



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:43 PM EDT

PDB ID : 6TOD / pdb_00006tod
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

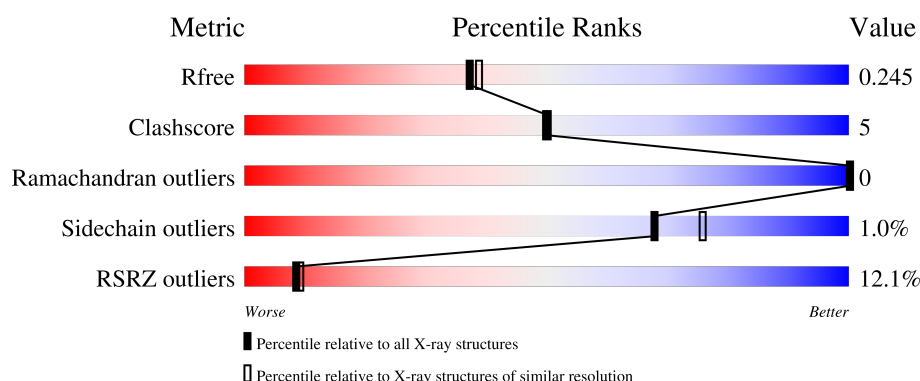
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

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
6	SOG	B	413	-	-	-	X
6	SOG	B	422	-	-	-	X
6	SOG	B	424	-	-	-	X

2 Entry composition

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
1	A	301	Total	C	N	O	S	0	0	0
			2390	1584	399	390	17			
1	B	311	Total	C	N	O	S	0	0	0
			2486	1652	411	406	17			

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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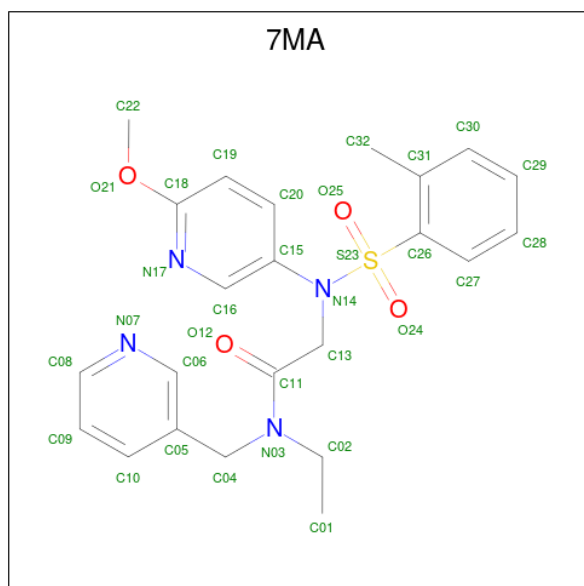
Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	ASN	engineered mutation	UNP O43613
B	198	ALA	LEU	engineered mutation	UNP O43613
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
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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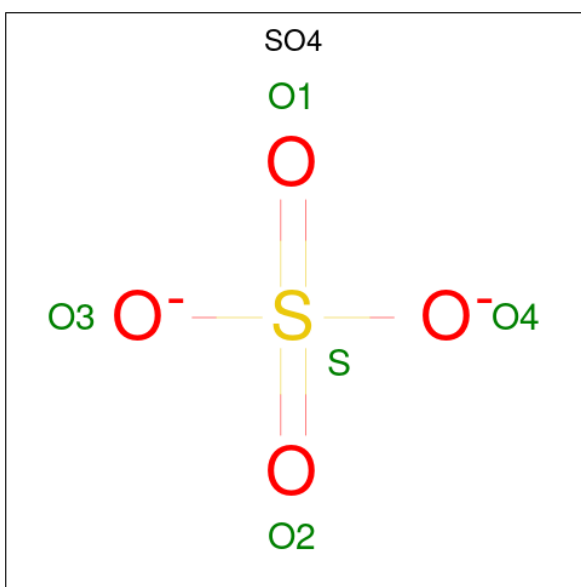
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	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 (CCD ID: 7MA) (formula: C₂₃H₂₆N₄O₄S) (labeled as "Ligand of Interest" by depositor).



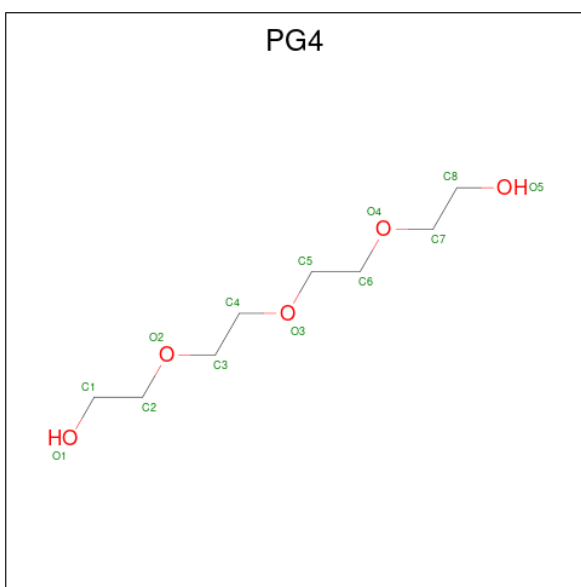
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			58	23	26	4	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			58	23	26	4	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



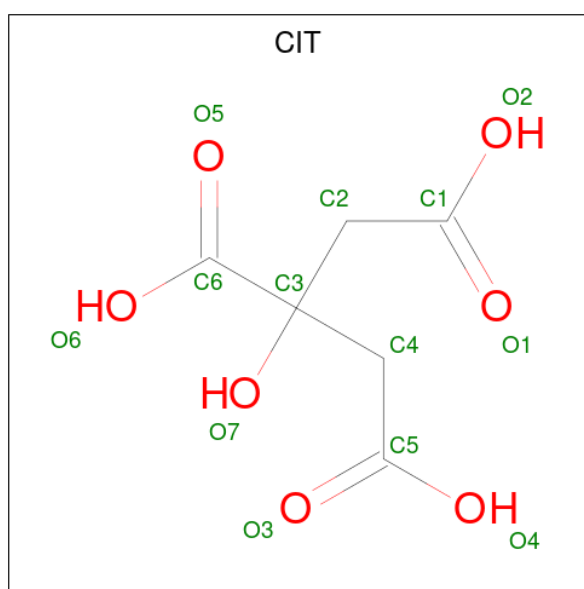
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

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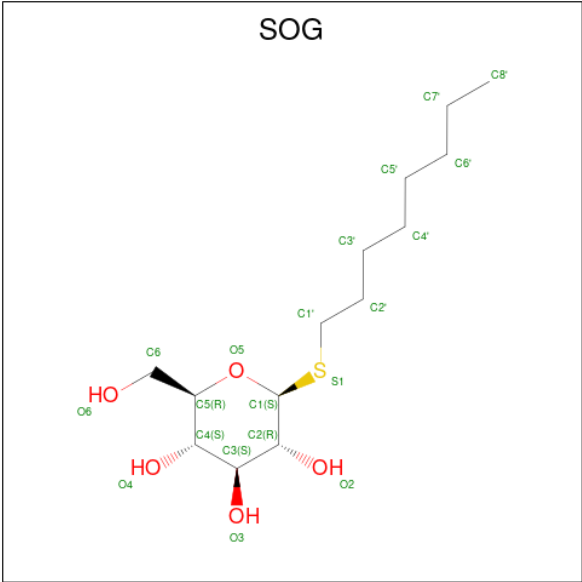
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			17	11	5	1		
6	A	1	Total	C	O	S	0	0
			16	10	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			14	8	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	O	S	0	0
			20	14	5	1		
6	A	1	Total	C	S		0	0
			7	6	1			
6	A	1	Total	C	S		0	0
			7	6	1			

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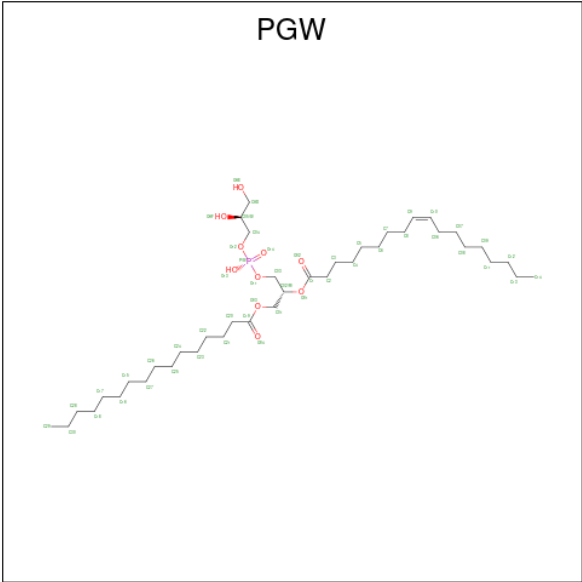
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	A	1	Total 7	C 6	S 1		0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 16	C 10	O 5	S 1	0	0
6	B	1	Total 20	C 14	O 5	S 1	0	0
6	B	1	Total 6	C 6			0	0
6	B	1	Total 10	C 9	S 1		0	0
6	B	1	Total 9	C 8	S 1		0	0
6	B	1	Total 8	C 7	S 1		0	0

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

- Molecule 7 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 9 is water.

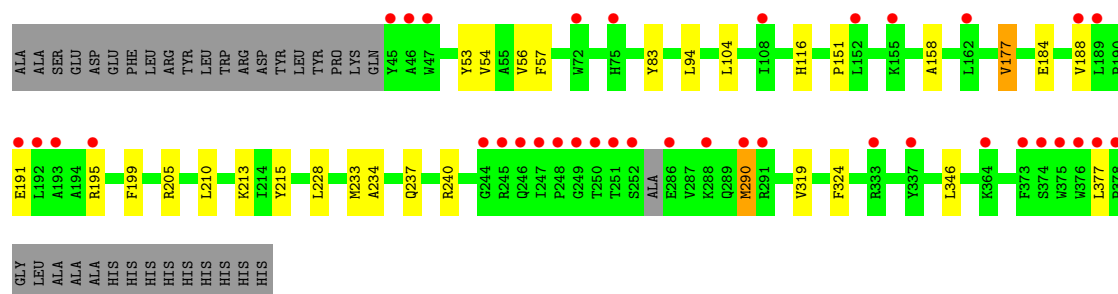
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	110	Total	O	0	0
			110	110		
9	B	101	Total	O	0	0
			101	101		

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.

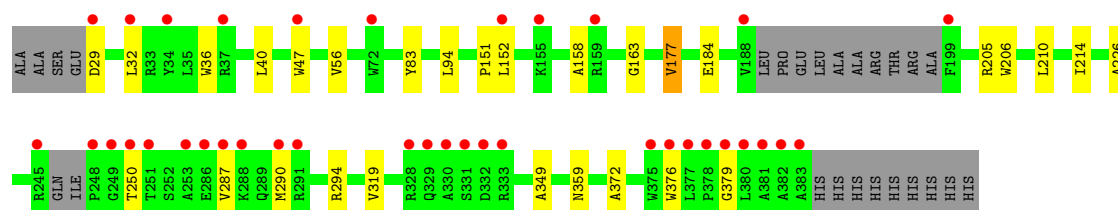
• Molecule 1: Orexin receptor type 1

Chain A: 



• Molecule 1: Orexin receptor type 1

Chain B: 



4 Data and refinement statistics

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 30.62 – 2.11	Depositor EDS
% Data completeness (in resolution range)	61.3 (30.62-2.11) 81.1 (30.62-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.188 , 0.208 0.224 , 0.245	Depositor DCC
R_{free} test set	4790 reflections (4.98%)	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)	0.31 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, SO4, CIT, 7MA, PG4, NA, SOG

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	0.86	1/2456 (0.0%)	1.33	2/3350 (0.1%)
1	B	0.87	1/2557 (0.0%)	1.32	4/3485 (0.1%)
All	All	0.87	2/5013 (0.0%)	1.33	6/6835 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	VAL	CA-C	6.07	1.57	1.52
1	A	177	VAL	CA-C	5.31	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PRO	N-CA-C	6.63	122.46	113.84
1	A	151	PRO	N-CA-C	6.07	121.73	113.84
1	A	177	VAL	N-CA-CB	5.49	113.96	110.50
1	B	151	PRO	CA-C-N	-5.42	114.57	122.86
1	B	151	PRO	C-N-CA	-5.42	114.57	122.86
1	B	177	VAL	N-CA-CB	5.35	113.87	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2390	0	2456	27	0
1	B	2486	0	2535	25	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
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	62	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.

