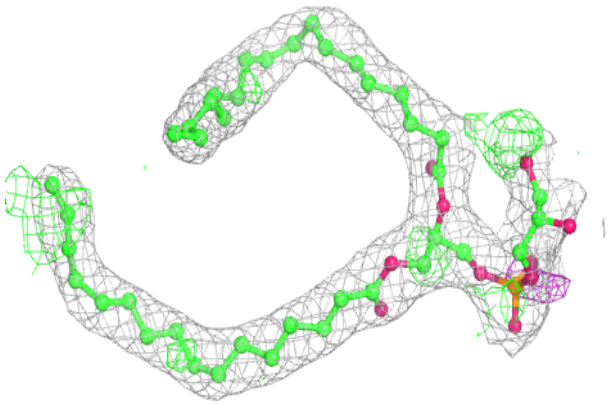


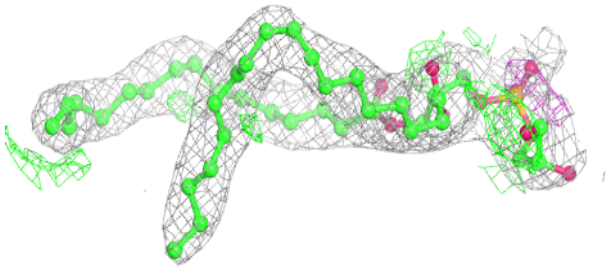


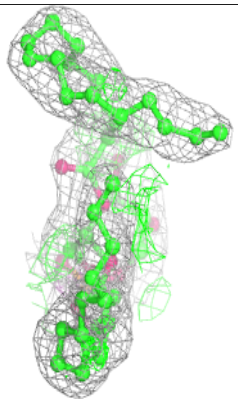


Electron density around PGW B 431:

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

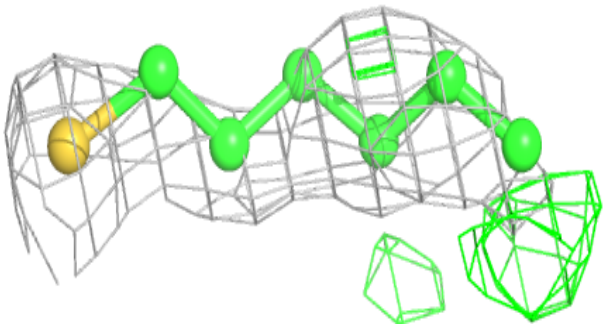


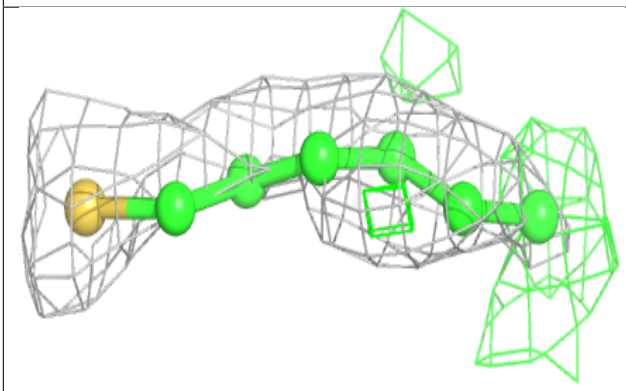


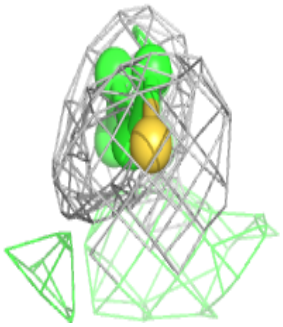


Electron density around SOG B 428:

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

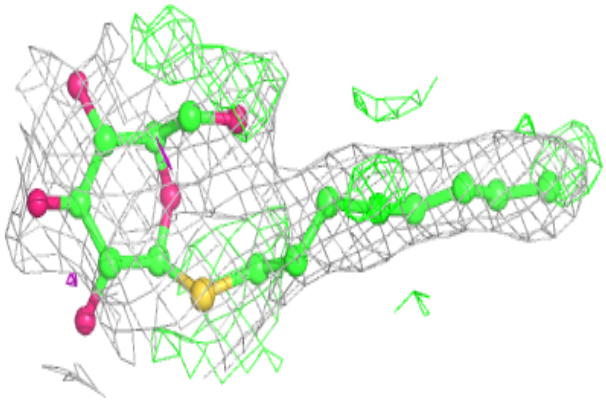


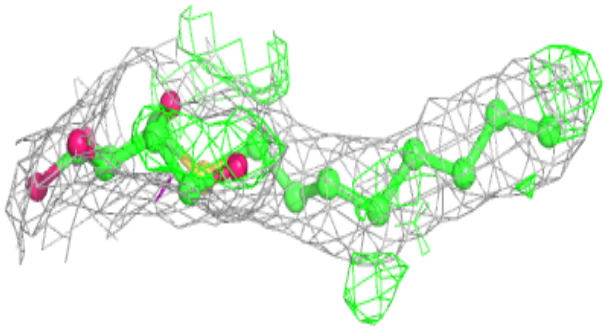


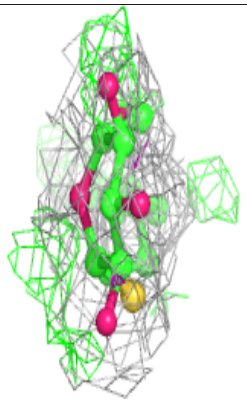


Electron density around SOG A 410:

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

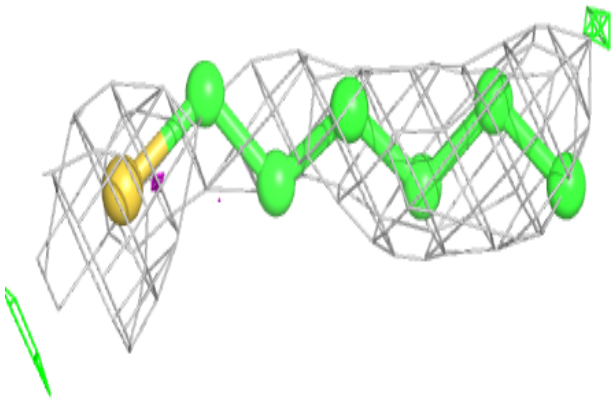


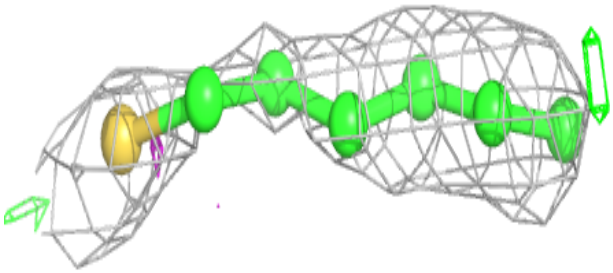


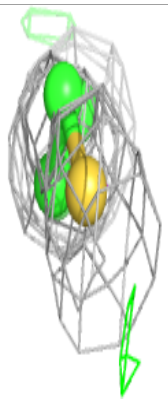


Electron density around SOG A 420:

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

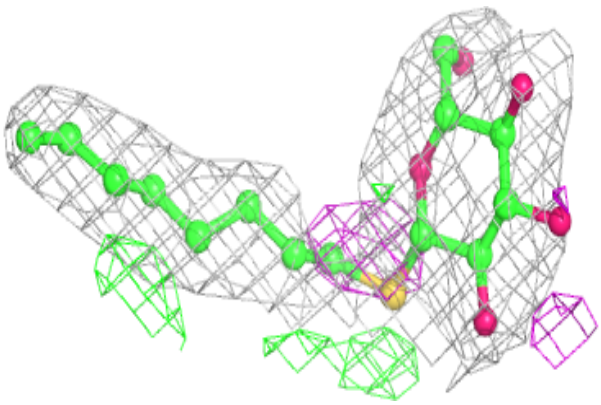


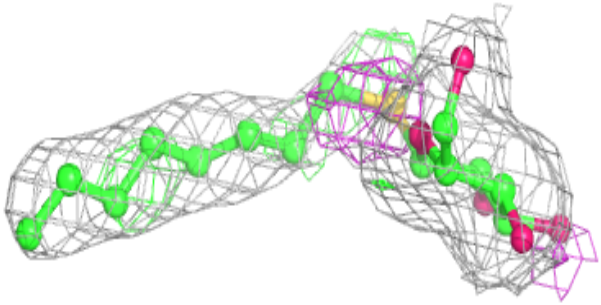


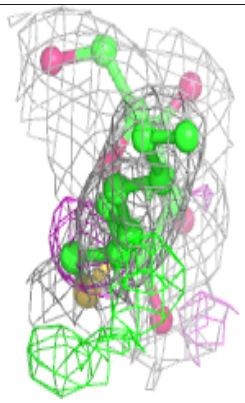


Electron density around SOG A 411:

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

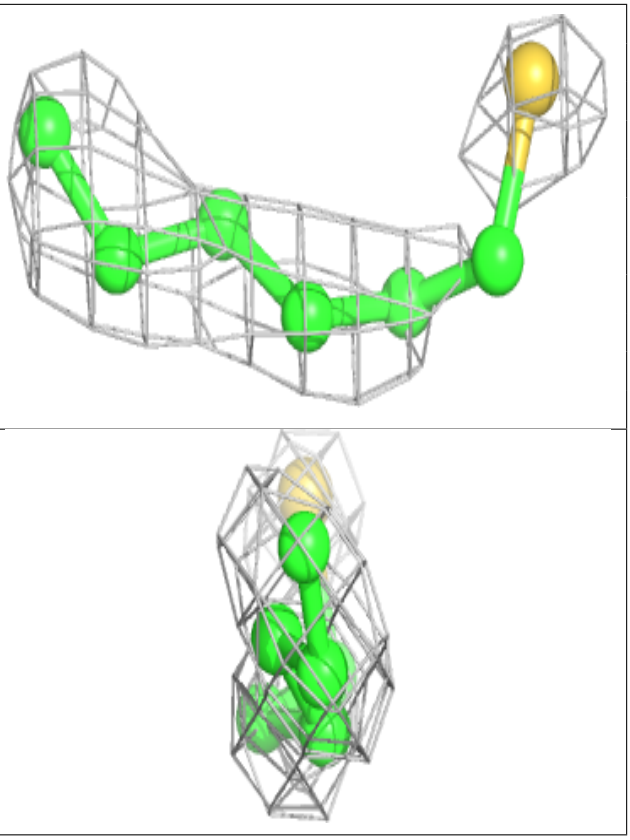


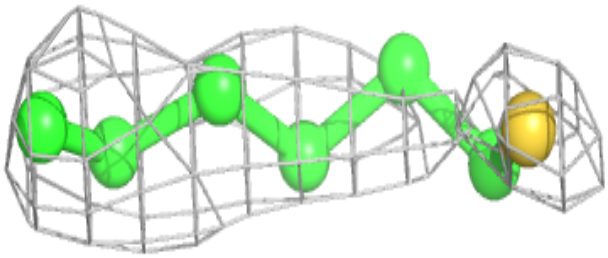




Electron density around SOG B 429:

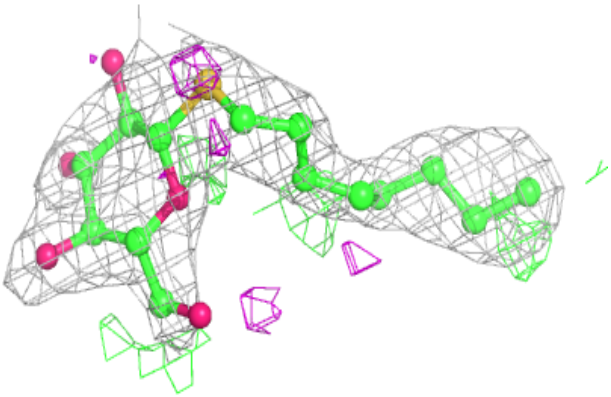
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

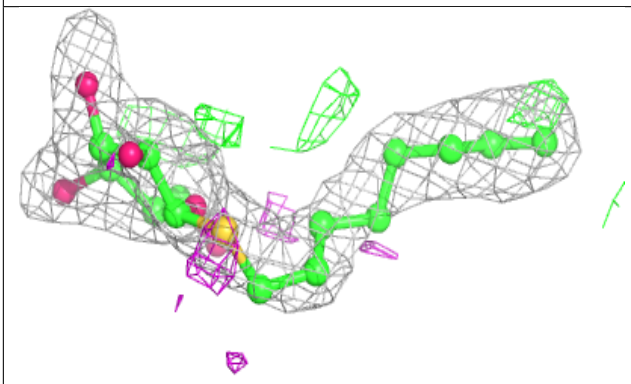


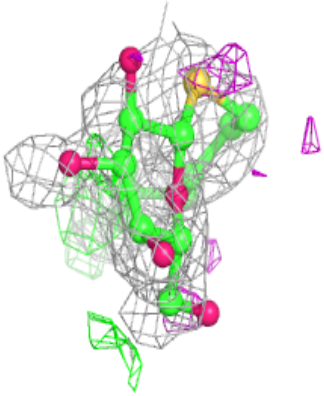


Electron density around SOG A 413:

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

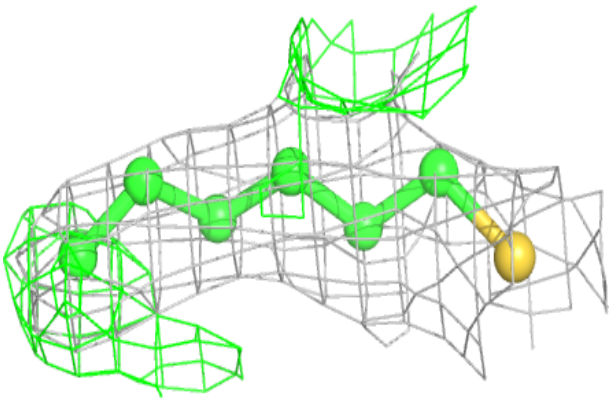


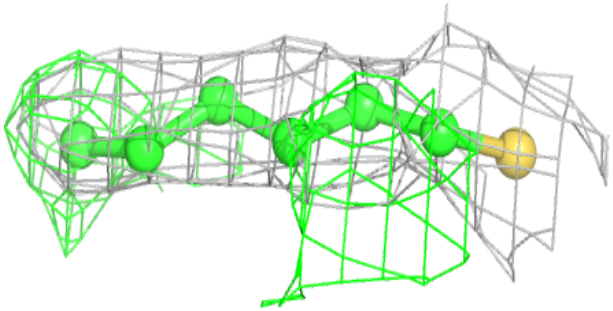


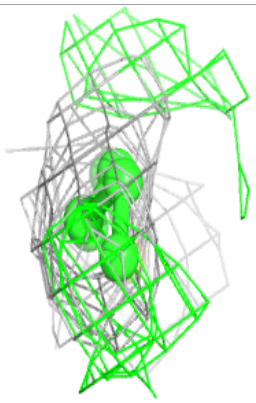


Electron density around SOG A 419:

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

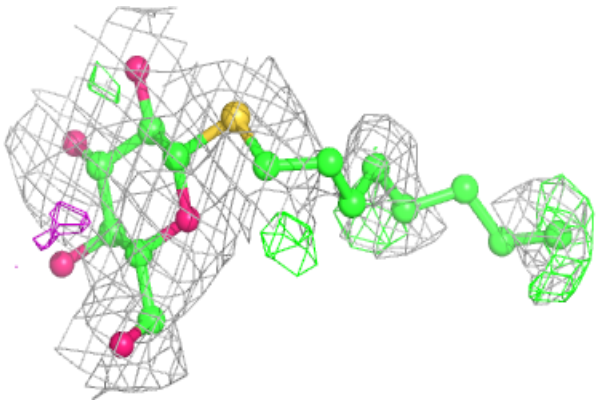


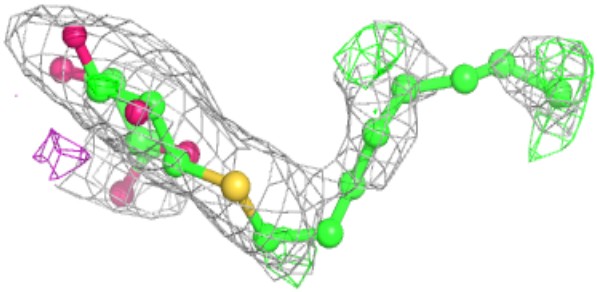


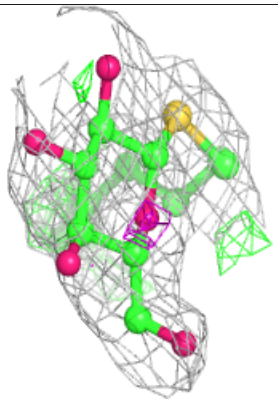


Electron density around SOG B 410:

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

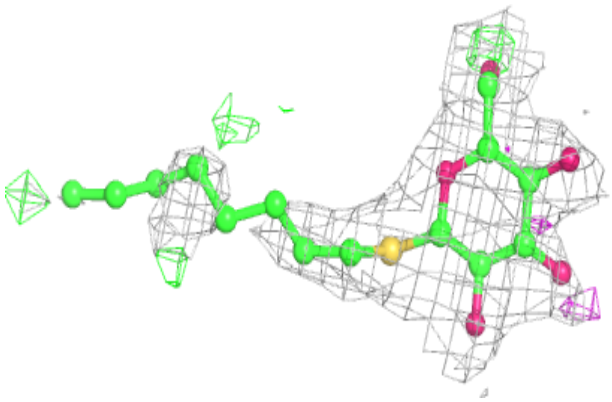


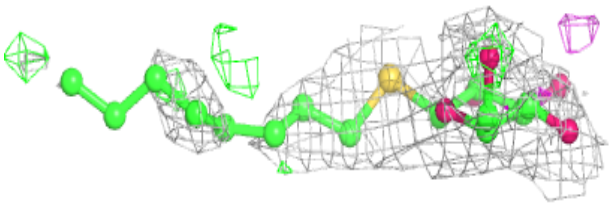


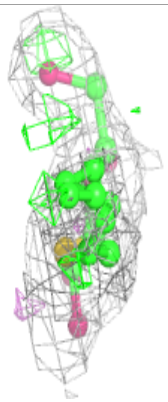


Electron density around SOG A 412:

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

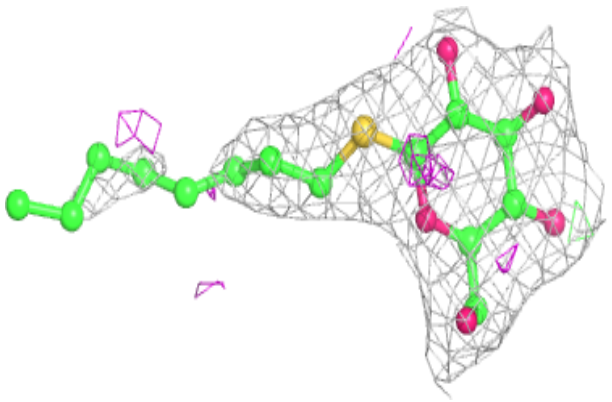


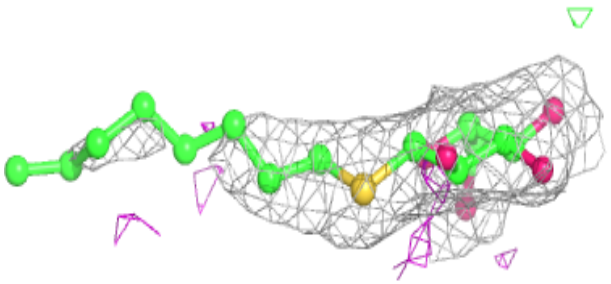


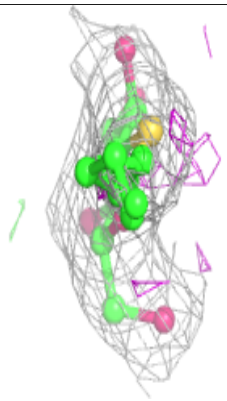


Electron density around SOG B 407:

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

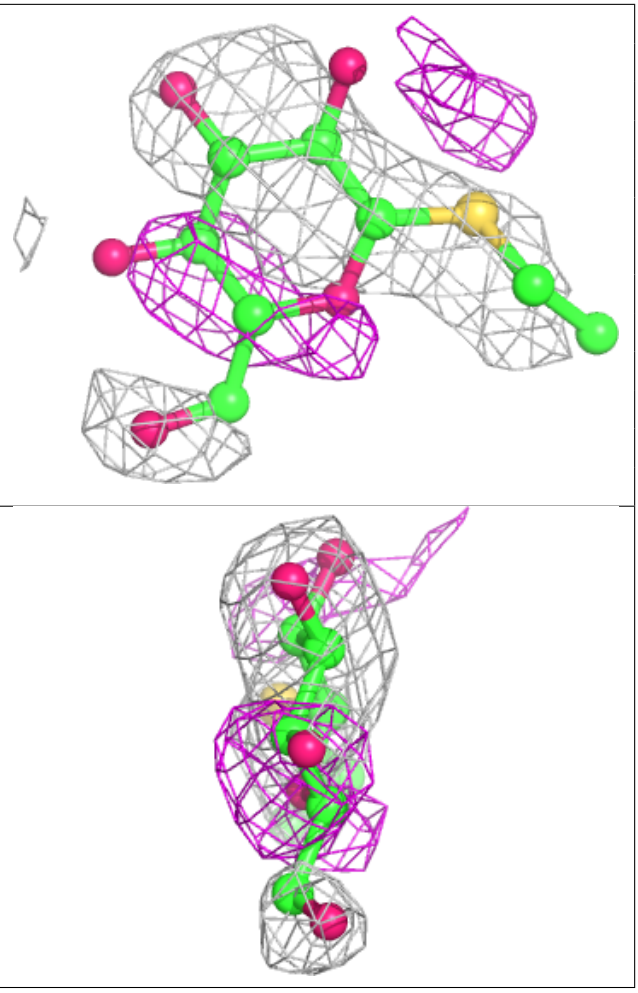






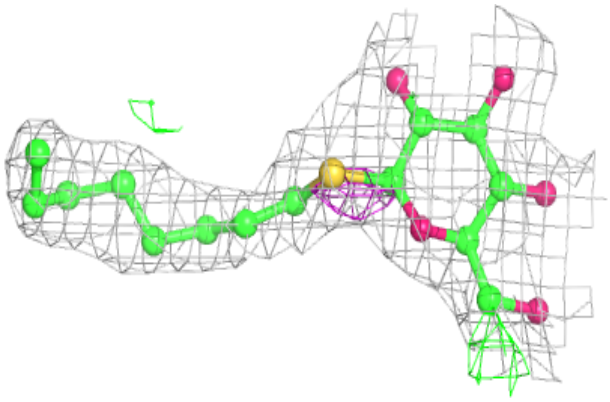
Electron density around SOG A 415:

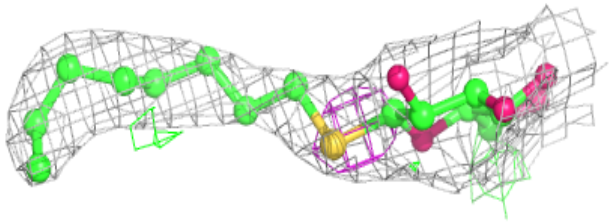
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

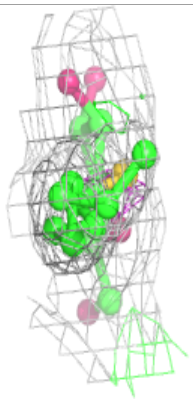


Electron density around SOG A 409:

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

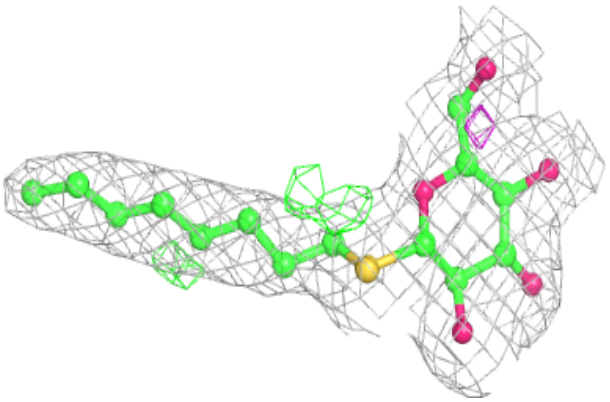


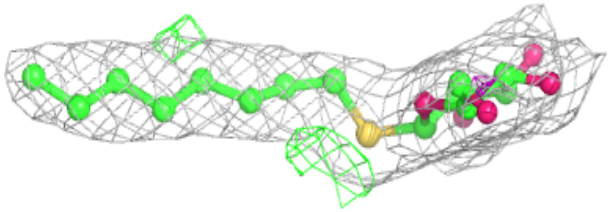


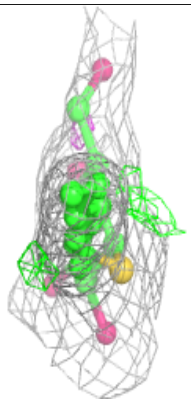


Electron density around SOG B 406:

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

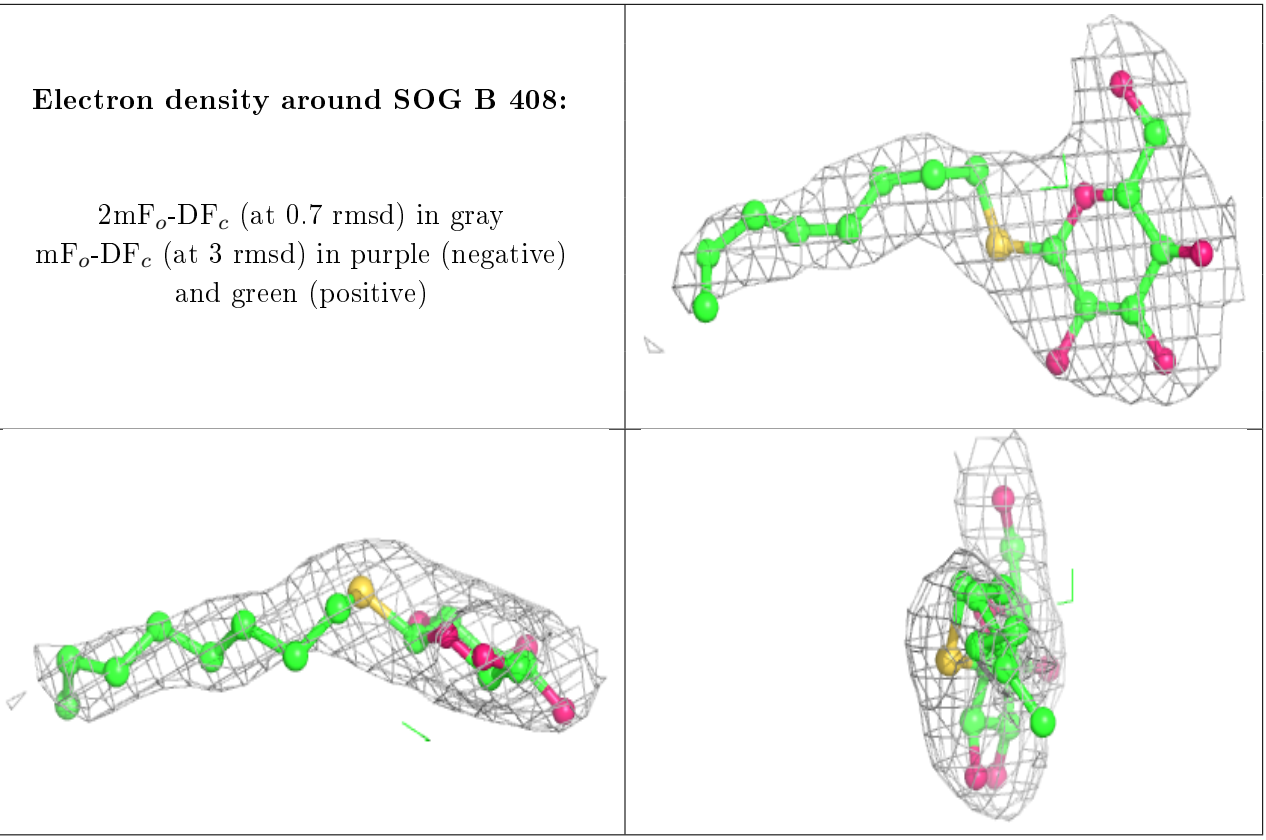






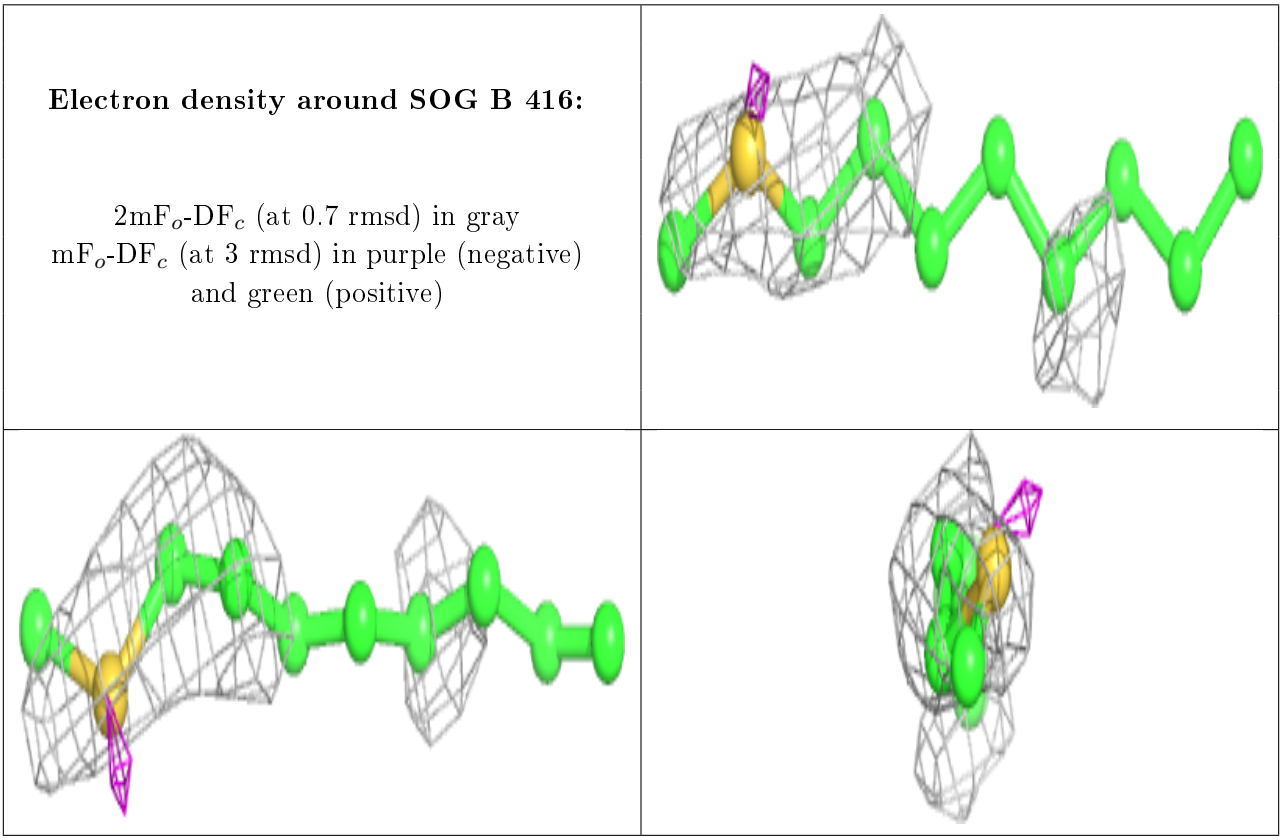
Electron density around SOG B 408:

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



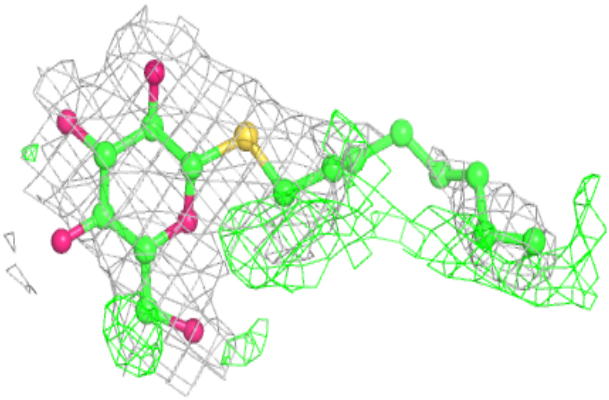
Electron density around SOG B 416:

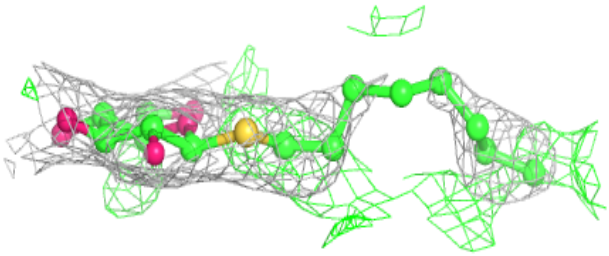
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

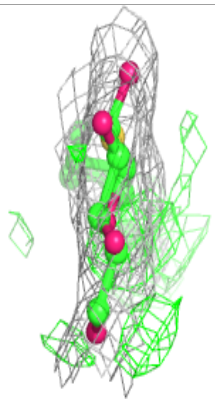


Electron density around SOG A 414:

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

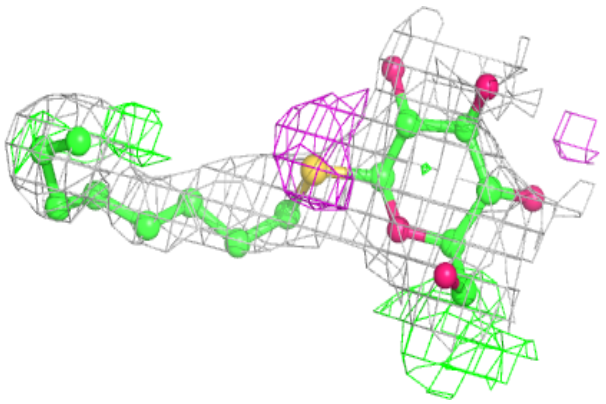


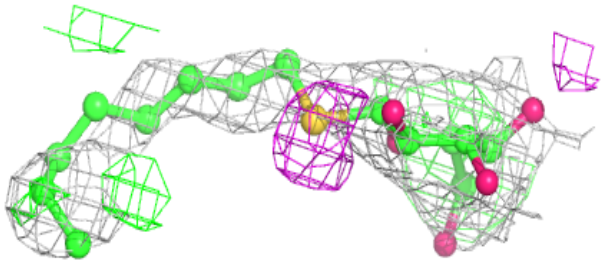


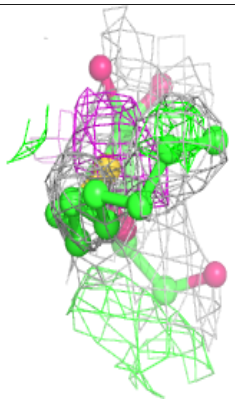


Electron density around SOG B 409:

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

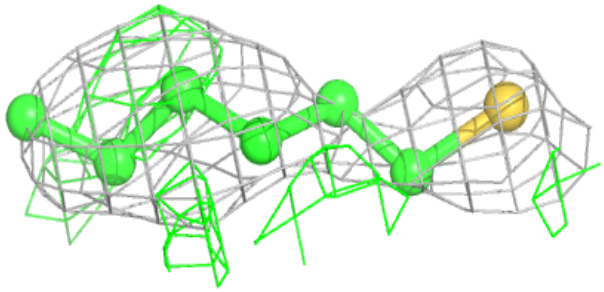


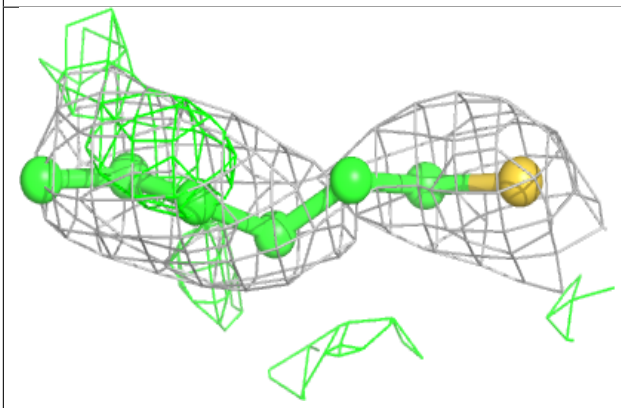


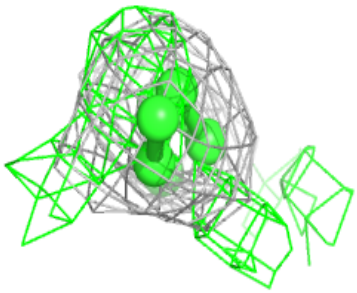


Electron density around SOG B 425:

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

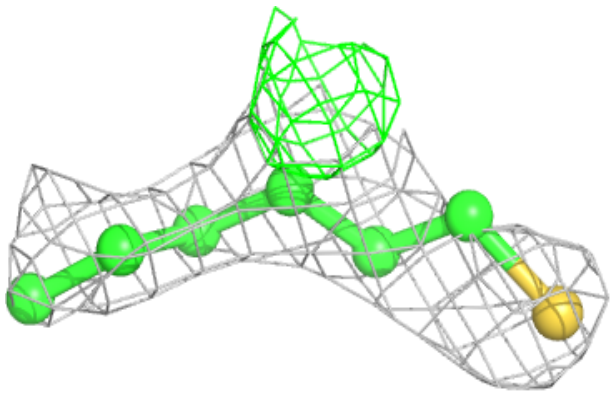


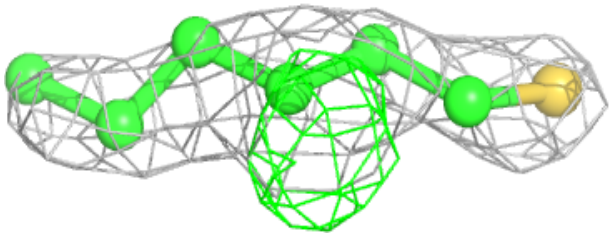


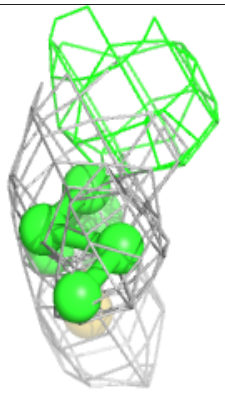


Electron density around SOG A 425:

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

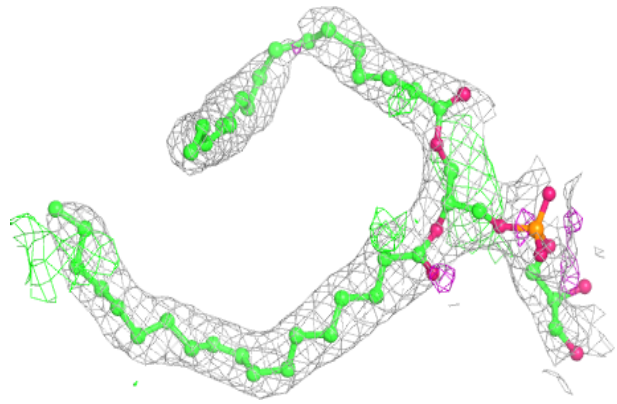


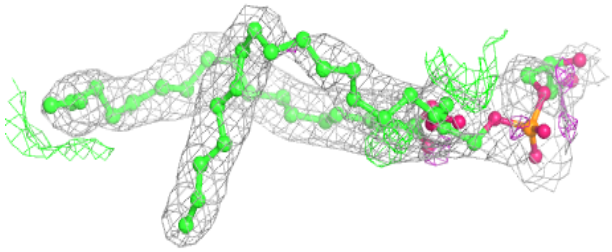




Electron density around PGW A 429:

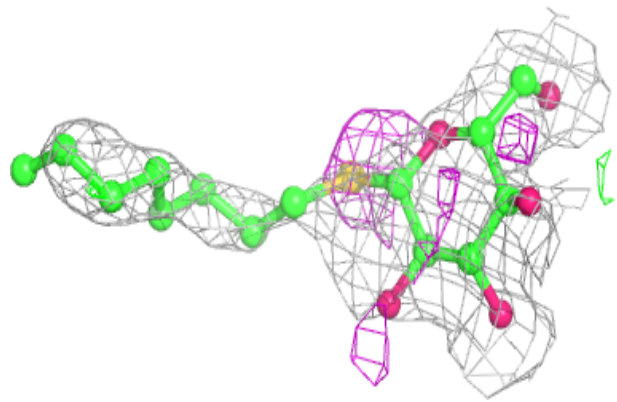
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

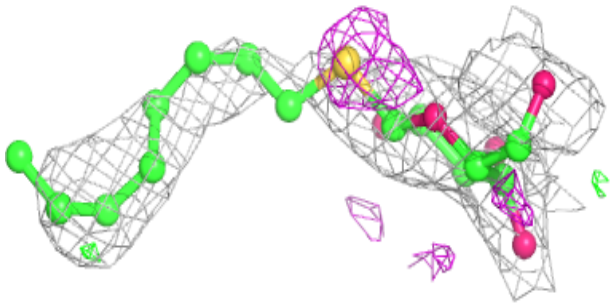


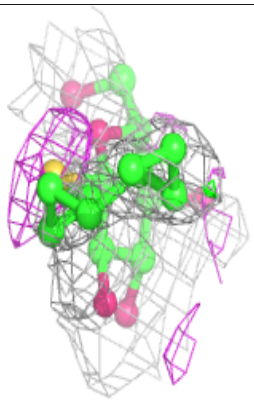


Electron density around SOG A 417:

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

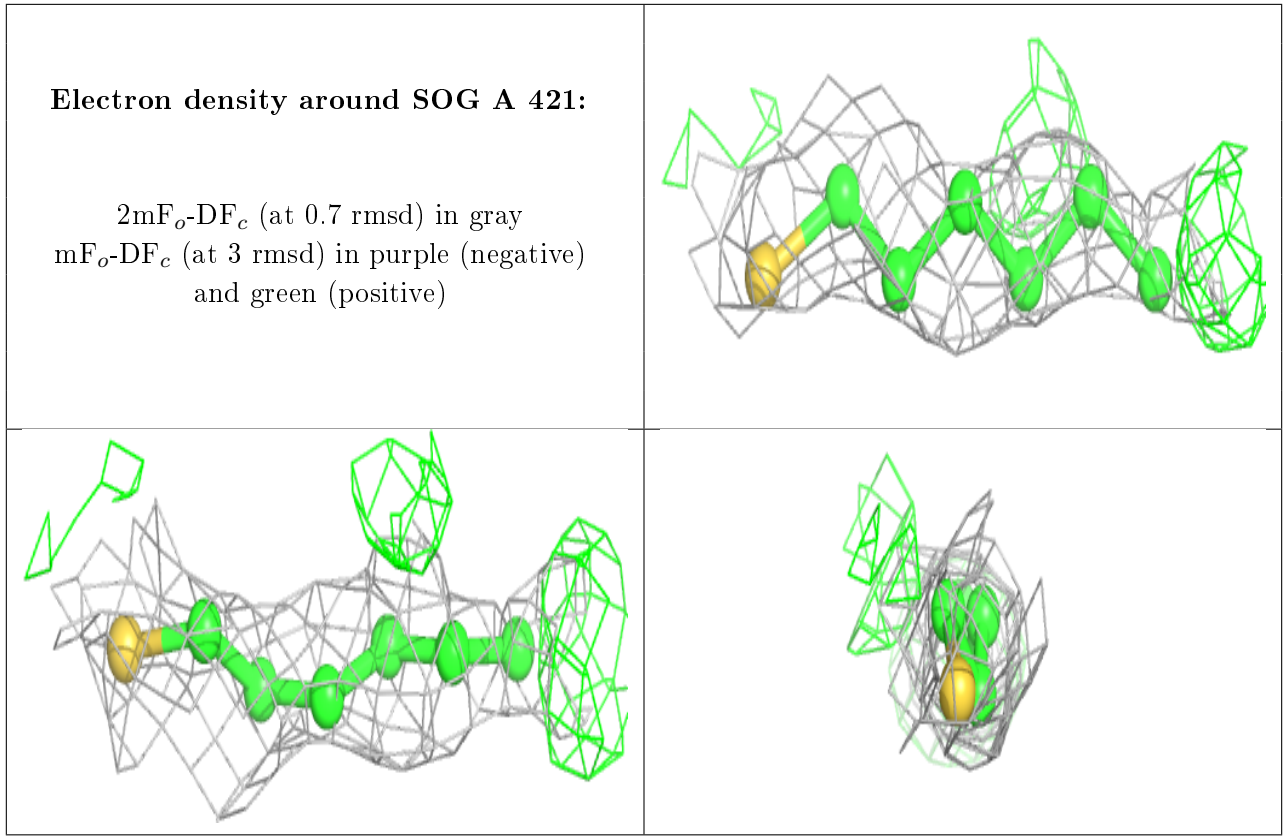






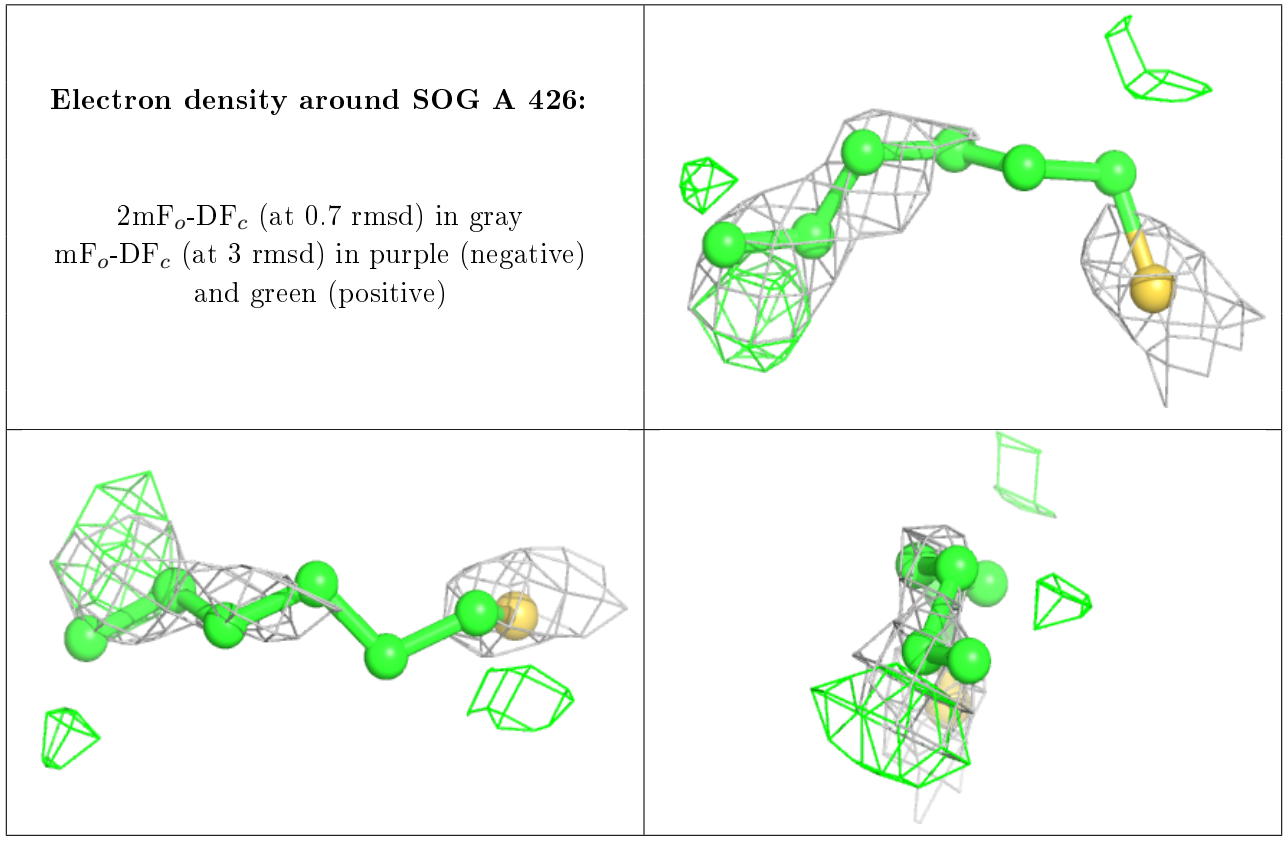
Electron density around SOG A 421:

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



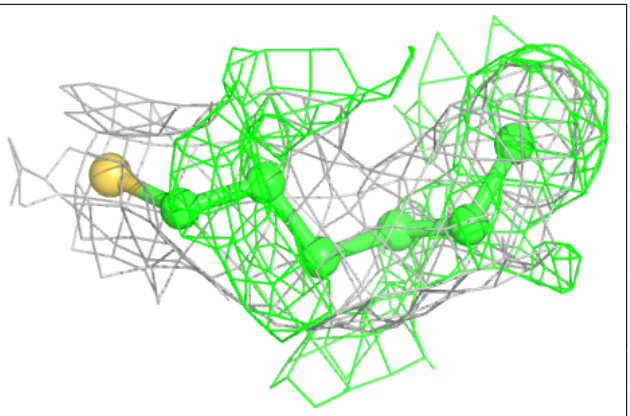
Electron density around SOG A 426:

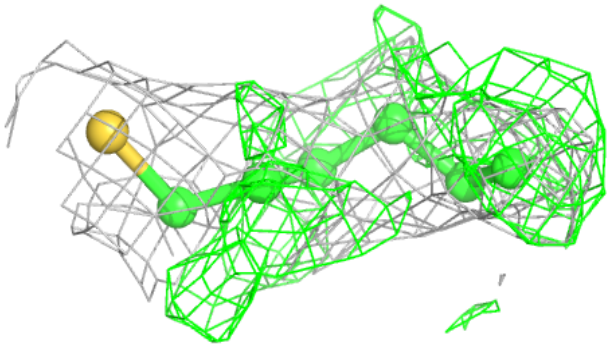
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

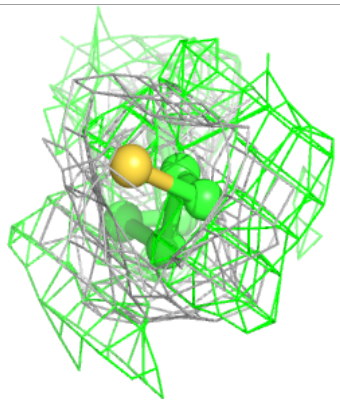


Electron density around SOG A 427:

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

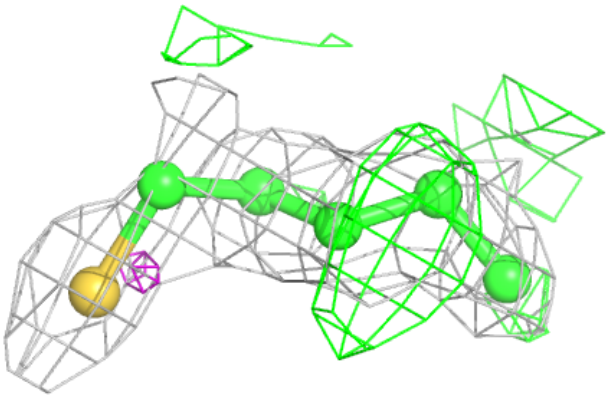


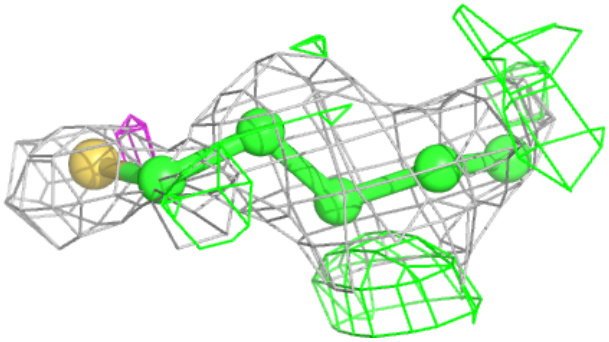


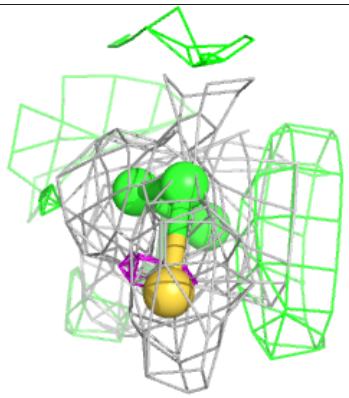


Electron density around SOG B 424:

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

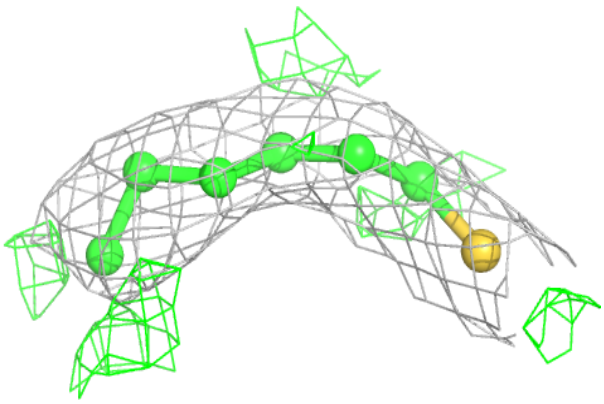


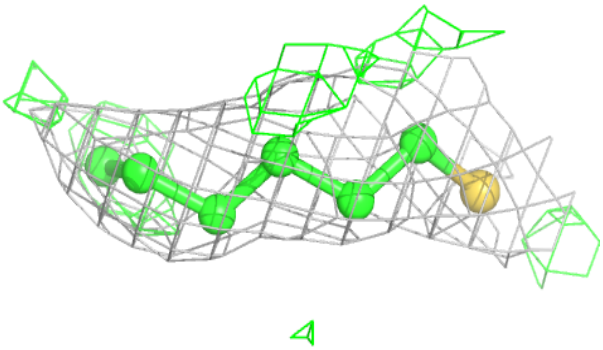


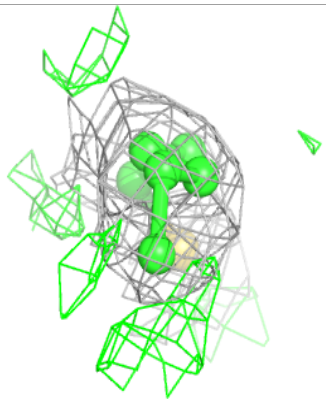


Electron density around SOG A 422:

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

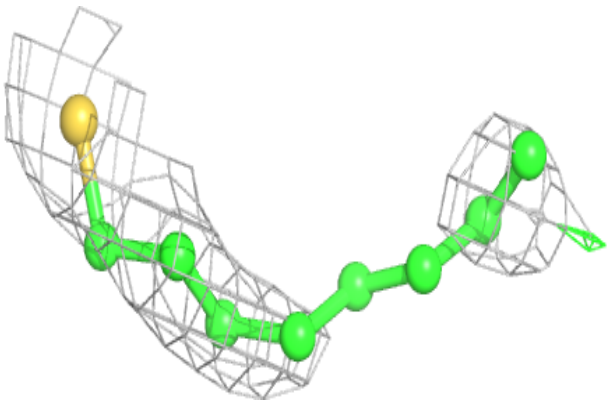


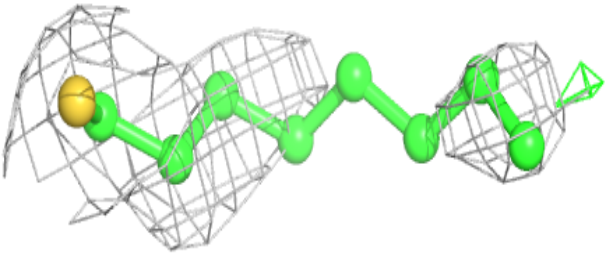


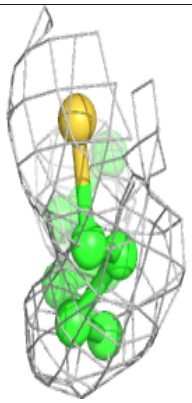


Electron density around SOG B 423:

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

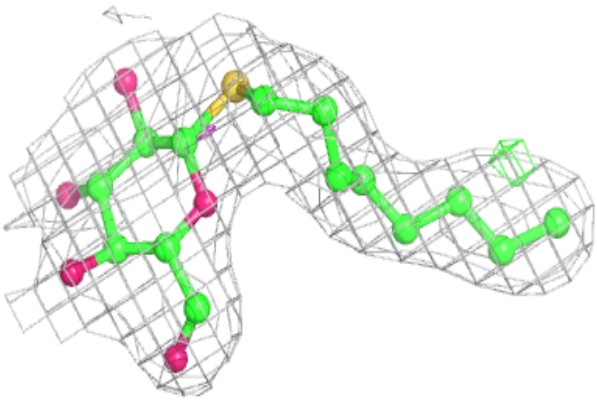


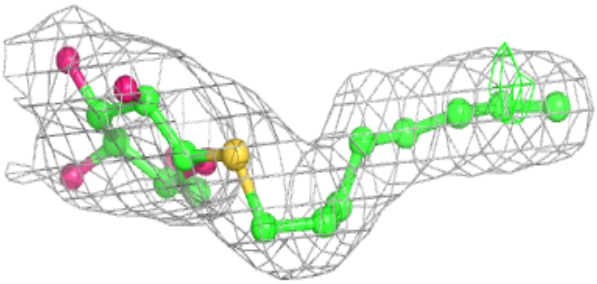


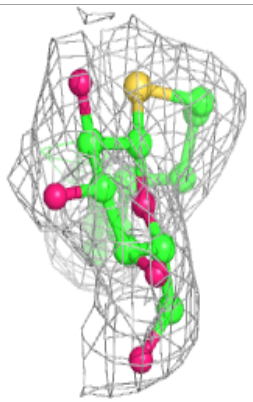


Electron density around SOG B 411:

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

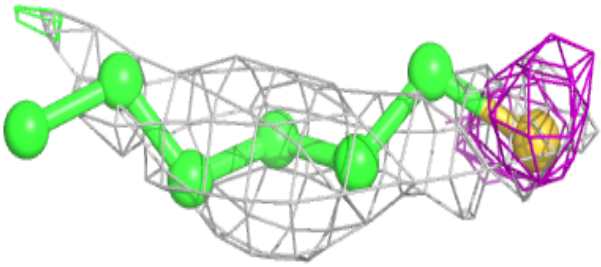


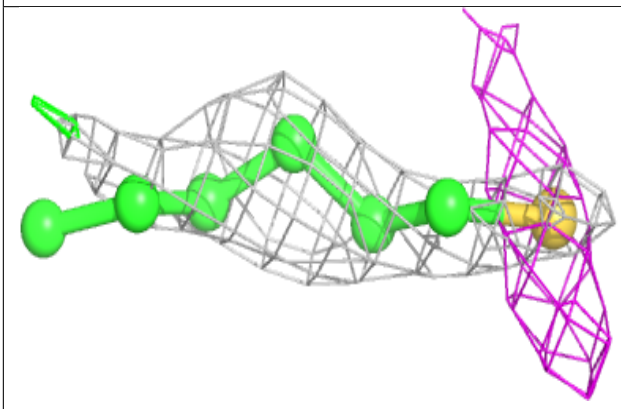


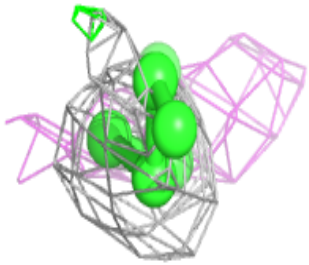


Electron density around SOG A 423:

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

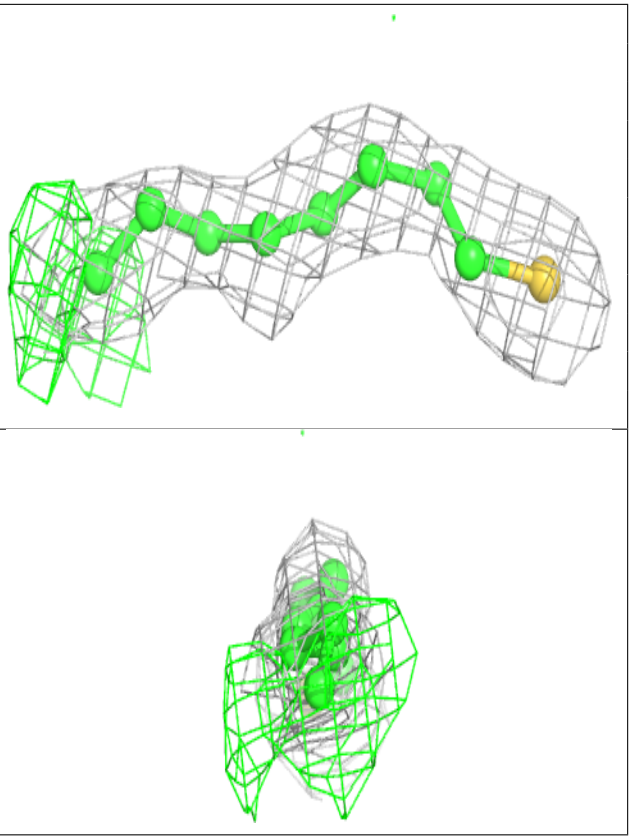






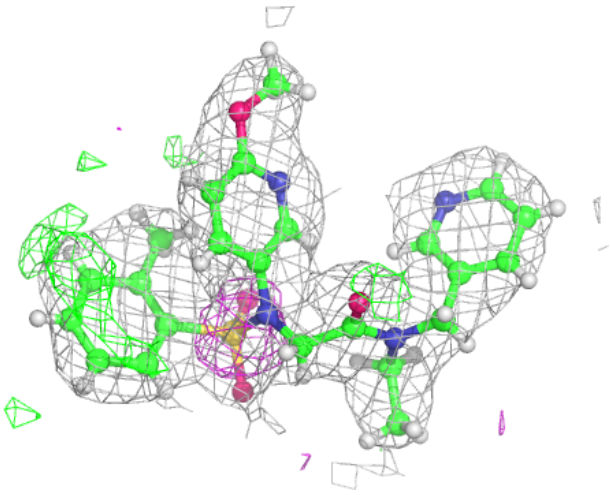
Electron density around SOG B 419:

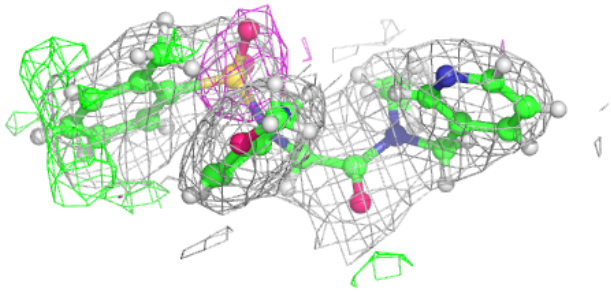
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

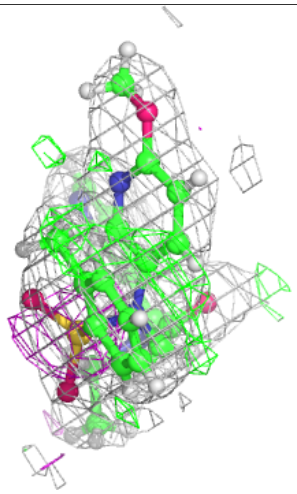


Electron density around 7MA B 401:

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

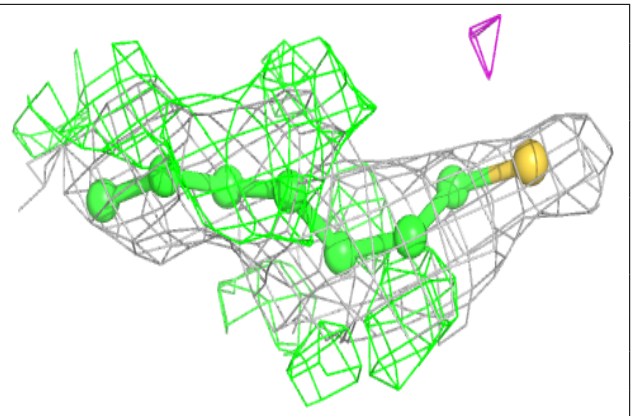


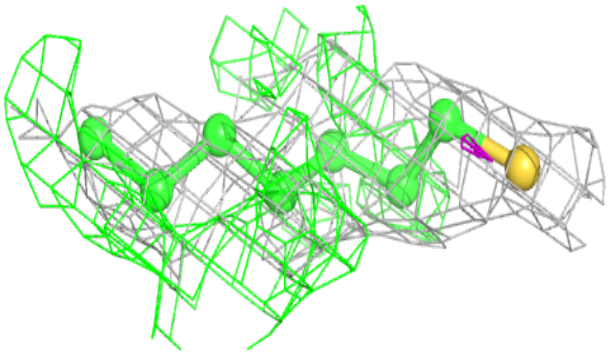


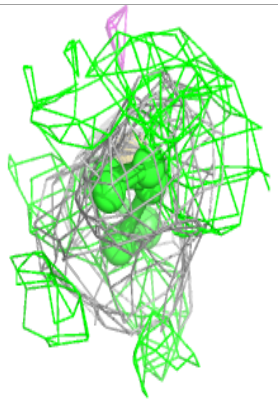


Electron density around SOG B 422:

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

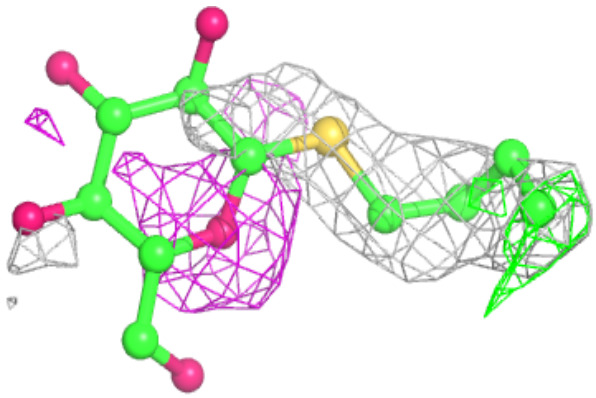


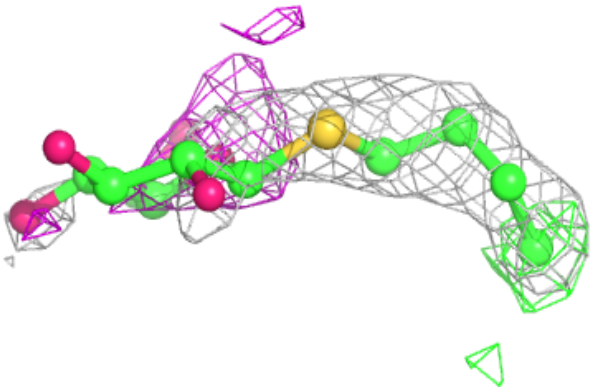


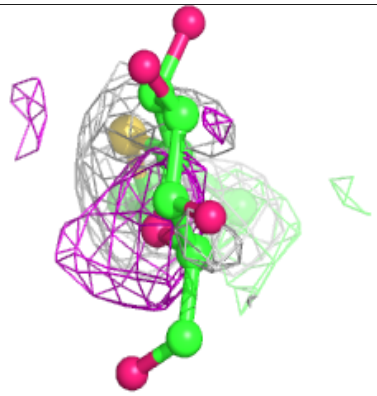


Electron density around SOG B 413:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.