All (62) 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:HH21	1.17	1.06
1:B:290:MET:HE3	1:B:294:ARG:NH2	1.74	1.01
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	0.85
1:B:290:MET:CE	1:B:294:ARG:NH2	2.41	0.83
1:A:324:PHE:CE1	6:A:410:SOG:H61	2.16	0.80
1:B:250:THR:HA	1:B:287:VAL:HG11	1.65	0.77
1:A:210:LEU:HD13	6:A:411:SOG:H62	1.75	0.68
1:A:234:ALA:HB2	7:A:429:PGW:H7A	1.77	0.66
1:A:346:LEU:HD21	4:A:405:PG4:H22	1.76	0.66
1:A:237:GLN:HE21	7:A:429:PGW:H04	1.64	0.63
1:B:359:ASN:HD21	6:B:424:SOG:H2'2	1.64	0.62
1:B:94:LEU:HB2	6:B:418:SOG:H1'2	1.82	0.62
1:B:290:MET:HE3	1:B:294:ARG:CZ	2.31	0.60
1:B:36:TRP:HA	1:B:40:LEU:HB2	1.85	0.58
1:A:57:PHE:CD2	6:A:415:SOG:H4	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:410:SOG:C5	6:A:411:SOG:S1	2.86	0.56
1:B:152:LEU:H	6:B:421:SOG:H62	1.71	0.55
1:B:319:VAL:HG11	6:B:409:SOG:H6'1	1.88	0.54
6:A:409:SOG:H3'1	6:A:417:SOG:H4'1	1.91	0.53
1:A:53:TYR:CD1	1:A:104:LEU:HD13	2.45	0.52
6:A:410:SOG:H7'1	6:B:409:SOG:H4'2	1.92	0.52
1:A:116:HIS:HD2	6:A:427:SOG:H2'2	1.75	0.52
6:B:407:SOG:H61	6:B:408:SOG:H3	1.93	0.51
1:A:54:VAL:HG22	6:A:415:SOG:O4	2.09	0.51
6:A:426:SOG:H4'2	6:B:414:SOG:H8'3	1.94	0.50
6:A:414:SOG:H3	1:B:163:GLY:HA3	1.92	0.50
1:A:188:VAL:HG22	1:A:199:PHE:HB3	1.95	0.49
1:A:184:GLU:HG2	1:A:205:ARG:CZ	2.43	0.49
1:A:233:MET:HB3	7:A:429:PGW:H2	1.94	0.48
1:A:213:LYS:HD3	6:A:411:SOG:C1'	2.31	0.47
1:A:215:TYR:HB2	7:B:431:PGW:H7	1.97	0.47
7:A:429:PGW:H23	6:B:414:SOG:H5'2	1.96	0.46
1:B:349:ALA:HB1	6:B:416:SOG:H3'1	1.97	0.46
1:A:177:VAL:HG22	6:A:413:SOG:H4'1	1.98	0.46
1:B:206:TRP:HA	6:B:414:SOG:H61	1.98	0.46
6:A:410:SOG:H1'1	6:B:409:SOG:H62	1.98	0.46
1:A:324:PHE:CD1	6:A:417:SOG:H3	2.51	0.45
1:B:184:GLU:HG2	1:B:205:ARG:CZ	2.47	0.45
1:B:47:TRP:CE2	6:B:408:SOG:H8'1	2.51	0.45
1:B:379:GLY:HA3	6:B:413:SOG:H3'1	1.98	0.45
1:A:191:GLU:H	1:A:191:GLU:CD	2.25	0.45
1:A:228:LEU:HB3	4:A:404:PG4:H21	1.98	0.45
1:A:290:MET:HE2	1:A:290:MET:HB2	1.85	0.45
1:A:319:VAL:HG11	6:A:417:SOG:H6'1	2.00	0.44
6:A:411:SOG:H3	6:B:409:SOG:H3	1.99	0.44
1:A:83:TYR:CE2	1:A:158:ALA:HB1	2.53	0.43
1:A:177:VAL:HB	7:B:431:PGW:H20A	2.00	0.43
1:B:372:ALA:HA	1:B:376:TRP:HB2	1.99	0.43
1:B:152:LEU:H	6:B:421:SOG:C6	2.30	0.43
6:A:410:SOG:O6	6:A:411:SOG:H2'2	2.19	0.43
1:B:210:LEU:HD23	6:B:428:SOG:H1'2	2.00	0.43
1:A:324:PHE:HD1	6:A:417:SOG:H3	1.84	0.42
6:A:412:SOG:H61	1:B:177:VAL:HG11	2.01	0.42
1:B:83:TYR:CE2	1:B:158:ALA:HB1	2.54	0.42
7:A:429:PGW:H26	1:B:214:ILE:HG22	2.01	0.42
1:B:29:ASP:HA	1:B:32:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:PHE:CD1	6:A:410:SOG:H61	2.54	0.42
1:A:240:ARG:HD2	7:A:429:PGW:OAF	2.20	0.41
1:B:226:ALA:HA	7:B:431:PGW:H08	2.03	0.41
1:A:94:LEU:HB2	6:A:416:SOG:H4'2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	248 (98%)	4 (2%)	55	63
1	B	260/280 (93%)	259 (100%)	1 (0%)	84	89
All	All	512/560 (91%)	507 (99%)	5 (1%)	68	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	195	ARG
1	A	290	MET
1	A	377	LEU
1	B	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	76	HIS
1	A	318	ASN
1	B	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	418	-	20,20,20	0.92	1 (5%)	24,25,25	0.89	0
6	SOG	B	408	-	20,20,20	0.93	2 (10%)	24,25,25	0.77	0
6	SOG	A	417	-	20,20,20	1.03	2 (10%)	24,25,25	1.29	4 (16%)
6	SOG	B	428	-	6,6,20	0.44	0	5,5,25	0.81	0
4	PG4	A	405	-	12,12,12	0.15	0	11,11,11	0.13	0
6	SOG	A	428	-	6,6,20	0.46	0	5,5,25	0.53	0
6	SOG	A	415	-	14,14,20	0.83	1 (7%)	18,19,25	1.06	1 (5%)
6	SOG	A	409	-	20,20,20	0.91	1 (5%)	24,25,25	0.90	1 (4%)
6	SOG	A	408	-	16,16,20	1.06	2 (12%)	20,21,25	1.02	2 (10%)
6	SOG	B	423	-	8,8,20	0.38	0	7,7,25	0.71	0
6	SOG	A	422	-	6,6,20	0.41	0	5,5,25	0.56	0
6	SOG	A	410	-	20,20,20	0.79	1 (5%)	24,25,25	1.71	3 (12%)
6	SOG	A	413	-	20,20,20	0.88	1 (5%)	24,25,25	1.34	4 (16%)
6	SOG	A	424	-	6,6,20	0.49	0	5,5,25	1.32	1 (20%)
6	SOG	B	425	-	6,6,20	0.45	0	5,5,25	0.92	0
6	SOG	B	409	-	20,20,20	1.03	1 (5%)	24,25,25	1.56	5 (20%)
3	SO4	A	402	-	4,4,4	0.32	0	6,6,6	0.19	0
7	PGW	B	431	-	50,50,50	0.98	2 (4%)	53,56,56	0.94	2 (3%)
6	SOG	B	420	-	4,4,20	0.57	0	3,3,25	0.76	0
4	PG4	A	404	-	12,12,12	0.58	0	11,11,11	0.17	0
6	SOG	B	407	-	20,20,20	1.04	2 (10%)	24,25,25	0.73	1 (4%)
6	SOG	A	416	-	20,20,20	0.95	1 (5%)	24,25,25	0.83	1 (4%)
5	CIT	A	406	-	12,12,12	1.01	0	17,17,17	1.51	4 (23%)
6	SOG	B	418	-	7,7,20	0.44	0	6,6,25	0.92	0
6	SOG	B	427	-	6,6,20	0.45	0	5,5,25	0.70	0
2	7MA	A	401	-	34,34,34	5.69	13 (38%)	46,47,47	2.64	22 (47%)
3	SO4	B	403	-	4,4,4	0.35	0	6,6,6	0.13	0
6	SOG	B	406	-	20,20,20	0.97	2 (10%)	24,25,25	1.08	1 (4%)
6	SOG	B	412	-	20,20,20	0.98	1 (5%)	24,25,25	0.73	0
6	SOG	A	425	-	6,6,20	0.46	0	5,5,25	0.73	0
6	SOG	A	426	-	6,6,20	0.44	0	5,5,25	0.66	0
6	SOG	B	417	-	8,8,20	0.40	0	7,7,25	0.70	0
2	7MA	B	401	-	34,34,34	5.82	12 (35%)	46,47,47	2.51	21 (45%)
4	PG4	B	405	-	12,12,12	0.50	0	11,11,11	0.33	0
6	SOG	A	412	-	20,20,20	1.02	2 (10%)	24,25,25	0.94	1 (4%)
6	SOG	A	423	-	6,6,20	0.44	0	5,5,25	0.83	0
6	SOG	B	411	-	20,20,20	0.91	1 (5%)	24,25,25	1.09	2 (8%)
6	SOG	B	419	-	8,8,20	0.43	0	7,7,25	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SOG	A	419	-	6,6,20	0.44	0	5,5,25	0.66	0
6	SOG	A	411	-	20,20,20	0.72	0	24,25,25	1.15	3 (12%)
6	SOG	B	421	-	16,16,20	1.04	1 (6%)	20,21,25	0.82	0
6	SOG	B	429	-	6,6,20	0.43	0	5,5,25	0.84	0
4	PG4	A	403	-	12,12,12	0.49	0	11,11,11	0.33	0
6	SOG	B	422	-	7,7,20	0.44	0	6,6,25	0.75	0
6	SOG	B	426	-	6,6,20	0.43	0	5,5,25	0.86	0
7	PGW	A	429	-	50,50,50	0.94	2 (4%)	53,56,56	1.16	4 (7%)
6	SOG	B	424	-	5,5,20	0.44	0	4,4,25	0.47	0
3	SO4	B	402	-	4,4,4	0.28	0	6,6,6	0.13	0
6	SOG	B	430	-	6,6,20	0.42	0	5,5,25	0.84	0
6	SOG	A	407	-	17,17,20	0.98	1 (5%)	21,22,25	1.16	2 (9%)
6	SOG	B	413	-	16,16,20	1.11	1 (6%)	20,21,25	0.93	2 (10%)
4	PG4	B	404	-	12,12,12	0.41	0	11,11,11	0.58	0
6	SOG	A	427	-	6,6,20	0.44	0	5,5,25	0.58	0
6	SOG	B	415	-	5,5,20	0.25	0	4,4,25	0.39	0
6	SOG	B	414	-	20,20,20	0.92	1 (5%)	24,25,25	1.08	2 (8%)
6	SOG	B	416	-	9,9,20	0.40	0	8,8,25	0.53	0
6	SOG	A	420	-	6,6,20	0.42	0	5,5,25	0.77	0
6	SOG	B	410	-	20,20,20	0.92	1 (5%)	24,25,25	0.78	0
6	SOG	A	414	-	20,20,20	1.02	2 (10%)	24,25,25	0.76	0
6	SOG	A	421	-	6,6,20	0.47	0	5,5,25	1.04	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	A	418	-	-	6/11/31/31	0/1/1/1
6	SOG	B	408	-	-	6/11/31/31	0/1/1/1
6	SOG	A	417	-	-	7/11/31/31	0/1/1/1
6	SOG	B	428	-	-	1/4/4/31	-
4	PG4	A	405	-	-	3/10/10/10	-
6	SOG	A	428	-	-	1/4/4/31	-
6	SOG	A	415	-	-	1/5/25/31	0/1/1/1
6	SOG	A	409	-	-	4/11/31/31	0/1/1/1
6	SOG	A	408	-	-	4/7/27/31	0/1/1/1
6	SOG	B	423	-	-	3/6/6/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	A	422	-	-	3/4/4/31	-
6	SOG	A	410	-	-	4/11/31/31	0/1/1/1
6	SOG	A	413	-	-	4/11/31/31	0/1/1/1
6	SOG	A	424	-	-	2/4/4/31	-
6	SOG	B	425	-	-	2/4/4/31	-
6	SOG	B	409	-	-	4/11/31/31	0/1/1/1
7	PGW	B	431	-	-	28/55/55/55	-
6	SOG	B	420	-	-	2/2/2/31	-
4	PG4	A	404	-	-	5/10/10/10	-
6	SOG	B	407	-	-	6/11/31/31	0/1/1/1
6	SOG	A	416	-	-	7/11/31/31	0/1/1/1
5	CIT	A	406	-	-	3/16/16/16	-
6	SOG	B	418	-	-	3/5/5/31	-
6	SOG	B	427	-	-	1/4/4/31	-
2	7MA	A	401	-	-	7/32/32/32	0/3/3/3
6	SOG	B	406	-	-	6/11/31/31	0/1/1/1
6	SOG	B	412	-	-	5/11/31/31	0/1/1/1
6	SOG	A	425	-	-	2/4/4/31	-
6	SOG	A	426	-	-	1/4/4/31	-
6	SOG	B	417	-	-	4/6/6/31	-
2	7MA	B	401	-	-	6/32/32/32	0/3/3/3
4	PG4	B	405	-	-	8/10/10/10	-
6	SOG	A	412	-	-	4/11/31/31	0/1/1/1
6	SOG	A	423	-	-	3/4/4/31	-
6	SOG	B	411	-	-	7/11/31/31	0/1/1/1
6	SOG	B	419	-	-	5/6/6/31	-
6	SOG	A	419	-	-	1/4/4/31	-
6	SOG	A	411	-	-	2/11/31/31	0/1/1/1
6	SOG	B	421	-	-	4/7/27/31	0/1/1/1
6	SOG	B	429	-	-	1/4/4/31	-
4	PG4	A	403	-	-	3/10/10/10	-
6	SOG	B	422	-	-	2/5/5/31	-
6	SOG	B	426	-	-	1/4/4/31	-
7	PGW	A	429	-	-	24/55/55/55	-
6	SOG	B	424	-	-	2/3/3/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	B	430	-	-	3/4/4/31	-
6	SOG	A	407	-	-	5/8/28/31	0/1/1/1
6	SOG	B	413	-	-	3/7/27/31	0/1/1/1
4	PG4	B	404	-	-	4/10/10/10	-
6	SOG	A	427	-	-	3/4/4/31	-
6	SOG	B	415	-	-	2/3/3/31	-
6	SOG	B	414	-	-	4/11/31/31	0/1/1/1
6	SOG	B	416	-	-	1/7/7/31	-
6	SOG	A	420	-	-	1/4/4/31	-
6	SOG	B	410	-	-	8/11/31/31	0/1/1/1
6	SOG	A	414	-	-	6/11/31/31	0/1/1/1
6	SOG	A	421	-	-	1/4/4/31	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7MA	O24-S23	20.83	1.65	1.43
2	A	401	7MA	O24-S23	20.48	1.65	1.43
2	B	401	7MA	O25-S23	17.92	1.62	1.43
2	A	401	7MA	O25-S23	17.73	1.62	1.43
2	B	401	7MA	S23-N14	13.57	1.84	1.65
2	A	401	7MA	S23-N14	13.42	1.84	1.65
2	B	401	7MA	C26-S23	8.91	1.89	1.78
2	A	401	7MA	C26-S23	8.01	1.88	1.78
2	A	401	7MA	C15-N14	5.50	1.52	1.44
2	B	401	7MA	C15-N14	5.48	1.52	1.44
2	B	401	7MA	C11-N03	5.19	1.45	1.35
2	A	401	7MA	C11-N03	4.85	1.44	1.35
7	B	431	PGW	O01-C1	4.64	1.47	1.34
7	A	429	PGW	O01-C1	4.30	1.46	1.34
7	A	429	PGW	O03-C19	4.18	1.45	1.33
7	B	431	PGW	O03-C19	4.06	1.45	1.33
6	B	409	SOG	C1'-S1	-3.82	1.76	1.81
6	A	417	SOG	C1'-S1	-3.46	1.76	1.81
6	B	413	SOG	C1'-S1	-3.40	1.76	1.81
6	A	412	SOG	C1'-S1	-3.38	1.76	1.81
6	A	414	SOG	C1'-S1	-3.35	1.76	1.81
6	B	407	SOG	C1'-S1	-3.35	1.76	1.81
6	B	406	SOG	C1'-S1	-3.32	1.76	1.81
6	A	416	SOG	C1'-S1	-3.21	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	408	SOG	C1'-S1	-3.21	1.76	1.81
6	B	412	SOG	C1'-S1	-3.17	1.77	1.81
6	B	421	SOG	C1'-S1	-3.07	1.77	1.81
6	B	408	SOG	C1'-S1	-3.04	1.77	1.81
6	A	418	SOG	C1'-S1	-3.03	1.77	1.81
2	B	401	7MA	C20-C15	3.02	1.45	1.39
6	A	409	SOG	C1'-S1	-3.00	1.77	1.81
6	B	414	SOG	C1'-S1	-2.99	1.77	1.81
6	B	410	SOG	C1'-S1	-2.97	1.77	1.81
6	A	413	SOG	C1'-S1	-2.92	1.77	1.81
2	A	401	7MA	O21-C18	2.91	1.39	1.35
6	B	411	SOG	C1'-S1	-2.90	1.77	1.81
2	B	401	7MA	C13-C11	2.80	1.57	1.53
6	A	407	SOG	C1'-S1	-2.79	1.77	1.81
2	B	401	7MA	O21-C18	2.72	1.39	1.35
2	A	401	7MA	C19-C18	2.69	1.45	1.39
2	B	401	7MA	C19-C18	2.60	1.45	1.39
2	A	401	7MA	C20-C15	2.60	1.44	1.39
2	A	401	7MA	C13-C11	2.44	1.56	1.53
6	B	407	SOG	C1-S1	-2.33	1.76	1.80
6	A	410	SOG	C1'-S1	-2.31	1.78	1.81
2	B	401	7MA	C18-N17	2.29	1.36	1.32
6	A	417	SOG	C1-S1	-2.20	1.77	1.80
6	A	415	SOG	C1-S1	-2.19	1.77	1.80
2	A	401	7MA	C29-C30	2.18	1.42	1.38
2	A	401	7MA	C18-N17	2.17	1.35	1.32
6	B	406	SOG	C1-S1	-2.16	1.77	1.80
6	B	408	SOG	C1-S1	-2.15	1.77	1.80
2	B	401	7MA	C29-C30	2.14	1.42	1.38
6	A	412	SOG	C1-S1	-2.14	1.77	1.80
6	A	414	SOG	C1-S1	-2.07	1.77	1.80
6	A	408	SOG	C1-S1	-2.03	1.77	1.80
2	A	401	7MA	C27-C26	2.00	1.41	1.39

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7MA	C16-N17-C18	6.20	122.36	116.72
2	A	401	7MA	O25-S23-O24	-6.06	110.13	119.59
6	A	410	SOG	C1-O5-C5	5.93	123.19	112.56
2	A	401	7MA	C16-N17-C18	5.72	121.92	116.72
7	A	429	PGW	O01-C1-C2	5.60	123.59	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7MA	C13-N14-C15	5.49	124.04	116.67
2	A	401	7MA	C13-C11-N03	5.38	123.57	117.04
2	B	401	7MA	O25-S23-O24	-5.26	111.38	119.59
2	A	401	7MA	O24-S23-N14	5.12	112.66	106.69
2	B	401	7MA	C13-C11-N03	5.06	123.18	117.04
2	A	401	7MA	C13-N14-C15	4.69	122.97	116.67
2	A	401	7MA	O25-S23-N14	4.35	111.76	106.69
2	B	401	7MA	C11-C13-N14	4.22	118.59	112.19
6	A	407	SOG	C1-O5-C5	4.06	119.84	112.56
6	B	409	SOG	C3-C4-C5	3.96	117.42	110.23
5	A	406	CIT	O6-C6-C3	3.96	120.73	113.14
2	B	401	7MA	O25-S23-N14	3.76	111.07	106.69
7	B	431	PGW	O01-C1-C2	3.66	119.41	111.48
2	B	401	7MA	C20-C15-N14	3.55	125.32	120.15
2	B	401	7MA	O24-S23-N14	3.51	110.78	106.69
6	A	413	SOG	C3-C4-C5	3.51	116.60	110.23
2	A	401	7MA	C27-C26-S23	-3.37	112.89	117.48
6	A	411	SOG	C1-O5-C5	3.31	118.49	112.56
2	A	401	7MA	C20-C15-N14	3.28	124.93	120.15
6	B	406	SOG	C1'-S1-C1	3.26	107.49	100.45
2	A	401	7MA	O12-C11-C13	-3.25	115.76	120.56
6	A	412	SOG	C1-O5-C5	3.17	118.25	112.56
2	A	401	7MA	C31-C26-S23	3.11	124.97	122.07
2	B	401	7MA	O12-C11-C13	-3.09	115.99	120.56
6	A	417	SOG	C4-C3-C2	3.06	116.20	110.83
6	B	409	SOG	O5-C5-C4	3.04	115.17	109.70
2	A	401	7MA	C11-C13-N14	3.03	116.79	112.19
6	B	409	SOG	C4-C3-C2	3.01	116.12	110.83
6	A	413	SOG	C4-C3-C2	2.99	116.08	110.83
6	A	415	SOG	C1-O5-C5	2.91	117.78	112.56
6	B	409	SOG	C1-O5-C5	2.90	117.77	112.56
2	B	401	7MA	C13-N14-S23	2.88	123.30	117.47
2	A	401	7MA	C05-C04-N03	2.88	117.67	113.15
2	A	401	7MA	C13-N14-S23	2.82	123.18	117.47
2	A	401	7MA	C08-N07-C06	2.80	121.76	116.85
6	A	410	SOG	C1'-S1-C1	2.76	106.42	100.45
2	A	401	7MA	C04-N03-C02	2.76	119.83	116.36
6	B	411	SOG	C3-C4-C5	2.71	115.15	110.23
2	A	401	7MA	C26-S23-N14	-2.71	101.39	106.16
6	A	407	SOG	O5-C1-C2	2.70	114.04	110.32
7	A	429	PGW	O03-C19-C20	2.67	119.98	111.83
6	A	410	SOG	O5-C5-C4	2.66	114.50	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7MA	C15-N14-S23	-2.62	112.46	117.72
2	A	401	7MA	C05-C06-N07	-2.61	118.77	123.75
2	A	401	7MA	C04-C05-C10	-2.60	115.96	120.75
2	B	401	7MA	C04-C05-C10	-2.59	115.97	120.75
2	A	401	7MA	O25-S23-C26	2.57	112.34	107.35
6	B	414	SOG	C4-C3-C2	2.56	115.33	110.83
2	B	401	7MA	C08-N07-C06	2.56	121.33	116.85
6	B	411	SOG	C4-C3-C2	2.53	115.28	110.83
7	A	429	PGW	O01-C1-O02	-2.53	117.80	123.70
2	B	401	7MA	C31-C26-S23	2.52	124.42	122.07
6	A	417	SOG	C3-C4-C5	2.51	114.79	110.23
2	B	401	7MA	O21-C18-C19	2.49	121.18	116.77
2	B	401	7MA	C30-C31-C26	2.48	118.89	116.27
6	A	409	SOG	C4-C3-C2	2.46	115.15	110.83
6	A	411	SOG	C1'-S1-C1	2.46	105.76	100.45
6	A	417	SOG	O5-C5-C4	2.45	114.12	109.70
6	A	413	SOG	O5-C1-C2	-2.44	106.95	110.32
7	B	431	PGW	O03-C19-C20	2.44	119.26	111.83
2	A	401	7MA	O21-C18-C19	2.43	121.06	116.77
2	B	401	7MA	C05-C06-N07	-2.42	119.14	123.75
6	B	414	SOG	C3-C4-C5	2.41	114.60	110.23
2	B	401	7MA	C10-C05-C06	2.38	120.60	117.10
6	A	408	SOG	C1-O5-C5	2.36	116.79	112.56
2	B	401	7MA	C27-C26-S23	-2.30	114.35	117.48
2	B	401	7MA	C05-C04-N03	2.30	116.77	113.15
6	A	417	SOG	C1-O5-C5	2.29	116.67	112.56
2	A	401	7MA	C10-C05-C06	2.28	120.45	117.10
6	B	413	SOG	C4-C3-C2	2.26	114.80	110.83
6	A	413	SOG	O5-C5-C4	2.17	113.61	109.70
2	A	401	7MA	C19-C20-C15	-2.14	117.59	120.30
6	A	408	SOG	O5-C5-C4	2.13	113.55	109.70
6	B	407	SOG	C1-O5-C5	2.13	116.39	112.56
6	A	424	SOG	C3'-C2'-C1'	-2.11	109.33	113.09
6	B	413	SOG	O5-C5-C6	2.09	111.63	106.44
5	A	406	CIT	O4-C5-C4	2.09	120.97	114.35
6	A	411	SOG	O5-C5-C4	2.05	113.39	109.70
5	A	406	CIT	O5-C6-C3	-2.04	118.13	122.09
2	B	401	7MA	C19-C20-C15	-2.04	117.72	120.30
7	A	429	PGW	O03-C19-O04	-2.02	118.58	123.63
6	A	416	SOG	C1-C2-C3	-2.01	106.63	110.55
5	A	406	CIT	O3-C5-C4	-2.00	117.28	122.95
6	B	409	SOG	C1'-S1-C1	2.00	104.78	100.45

There are no chirality outliers.

All (249) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	7MA	O12-C11-C13-N14
2	A	401	7MA	N03-C11-C13-N14
2	B	401	7MA	O12-C11-C13-N14
2	B	401	7MA	N03-C11-C13-N14
6	A	410	SOG	O5-C1-S1-C1'
6	A	413	SOG	C2'-C1'-S1-C1
6	A	417	SOG	O5-C1-S1-C1'
6	A	419	SOG	S1-C1'-C2'-C3'
6	A	420	SOG	S1-C1'-C2'-C3'
6	A	422	SOG	S1-C1'-C2'-C3'
6	A	423	SOG	S1-C1'-C2'-C3'
6	B	406	SOG	C2-C1-S1-C1'
6	B	406	SOG	O5-C1-S1-C1'
6	B	414	SOG	O5-C1-S1-C1'
6	B	418	SOG	S1-C1'-C2'-C3'
6	B	420	SOG	S1-C1'-C2'-C3'
6	B	423	SOG	S1-C1'-C2'-C3'
6	B	425	SOG	S1-C1'-C2'-C3'
7	A	429	PGW	C04-O12-P-O14
7	A	429	PGW	C2-C1-O01-C02
7	A	429	PGW	O12-C04-C05-OAF
7	B	431	PGW	OAF-C05-CAD-OAE
7	B	431	PGW	C04-C05-CAD-OAE
7	B	431	PGW	C03-O11-P-O12
7	B	431	PGW	C03-O11-P-O13
7	B	431	PGW	C03-O11-P-O14
6	B	411	SOG	C4-C5-C6-O6
7	A	429	PGW	O02-C1-O01-C02
7	A	429	PGW	C20-C19-O03-C01
6	B	410	SOG	O5-C5-C6-O6
6	B	411	SOG	O5-C5-C6-O6
6	B	413	SOG	O5-C5-C6-O6
7	A	429	PGW	O04-C19-O03-C01
6	B	412	SOG	O5-C5-C6-O6
6	B	406	SOG	O5-C5-C6-O6
6	B	421	SOG	O5-C5-C6-O6
6	A	412	SOG	S1-C1'-C2'-C3'
6	A	418	SOG	S1-C1'-C2'-C3'
6	B	416	SOG	S1-C1'-C2'-C3'
6	A	418	SOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	410	SOG	C4-C5-C6-O6
6	A	416	SOG	O5-C5-C6-O6
6	B	413	SOG	C4-C5-C6-O6
4	B	405	PG4	O3-C5-C6-O4
6	A	417	SOG	S1-C1'-C2'-C3'
7	A	429	PGW	O12-C04-C05-CAD
7	A	429	PGW	C16-C15-C27-C26
6	B	412	SOG	C4-C5-C6-O6
6	A	407	SOG	O5-C5-C6-O6
6	A	416	SOG	S1-C1'-C2'-C3'
6	B	406	SOG	S1-C1'-C2'-C3'
6	B	414	SOG	C4-C5-C6-O6
6	B	414	SOG	O5-C5-C6-O6
6	A	414	SOG	O5-C5-C6-O6
4	A	404	PG4	O3-C5-C6-O4
6	B	406	SOG	C4-C5-C6-O6
4	B	405	PG4	O1-C1-C2-O2
4	A	403	PG4	O1-C1-C2-O2
6	B	408	SOG	C1'-C2'-C3'-C4'
2	A	401	7MA	C13-N14-S23-O25
2	B	401	7MA	C13-N14-S23-O25
4	A	405	PG4	C3-C4-O3-C5
6	A	407	SOG	C1'-C2'-C3'-C4'
6	A	411	SOG	C1'-C2'-C3'-C4'
6	B	426	SOG	C1'-C2'-C3'-C4'
6	B	429	SOG	C1'-C2'-C3'-C4'
6	B	407	SOG	S1-C1'-C2'-C3'
6	A	408	SOG	C4-C5-C6-O6
4	B	404	PG4	O1-C1-C2-O2
6	A	421	SOG	C1'-C2'-C3'-C4'
6	B	410	SOG	C1'-C2'-C3'-C4'
6	B	411	SOG	C1'-C2'-C3'-C4'
6	B	418	SOG	C1'-C2'-C3'-C4'
6	B	422	SOG	C1'-C2'-C3'-C4'
6	B	430	SOG	C1'-C2'-C3'-C4'
6	A	407	SOG	S1-C1'-C2'-C3'
6	A	410	SOG	S1-C1'-C2'-C3'
6	A	416	SOG	C2'-C3'-C4'-C5'
6	A	426	SOG	C2'-C3'-C4'-C5'
6	B	409	SOG	C4'-C5'-C6'-C7'
6	B	412	SOG	C4'-C5'-C6'-C7'
6	B	423	SOG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
7	B	431	PGW	C16-C17-C18-C28
6	A	424	SOG	C1'-C2'-C3'-C4'
6	B	419	SOG	C1'-C2'-C3'-C4'
6	B	418	SOG	C3'-C4'-C5'-C6'
7	A	429	PGW	C09-C11-C12-C13
6	B	408	SOG	O5-C5-C6-O6
6	A	410	SOG	C2'-C3'-C4'-C5'
6	A	417	SOG	C4'-C5'-C6'-C7'
4	A	404	PG4	O2-C3-C4-O3
7	B	431	PGW	C08-C09-C11-C12
4	A	404	PG4	O4-C7-C8-O5
6	A	416	SOG	C4'-C5'-C6'-C7'
6	A	414	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C09-C11-C12-C13
6	A	417	SOG	C2'-C3'-C4'-C5'
6	A	428	SOG	C2'-C3'-C4'-C5'
6	B	408	SOG	C3'-C4'-C5'-C6'
7	A	429	PGW	C22-C23-C24-C25
6	A	427	SOG	C2'-C3'-C4'-C5'
6	B	411	SOG	C3'-C4'-C5'-C6'
6	A	409	SOG	C2'-C3'-C4'-C5'
6	B	410	SOG	C3'-C4'-C5'-C6'
6	A	414	SOG	C4'-C5'-C6'-C7'
7	A	429	PGW	C25-C26-C27-C15
6	A	416	SOG	C3'-C4'-C5'-C6'
6	A	413	SOG	C4'-C5'-C6'-C7'
6	A	418	SOG	C4-C5-C6-O6
6	B	421	SOG	C4-C5-C6-O6
7	B	431	PGW	C06-C07-C08-C09
6	A	423	SOG	C2'-C3'-C4'-C5'
6	A	413	SOG	C2'-C3'-C4'-C5'
7	A	429	PGW	C23-C24-C25-C26
6	A	415	SOG	O5-C5-C6-O6
6	A	414	SOG	C3'-C4'-C5'-C6'
6	B	407	SOG	C1'-C2'-C3'-C4'
6	B	425	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C17-C18-C28-C30
6	A	425	SOG	C2'-C3'-C4'-C5'
6	A	407	SOG	C4-C5-C6-O6
4	B	405	PG4	O4-C7-C8-O5
6	A	417	SOG	C1'-C2'-C3'-C4'
7	B	431	PGW	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	A	412	SOG	C4'-C5'-C6'-C7'
6	B	408	SOG	S1-C1'-C2'-C3'
7	A	429	PGW	O03-C01-C02-C03
7	B	431	PGW	O03-C01-C02-C03
6	A	409	SOG	O5-C5-C6-O6
6	A	411	SOG	C3'-C4'-C5'-C6'
6	B	417	SOG	C3'-C4'-C5'-C6'
7	B	431	PGW	C21-C22-C23-C24
7	A	429	PGW	C21-C22-C23-C24
6	A	424	SOG	C3'-C4'-C5'-C6'
6	A	422	SOG	C3'-C4'-C5'-C6'
6	A	422	SOG	C1'-C2'-C3'-C4'
6	A	409	SOG	C4'-C5'-C6'-C7'
6	A	413	SOG	C3'-C4'-C5'-C6'
6	B	415	SOG	C3'-C4'-C5'-C6'
6	B	408	SOG	C5'-C6'-C7'-C8'
6	A	412	SOG	C2'-C3'-C4'-C5'
6	B	424	SOG	C2'-C3'-C4'-C5'
6	B	414	SOG	C5'-C6'-C7'-C8'
6	B	420	SOG	C1'-C2'-C3'-C4'
6	A	414	SOG	C4-C5-C6-O6
6	A	408	SOG	O5-C5-C6-O6
7	B	431	PGW	C11-C12-C13-C14
6	B	428	SOG	C2'-C3'-C4'-C5'
2	A	401	7MA	C13-N14-S23-C26
2	B	401	7MA	C13-N14-S23-O24
6	B	408	SOG	C4'-C5'-C6'-C7'
6	B	413	SOG	S1-C1'-C2'-C3'
7	B	431	PGW	C25-C26-C27-C15
6	A	417	SOG	C5'-C6'-C7'-C8'
6	B	409	SOG	C5'-C6'-C7'-C8'
7	A	429	PGW	C4-C5-C6-C7
6	A	427	SOG	C3'-C4'-C5'-C6'
6	B	419	SOG	C5'-C6'-C7'-C8'
7	A	429	PGW	C19-C20-C21-C22
4	B	405	PG4	C1-C2-O2-C3
7	B	431	PGW	C20-C19-O03-C01
6	B	417	SOG	C5'-C6'-C7'-C8'
6	B	427	SOG	C2'-C3'-C4'-C5'
2	A	401	7MA	C13-N14-S23-O24
7	B	431	PGW	O04-C19-O03-C01
6	B	407	SOG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
4	B	404	PG4	O4-C7-C8-O5
6	A	417	SOG	C2-C1-S1-C1'
6	A	425	SOG	S1-C1'-C2'-C3'
6	B	424	SOG	S1-C1'-C2'-C3'
6	A	416	SOG	C4-C5-C6-O6
6	B	411	SOG	C2'-C3'-C4'-C5'
6	B	422	SOG	C3'-C4'-C5'-C6'
7	B	431	PGW	C15-C16-C17-C18
4	B	405	PG4	C3-C4-O3-C5
6	A	423	SOG	C1'-C2'-C3'-C4'
2	B	401	7MA	C13-N14-S23-C26
4	B	405	PG4	C5-C6-O4-C7
6	A	409	SOG	C3'-C4'-C5'-C6'
6	A	407	SOG	C2'-C3'-C4'-C5'
6	A	408	SOG	C1'-C2'-C3'-C4'
7	B	431	PGW	O03-C01-C02-O01
4	A	404	PG4	C6-C5-O3-C4
6	A	418	SOG	C1'-C2'-C3'-C4'
4	B	405	PG4	C6-C5-O3-C4
6	B	407	SOG	C4-C5-C6-O6
6	B	415	SOG	C4'-C5'-C6'-C7'
7	A	429	PGW	C03-O11-P-O14
7	B	431	PGW	C04-O12-P-O11
7	B	431	PGW	C04-O12-P-O13
7	B	431	PGW	C04-O12-P-O14
6	B	412	SOG	C3'-C4'-C5'-C6'
6	B	410	SOG	C5'-C6'-C7'-C8'
4	A	403	PG4	C8-C7-O4-C6
6	B	430	SOG	C3'-C4'-C5'-C6'
6	B	419	SOG	C3'-C4'-C5'-C6'
6	A	408	SOG	S1-C1'-C2'-C3'
6	B	410	SOG	S1-C1'-C2'-C3'
6	A	412	SOG	C3'-C4'-C5'-C6'
7	A	429	PGW	O03-C01-C02-O01
7	A	429	PGW	C10-C06-C07-C08
6	B	410	SOG	C4'-C5'-C6'-C7'
6	A	410	SOG	C1'-C2'-C3'-C4'
7	B	431	PGW	C07-C08-C09-C11
7	A	429	PGW	C17-C18-C28-C30
4	B	405	PG4	O2-C3-C4-O3
7	A	429	PGW	C24-C25-C26-C27
6	B	411	SOG	S1-C1'-C2'-C3'

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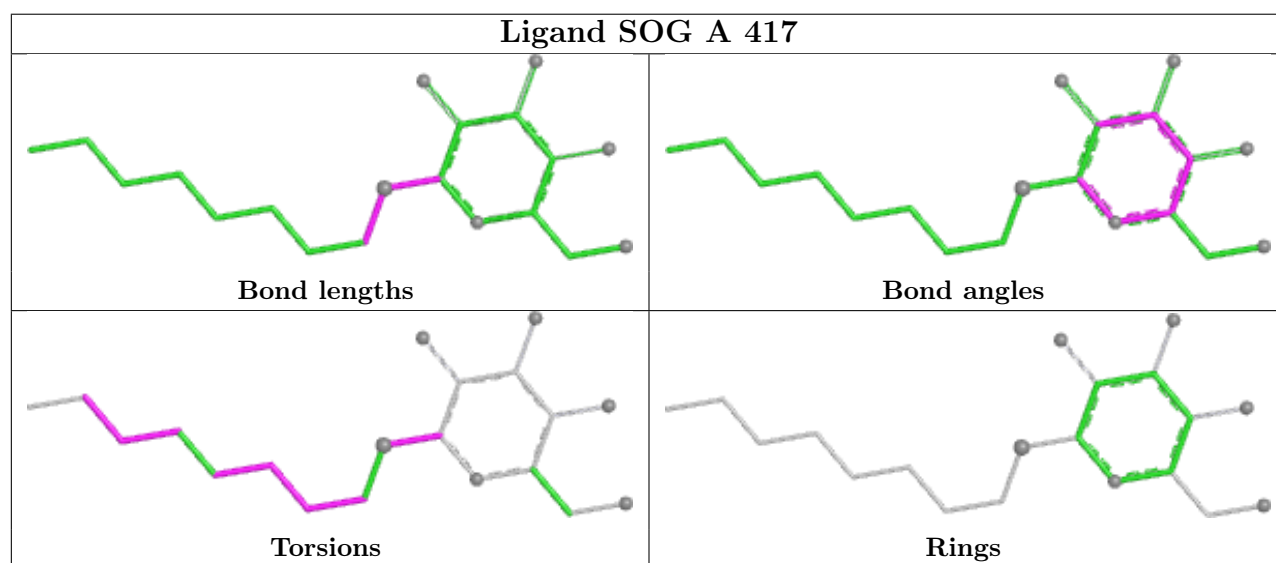
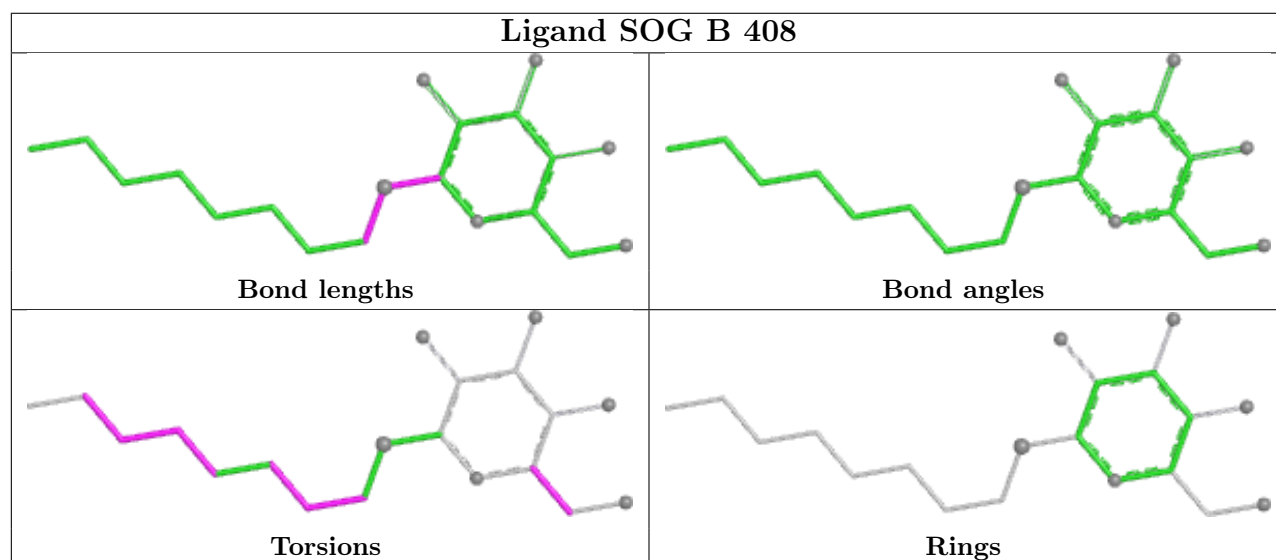
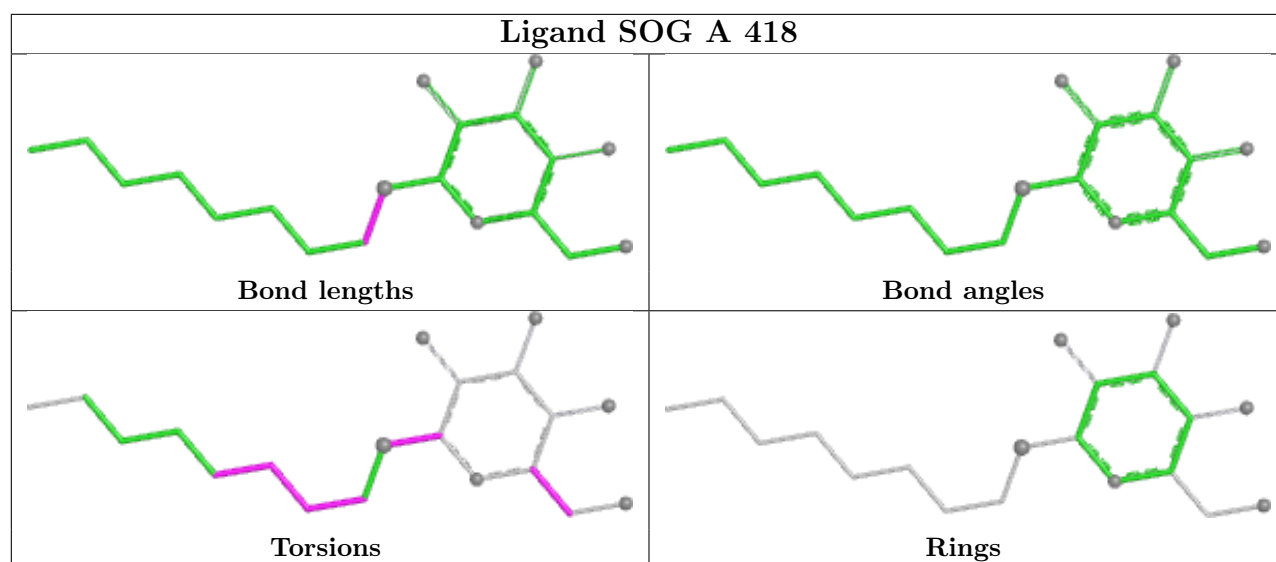
Mol	Chain	Res	Type	Atoms
5	A	406	CIT	C3-C4-C5-O4
6	B	409	SOG	S1-C1'-C2'-C3'
6	B	407	SOG	C2'-C3'-C4'-C5'
5	A	406	CIT	O7-C3-C4-C5
7	B	431	PGW	C7-C8-C9-C10
6	B	410	SOG	O5-C1-S1-C1'
6	B	417	SOG	C2'-C3'-C4'-C5'
4	A	403	PG4	C1-C2-O2-C3
7	B	431	PGW	C05-C04-O12-P
5	A	406	CIT	C3-C4-C5-O3
4	B	404	PG4	C5-C6-O4-C7
6	B	419	SOG	C4'-C5'-C6'-C7'
6	B	423	SOG	C5'-C6'-C7'-C8'
4	B	404	PG4	C3-C4-O3-C5
4	A	404	PG4	C5-C6-O4-C7
6	A	416	SOG	C5'-C6'-C7'-C8'
6	B	406	SOG	C1'-C2'-C3'-C4'
6	A	418	SOG	C2-C1-S1-C1'
6	A	427	SOG	S1-C1'-C2'-C3'
6	B	417	SOG	S1-C1'-C2'-C3'
6	B	421	SOG	C1'-C2'-C3'-C4'
6	B	409	SOG	C2'-C1'-S1-C1
6	B	411	SOG	C2'-C1'-S1-C1
6	B	421	SOG	C2'-C1'-S1-C1
7	A	429	PGW	C15-C16-C17-C18
7	B	431	PGW	C23-C24-C25-C26
6	A	418	SOG	C2'-C3'-C4'-C5'
7	A	429	PGW	C06-C07-C08-C09
6	B	419	SOG	C2'-C3'-C4'-C5'
6	B	412	SOG	S1-C1'-C2'-C3'
2	A	401	7MA	C11-C13-N14-C15
2	B	401	7MA	C11-C13-N14-C15
6	B	407	SOG	C5'-C6'-C7'-C8'
6	B	430	SOG	C2'-C3'-C4'-C5'
2	A	401	7MA	C15-N14-S23-O25
7	B	431	PGW	O01-C1-C2-C3
4	A	405	PG4	O2-C3-C4-O3
7	A	429	PGW	O03-C19-C20-C21
7	B	431	PGW	O02-C1-C2-C3
6	A	414	SOG	C5'-C6'-C7'-C8'
4	A	405	PG4	O3-C5-C6-O4

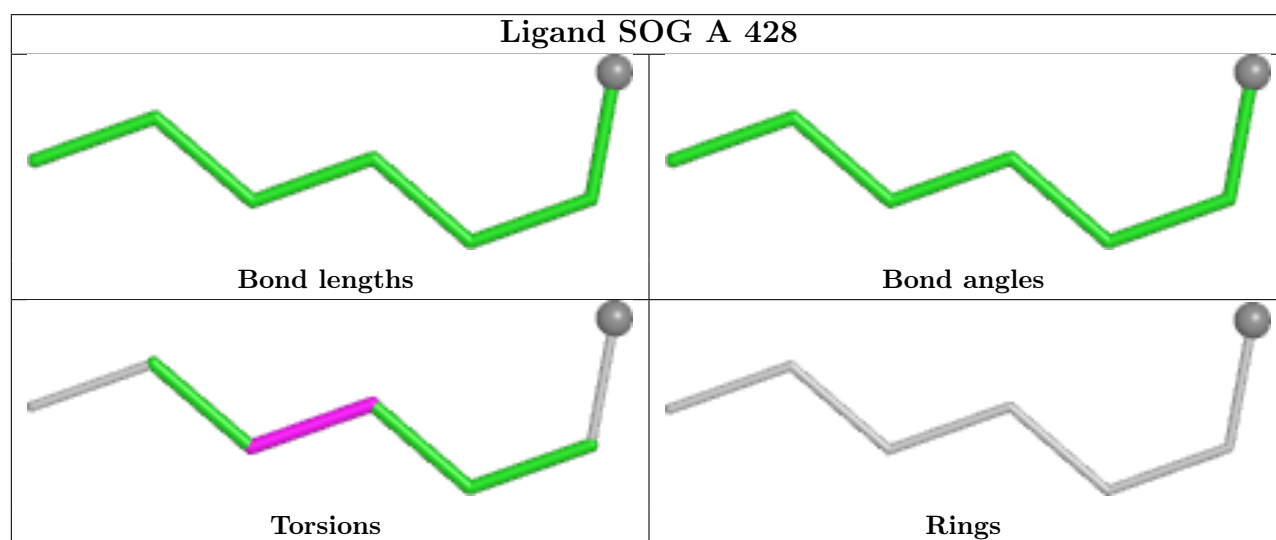
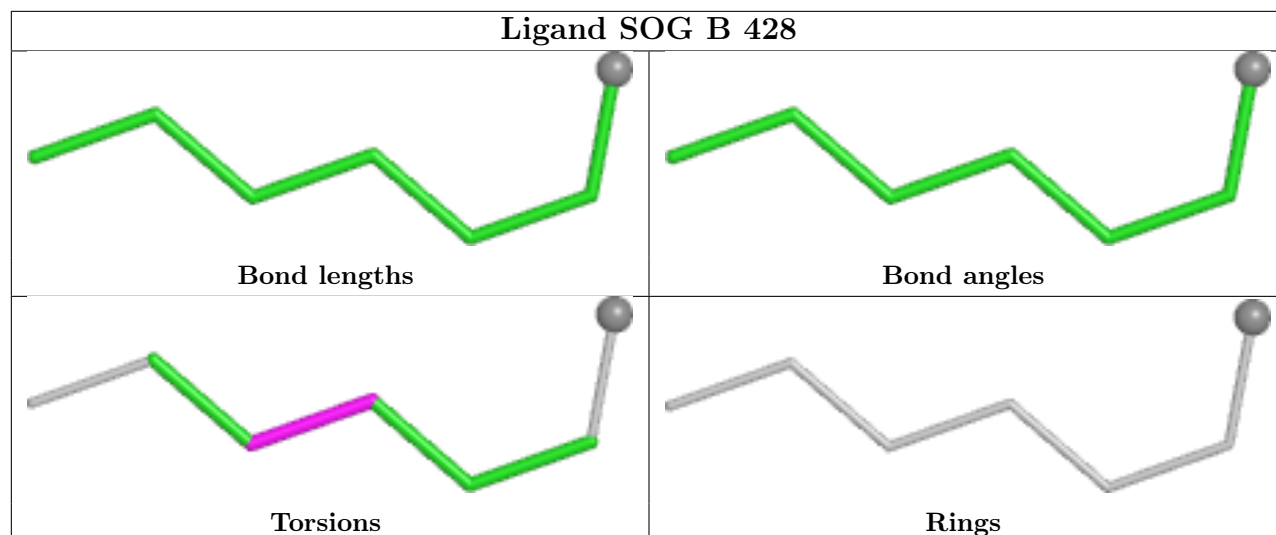
There are no ring outliers.

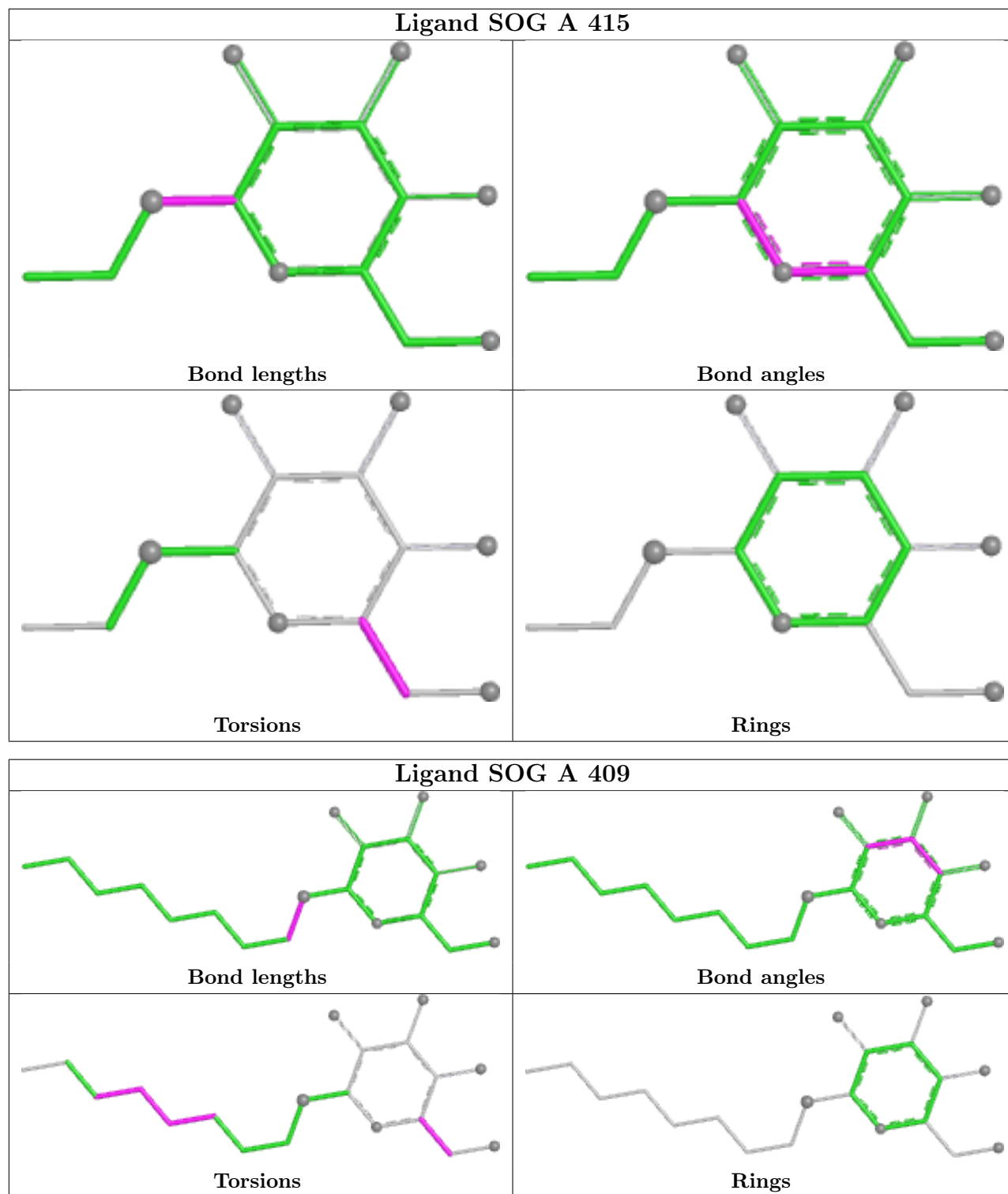
25 monomers are involved in 45 short contacts:

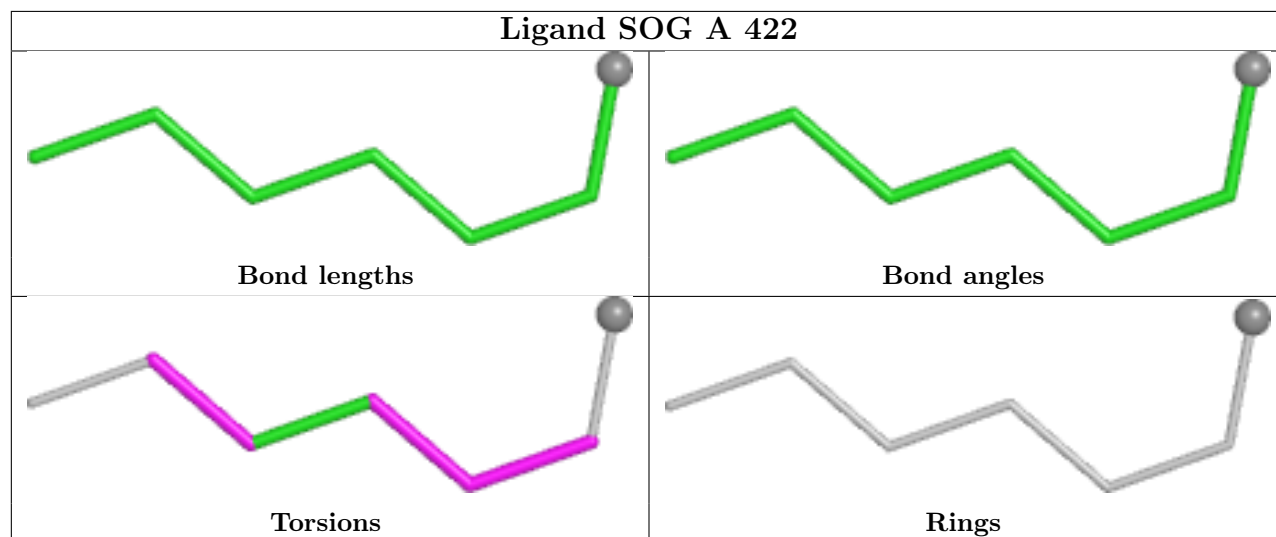
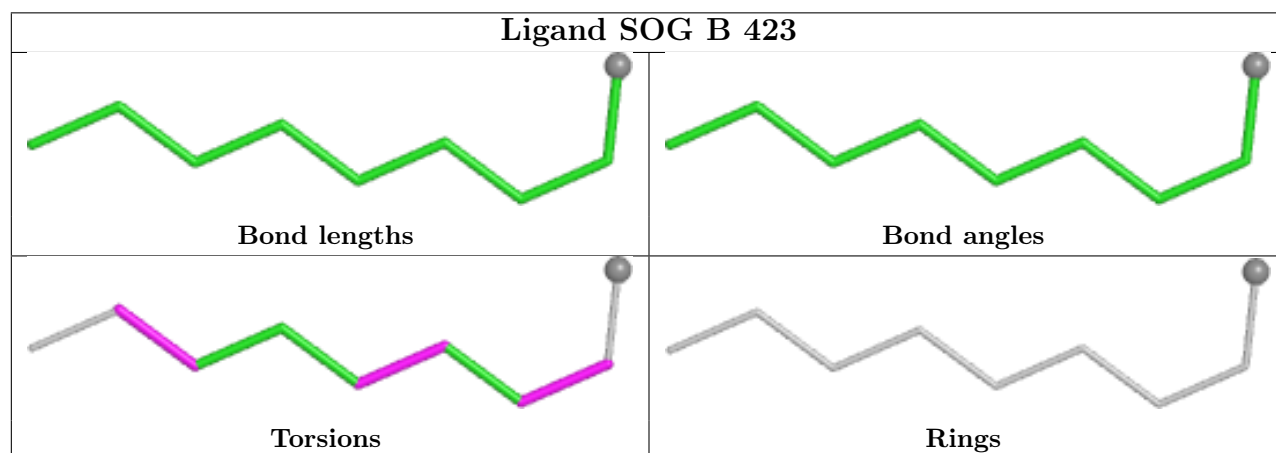
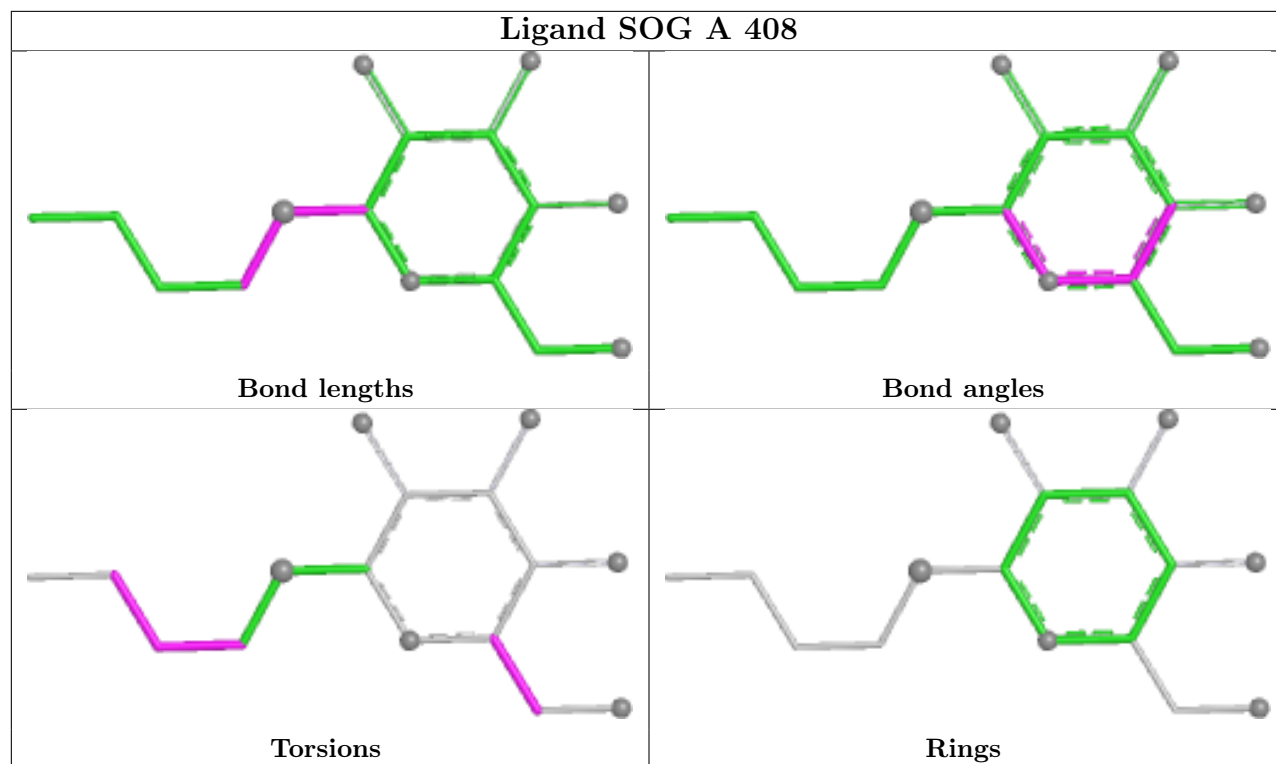
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	408	SOG	2	0
6	A	417	SOG	4	0
6	B	428	SOG	1	0
4	A	405	PG4	1	0
6	A	415	SOG	2	0
6	A	409	SOG	1	0
6	A	410	SOG	7	0
6	A	413	SOG	1	0
6	B	409	SOG	4	0
7	B	431	PGW	3	0
4	A	404	PG4	1	0
6	B	407	SOG	1	0
6	A	416	SOG	1	0
6	B	418	SOG	1	0
6	A	426	SOG	1	0
6	A	412	SOG	1	0
6	A	411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

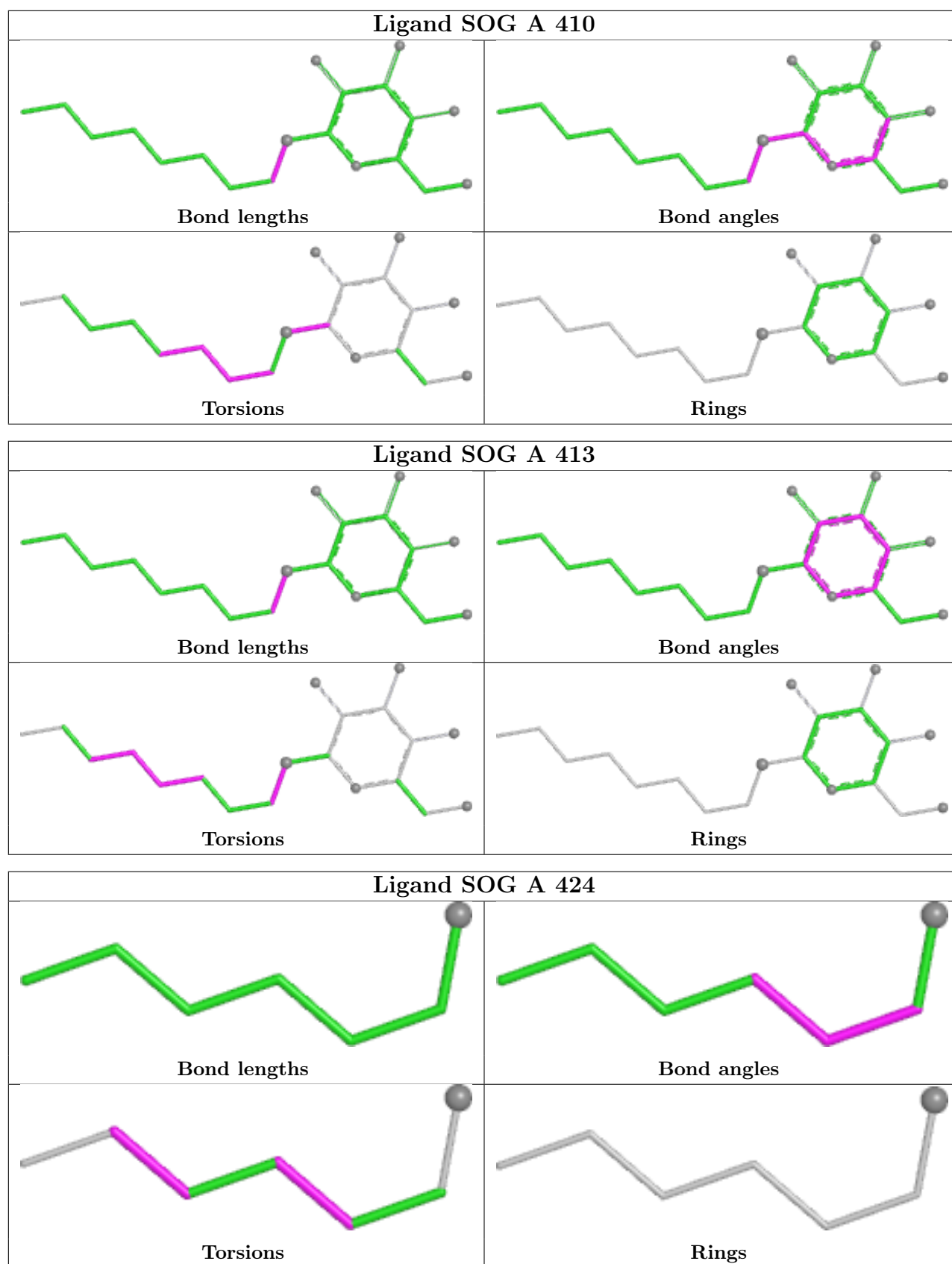
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

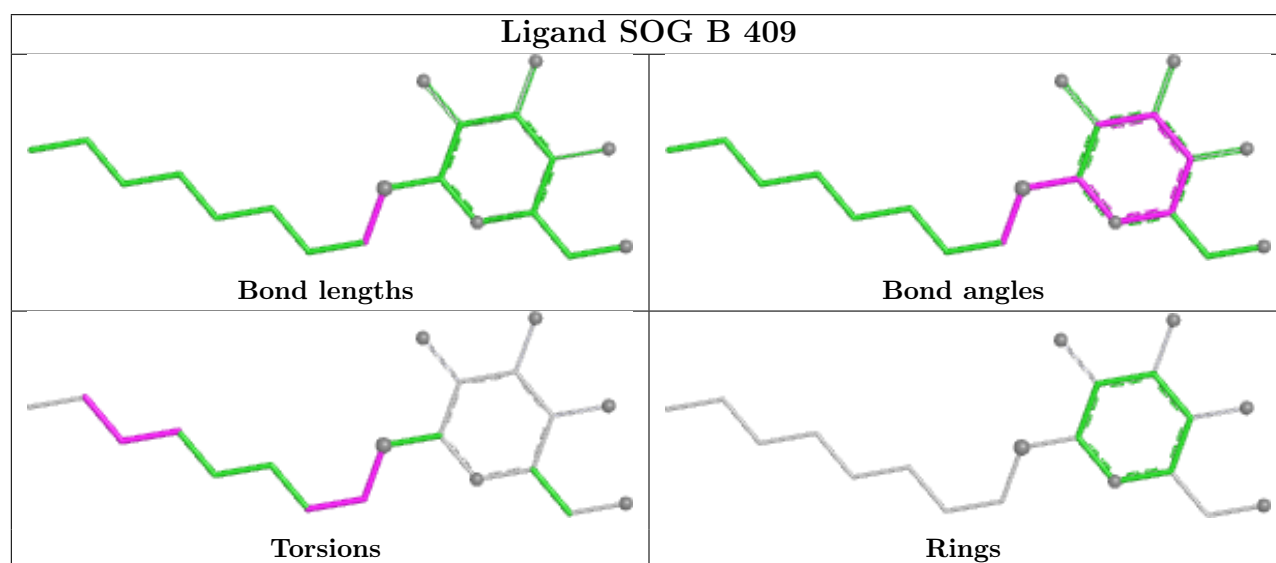
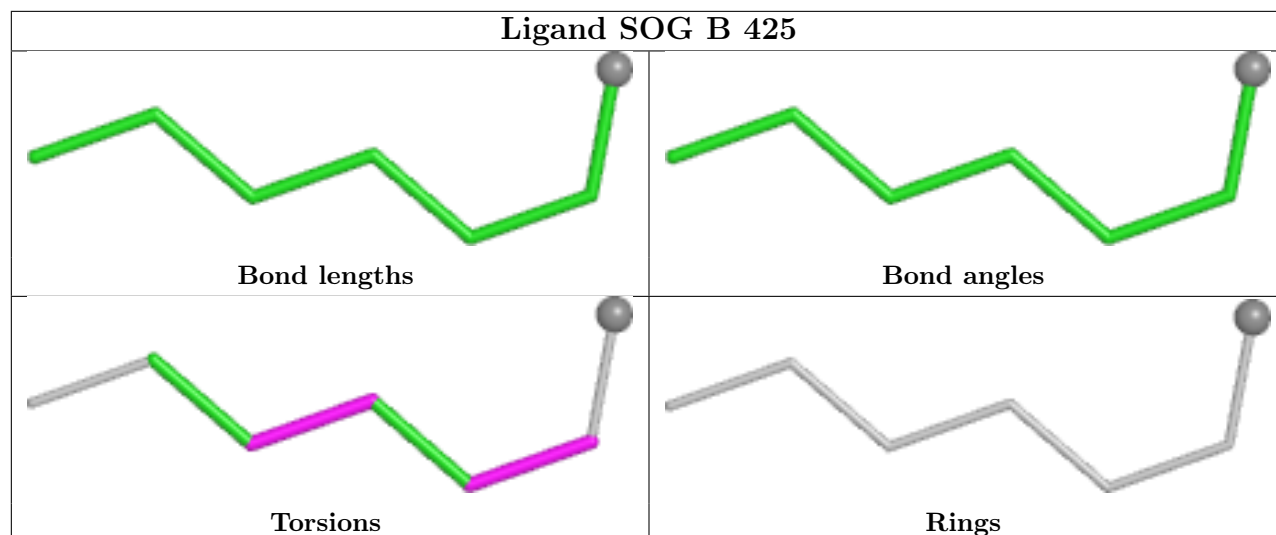


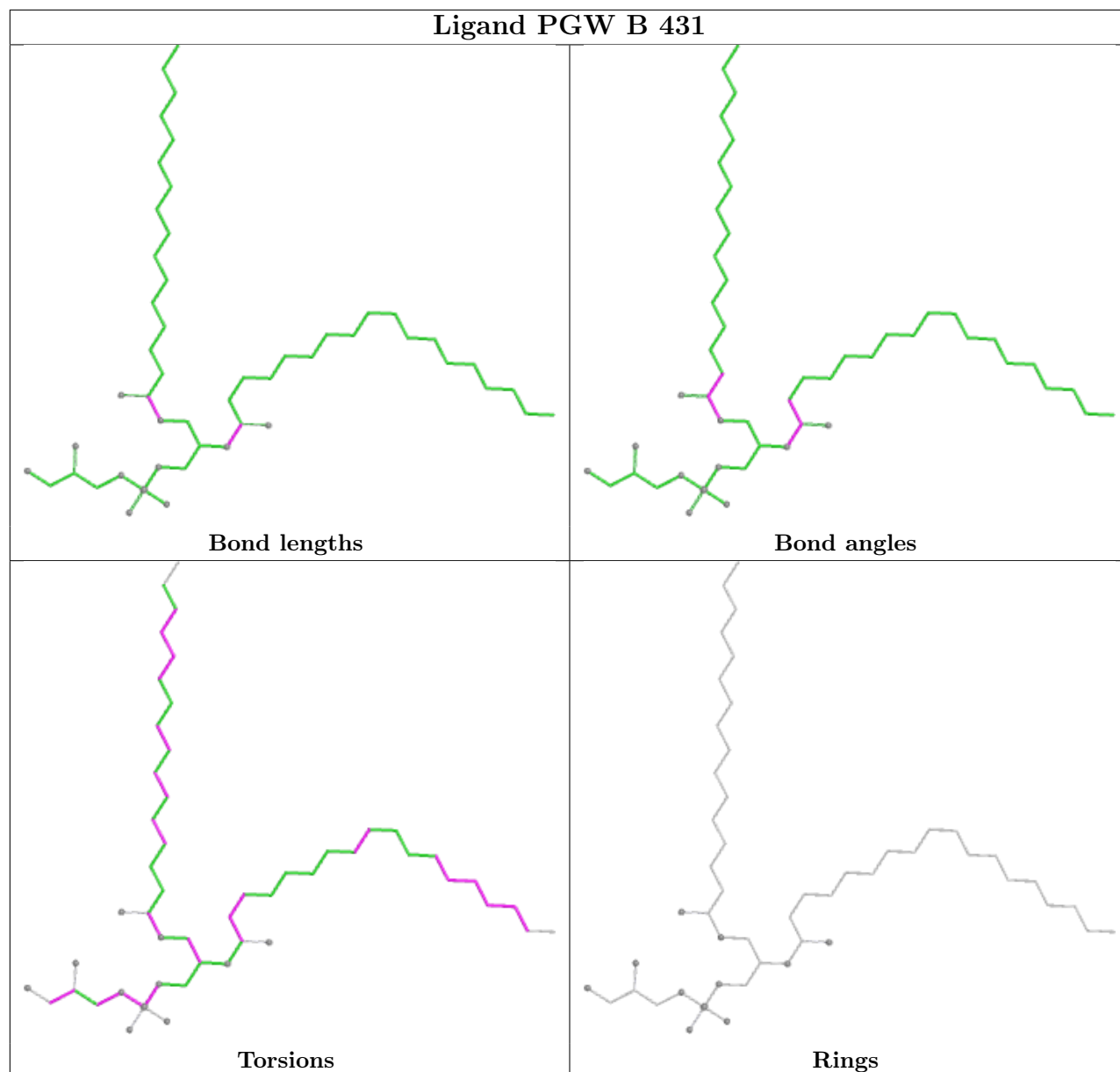


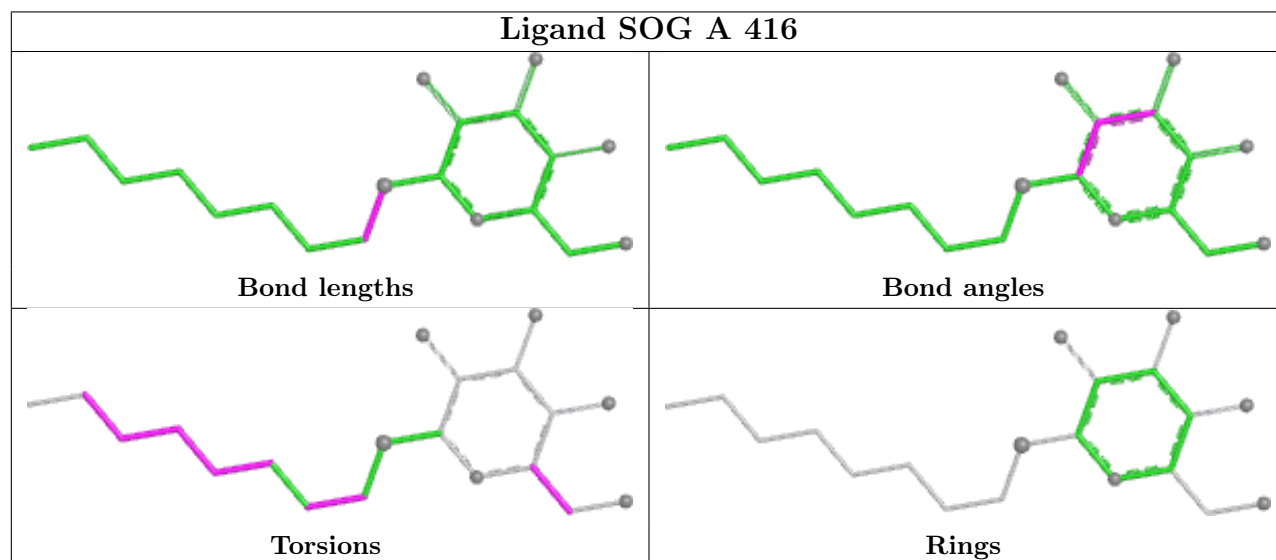
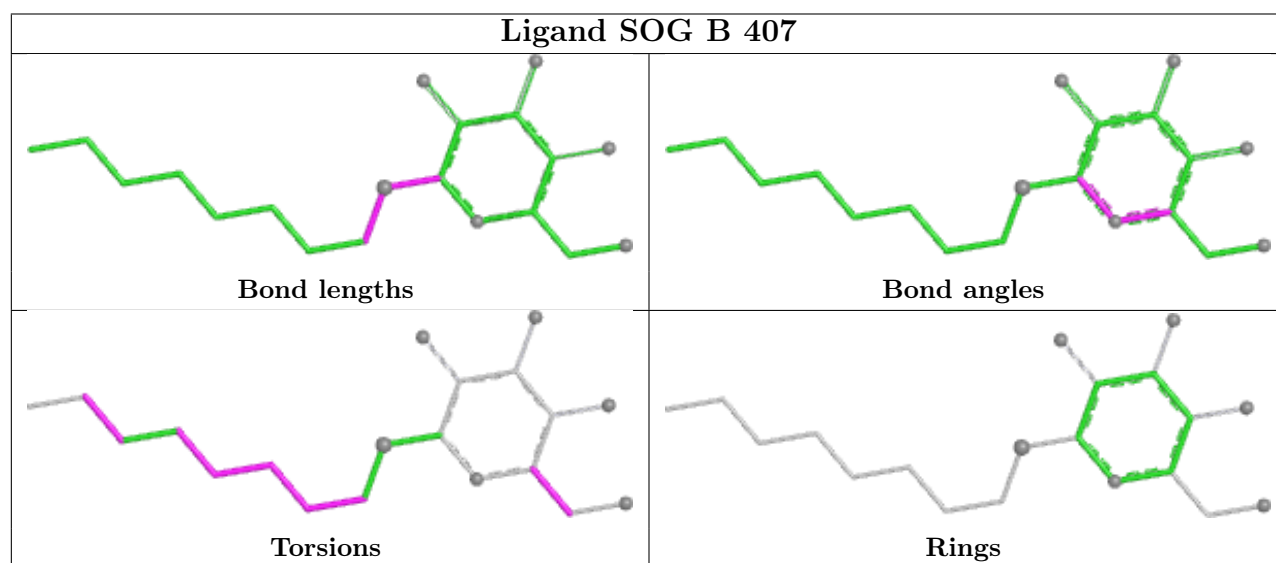
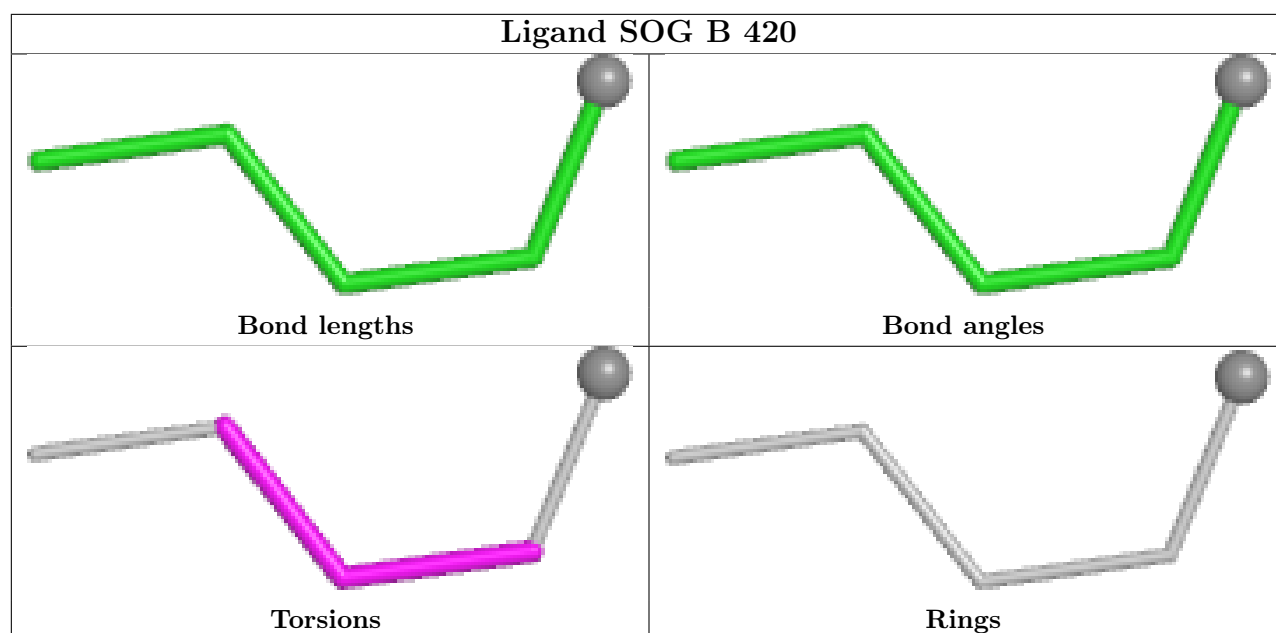


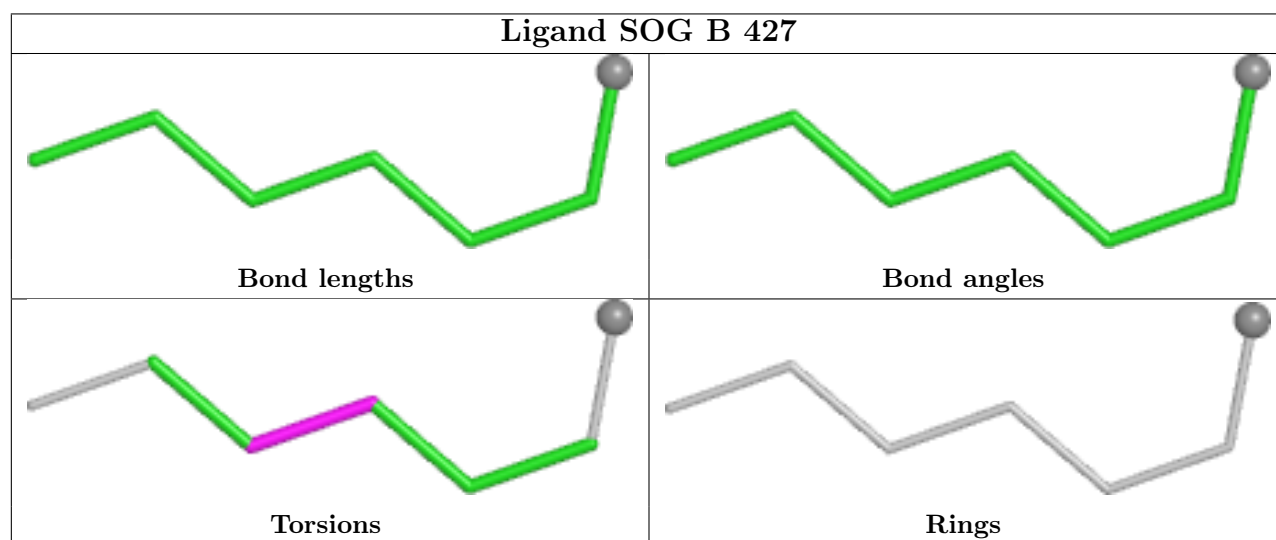
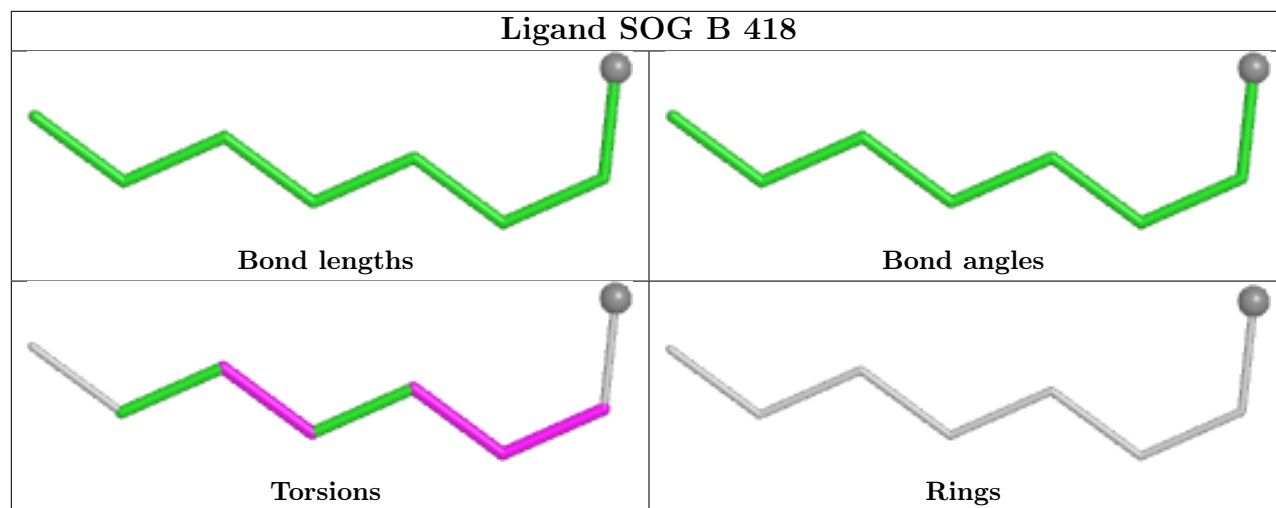




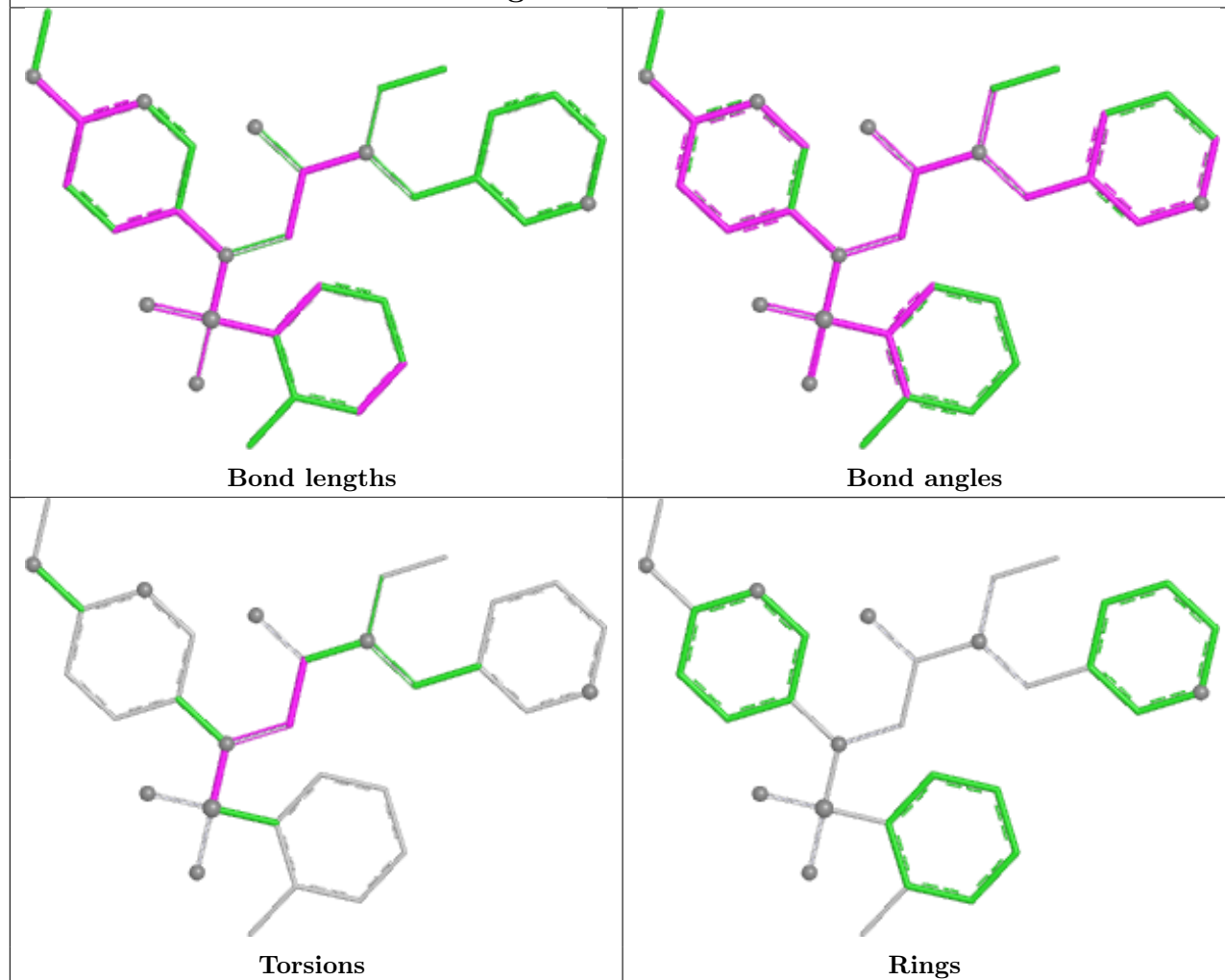




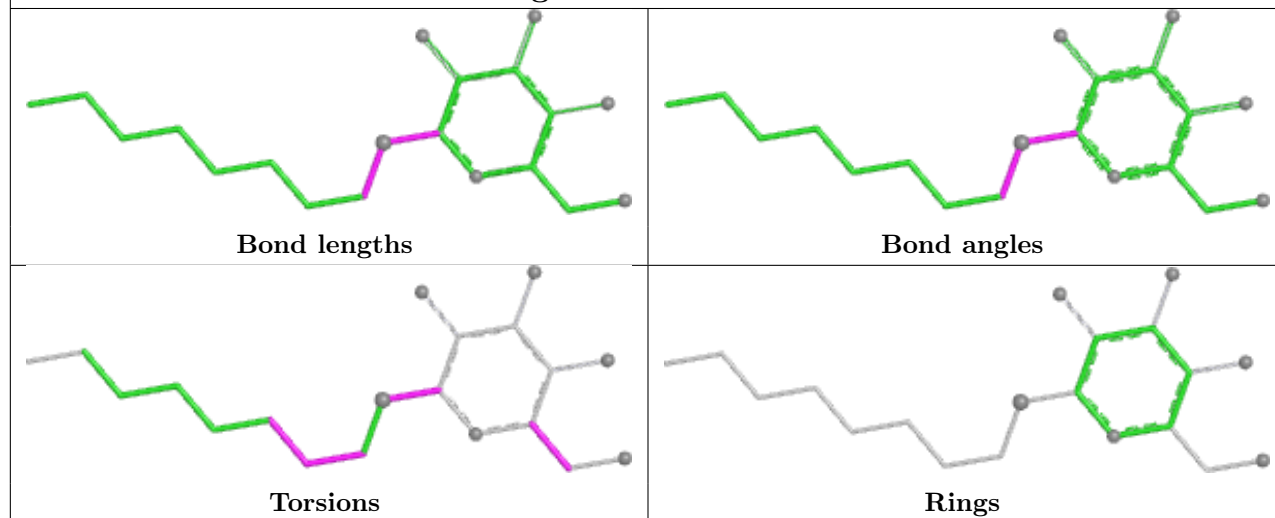


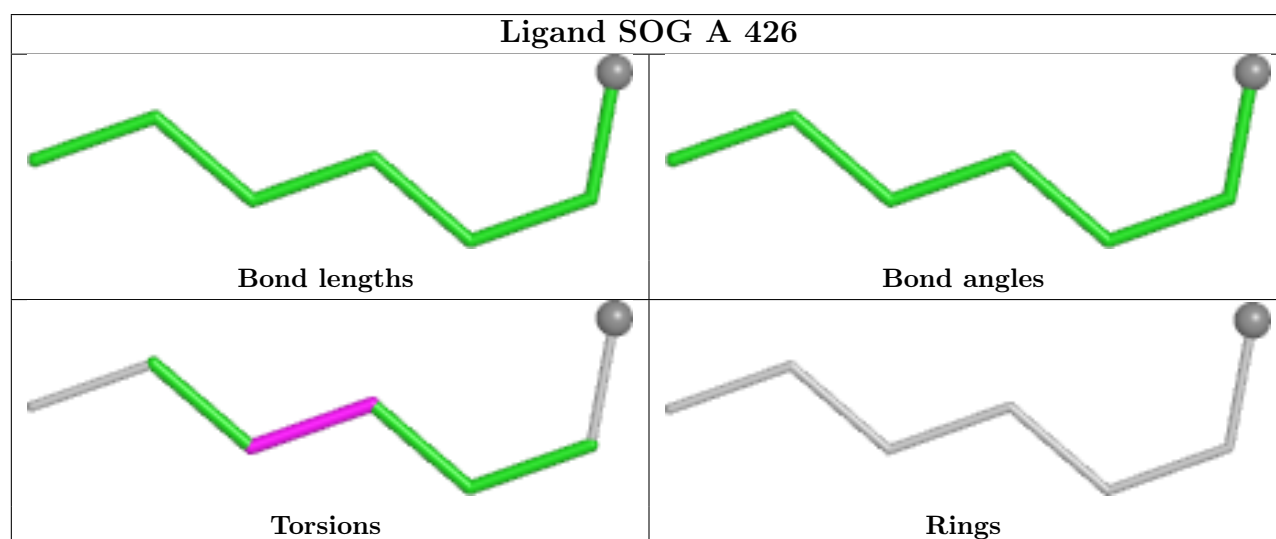
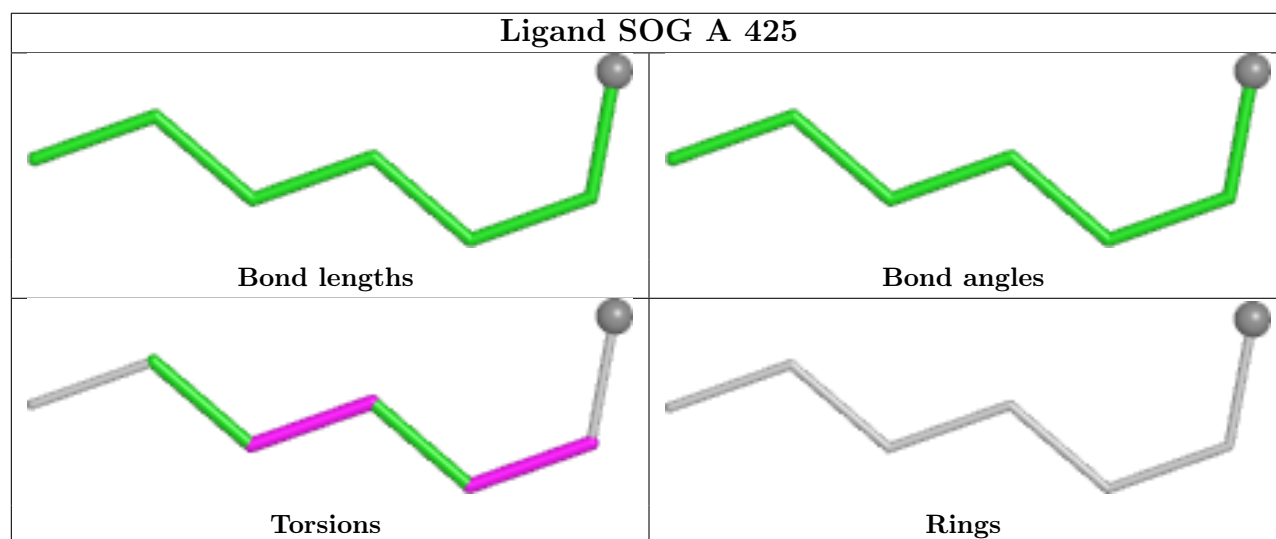
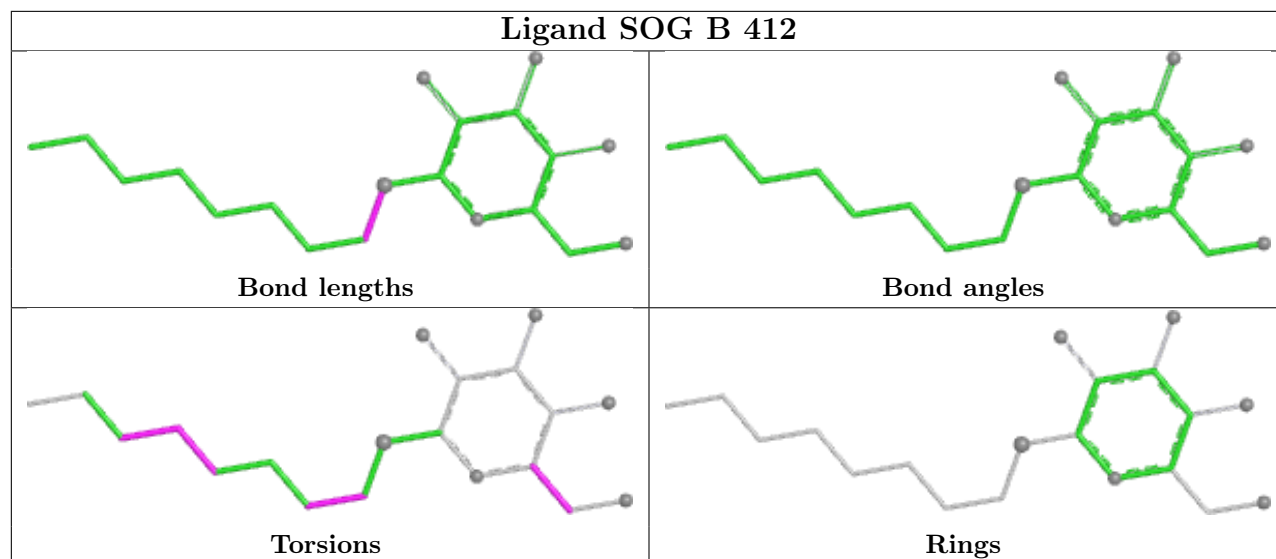


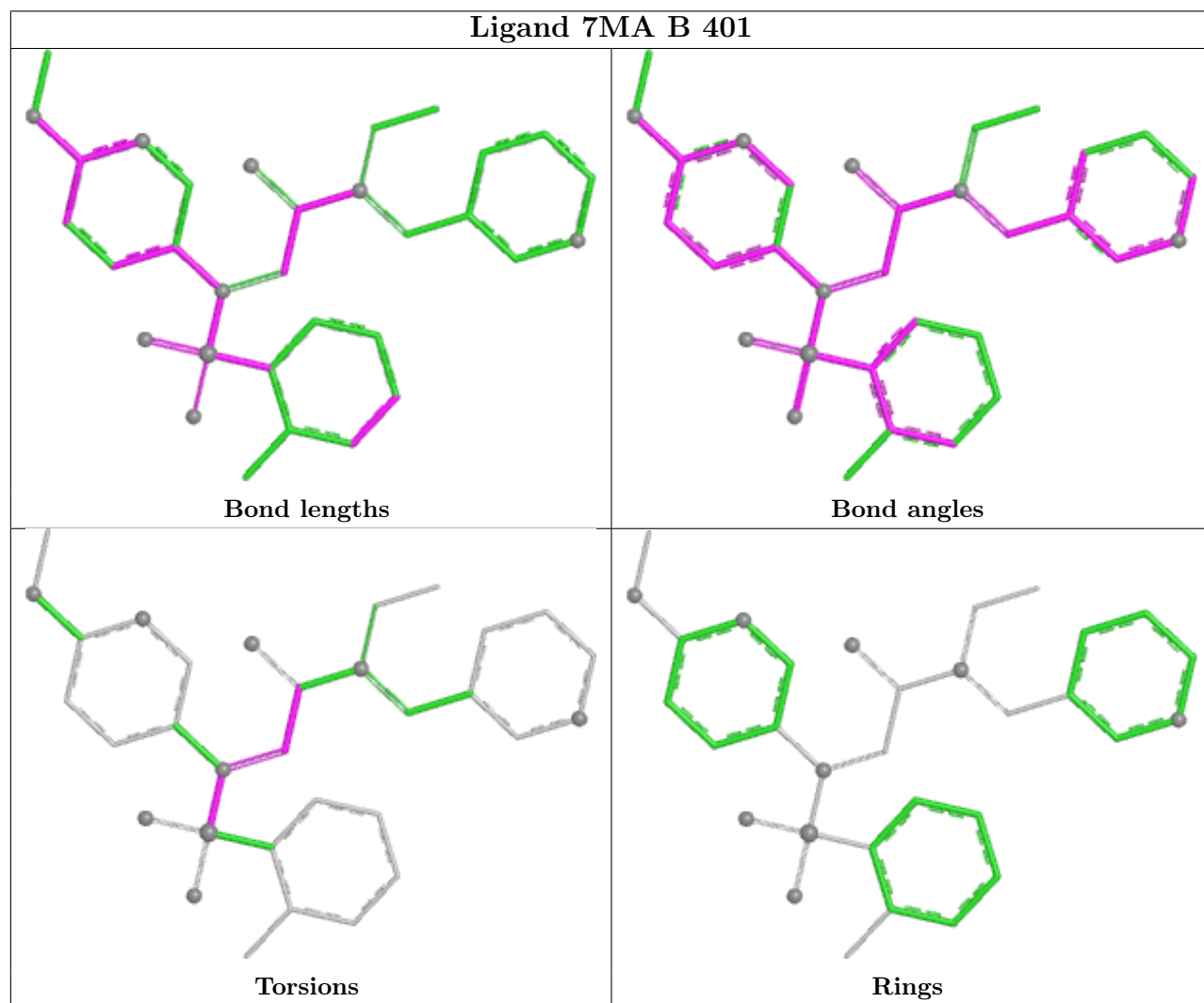
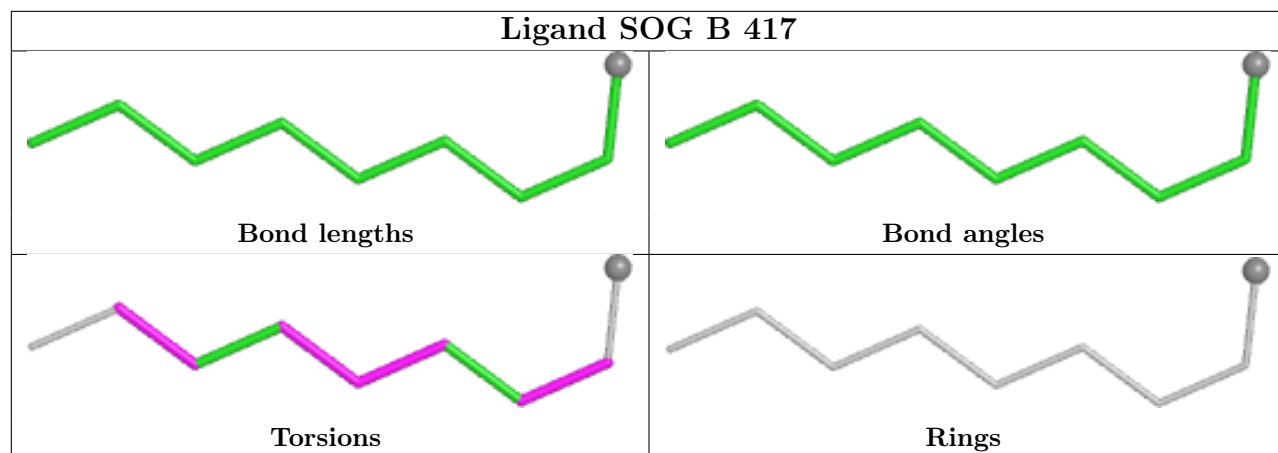
Ligand 7MA A 401

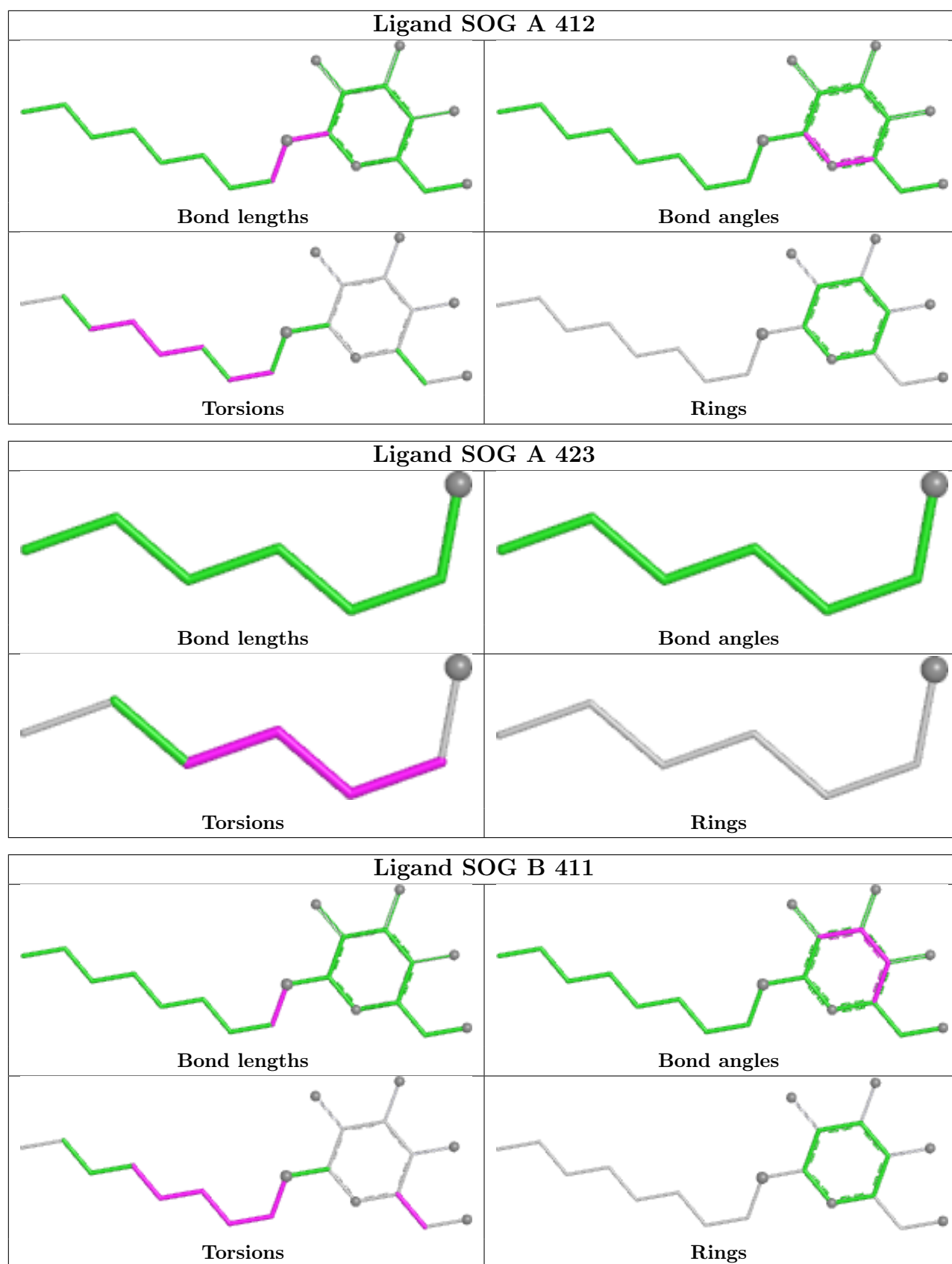


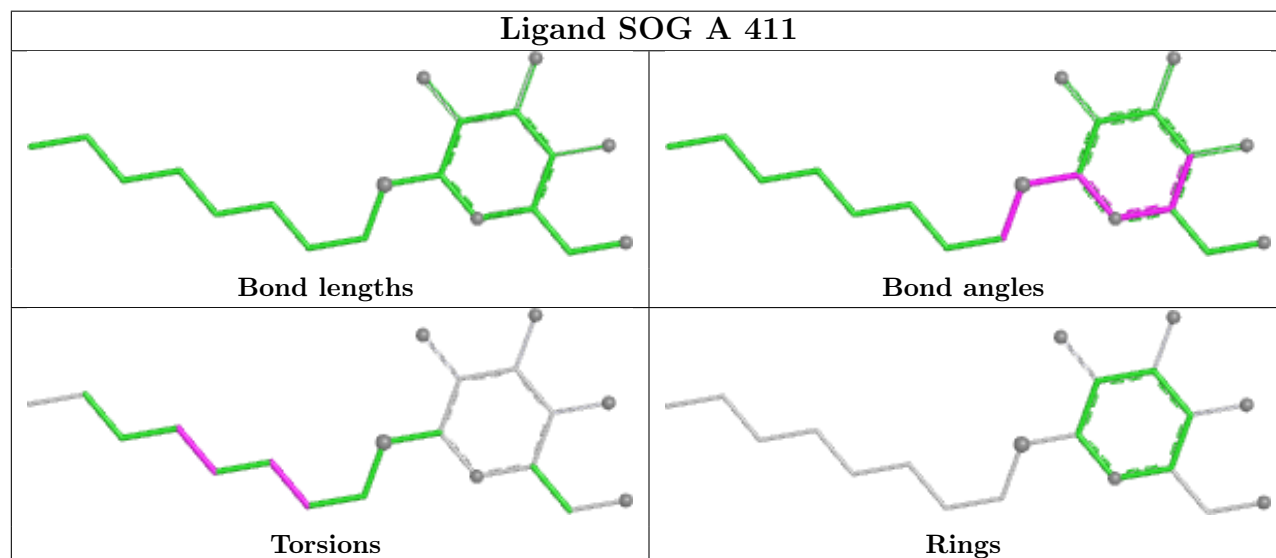
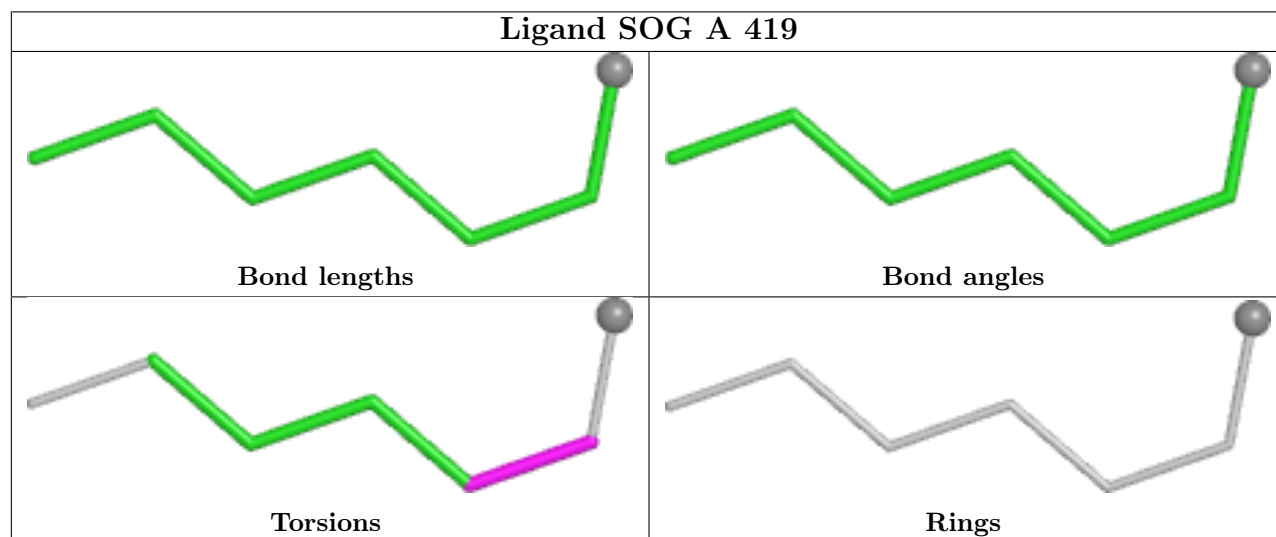
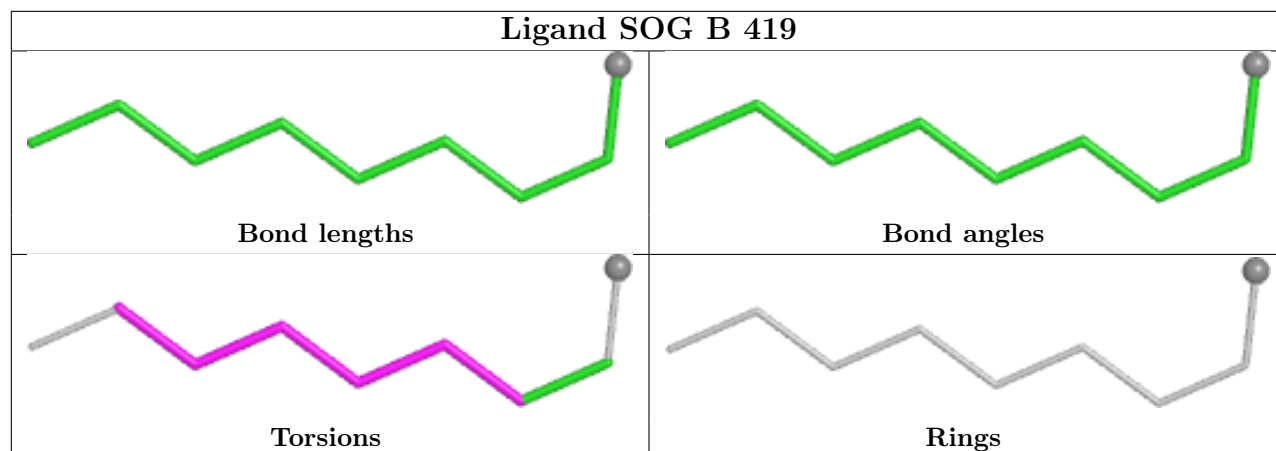
Ligand SOG B 406

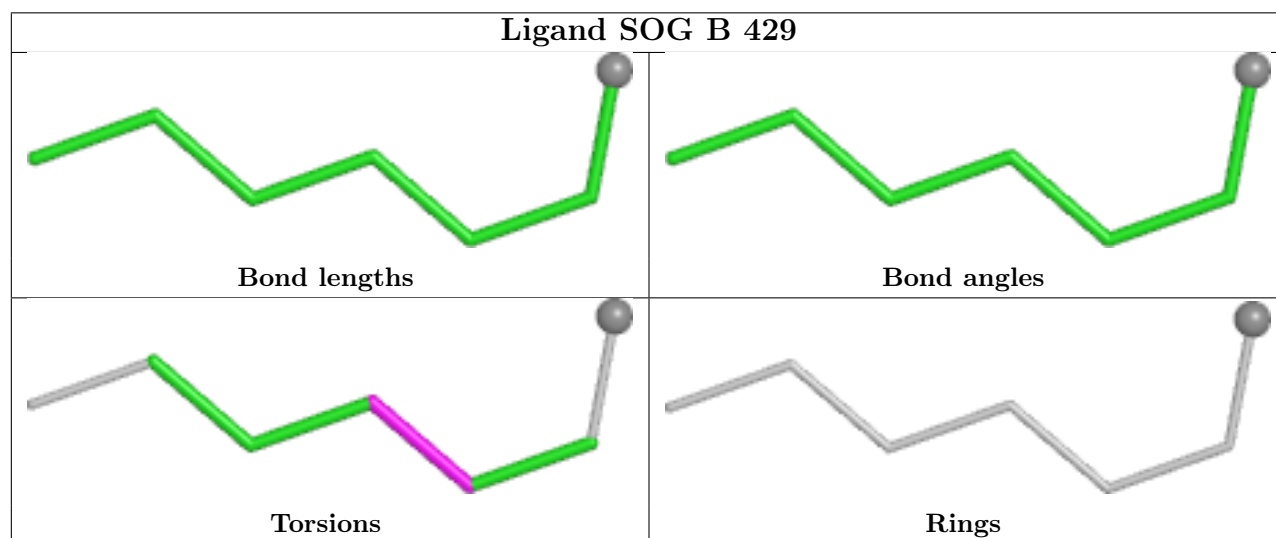
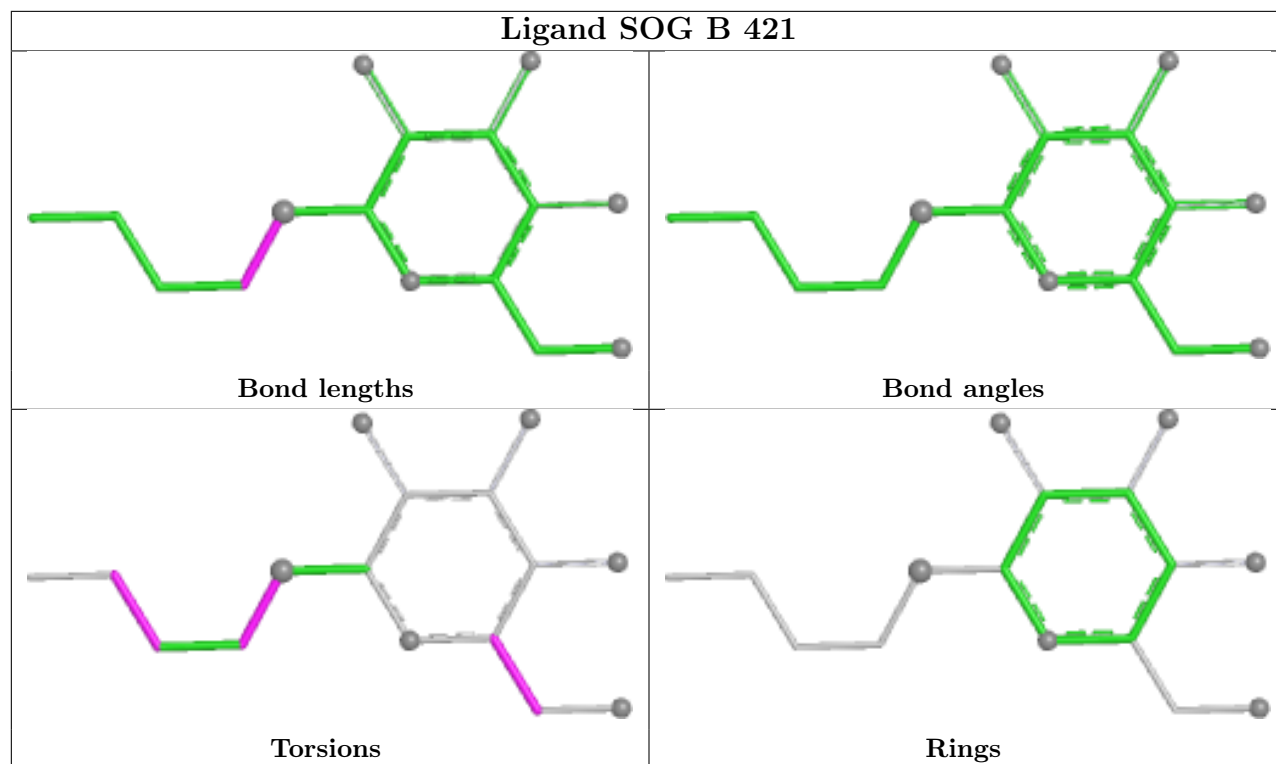


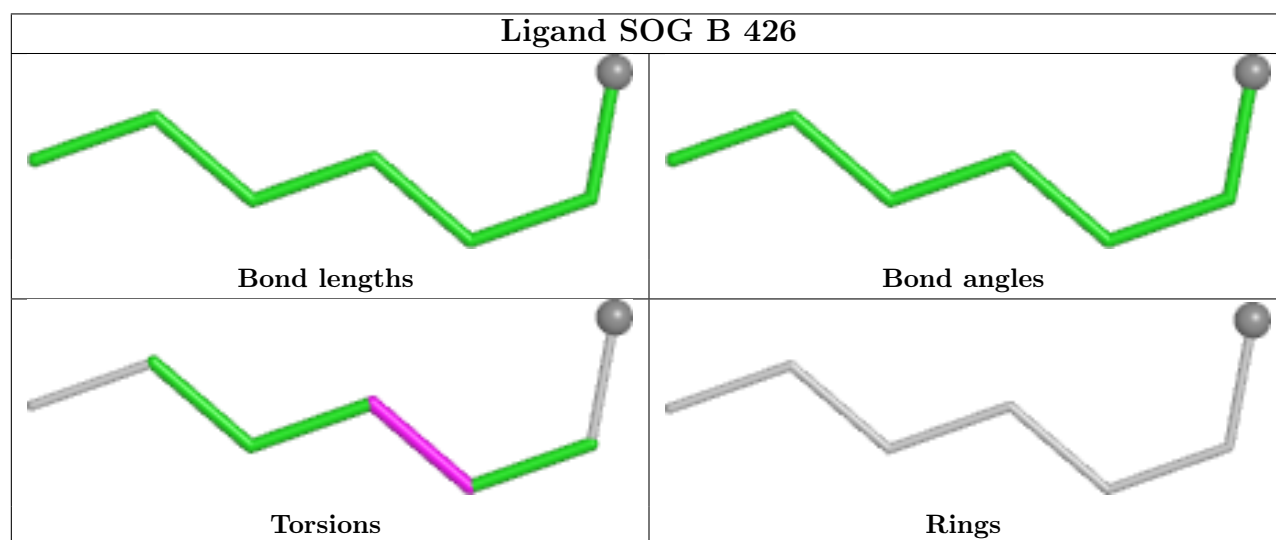
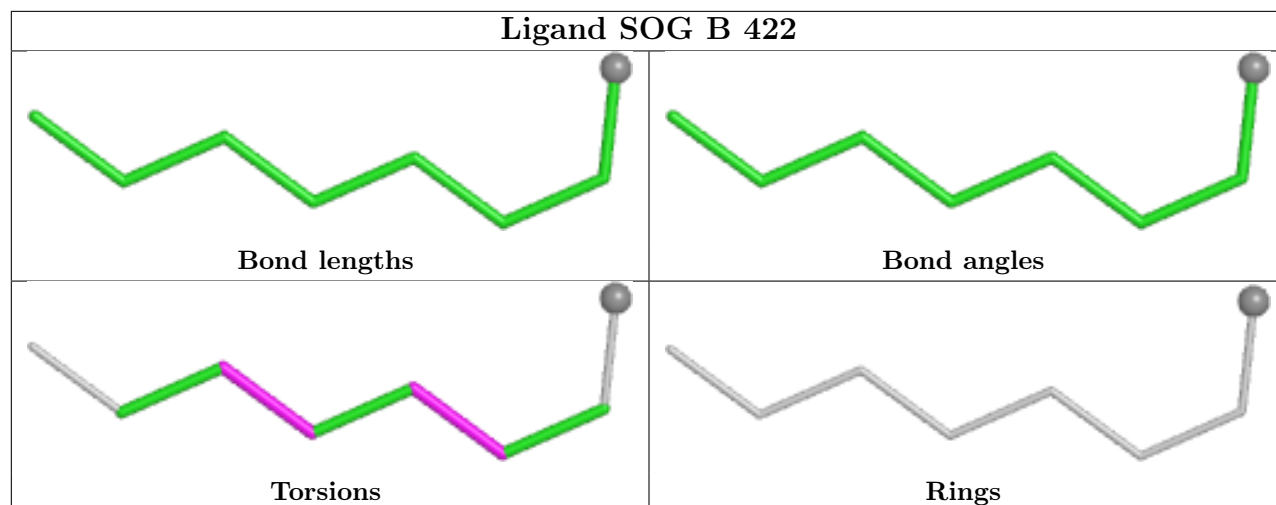


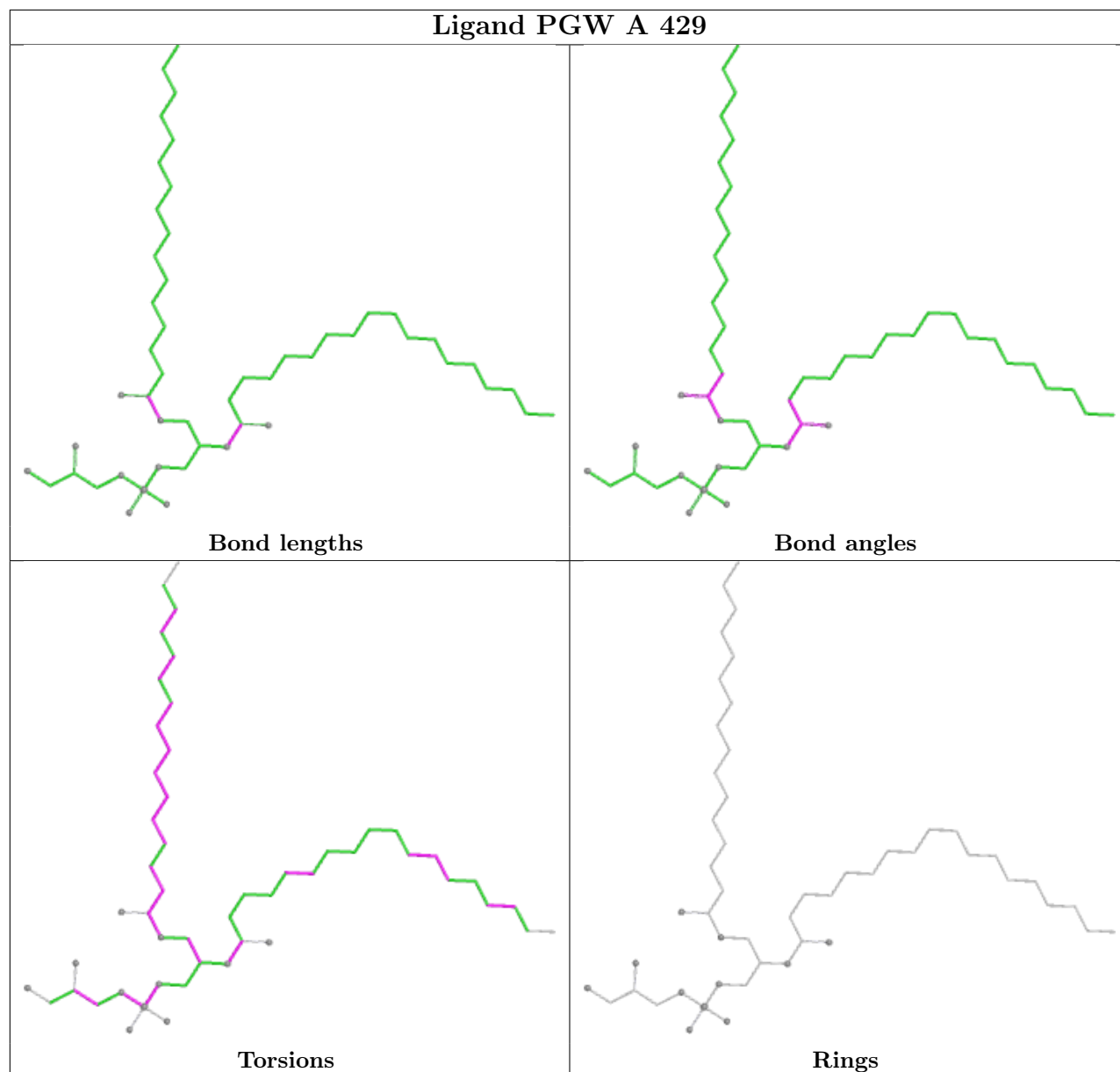


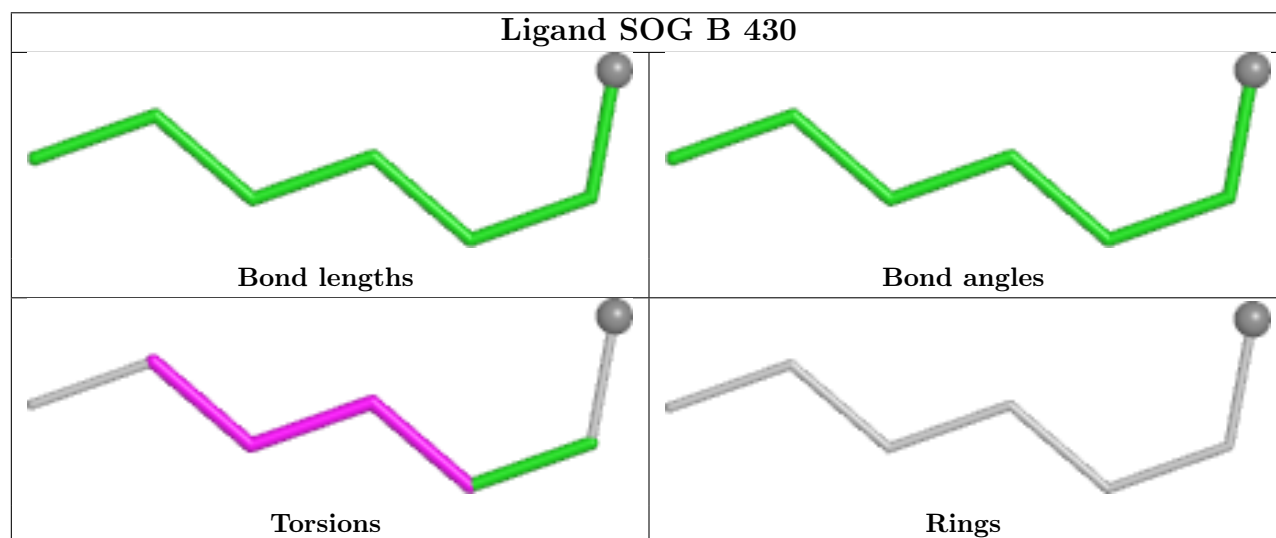
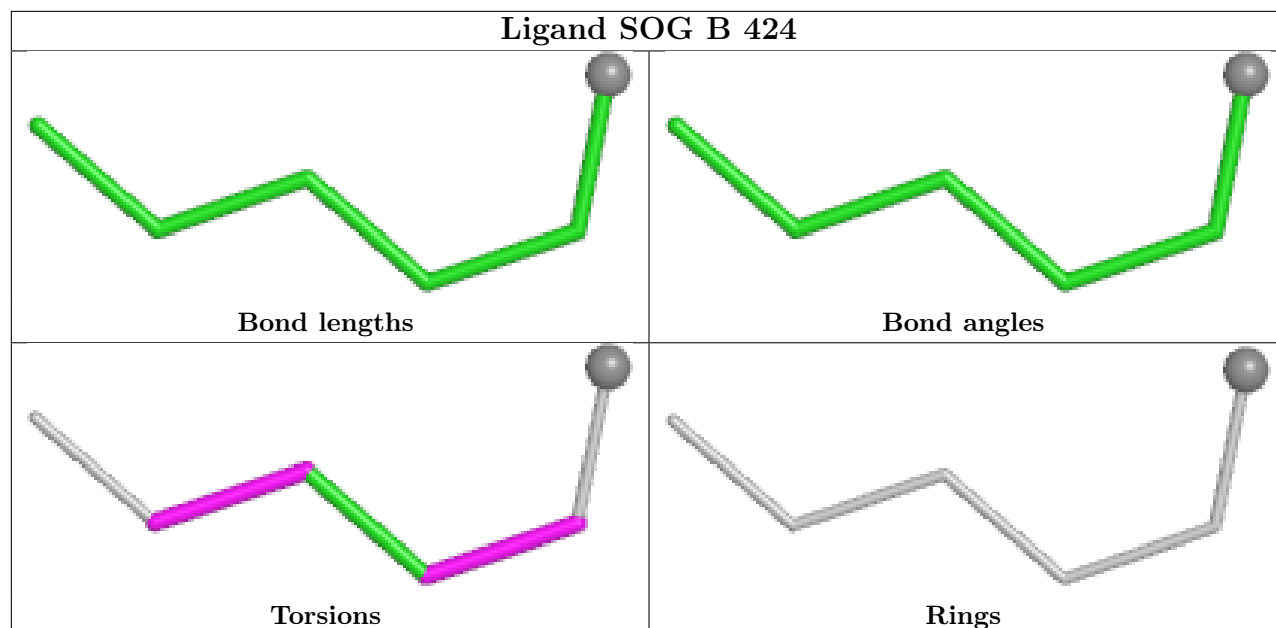


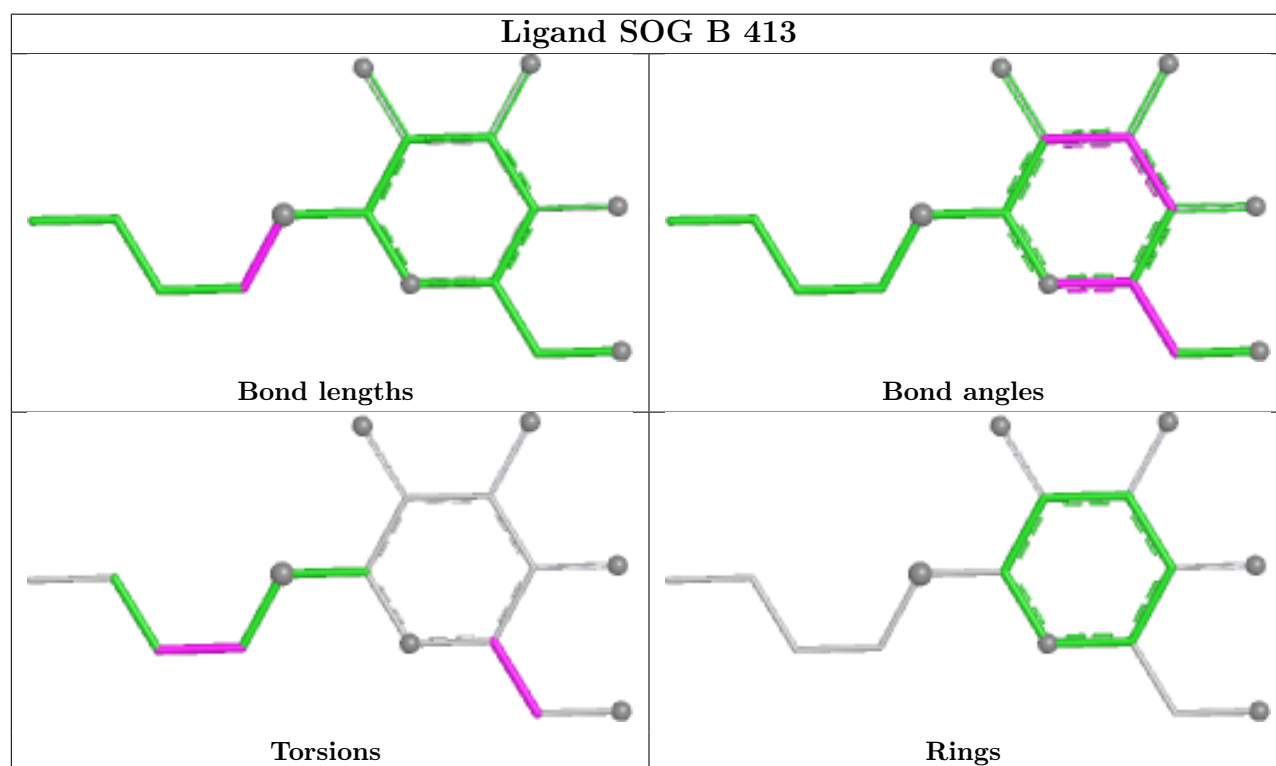
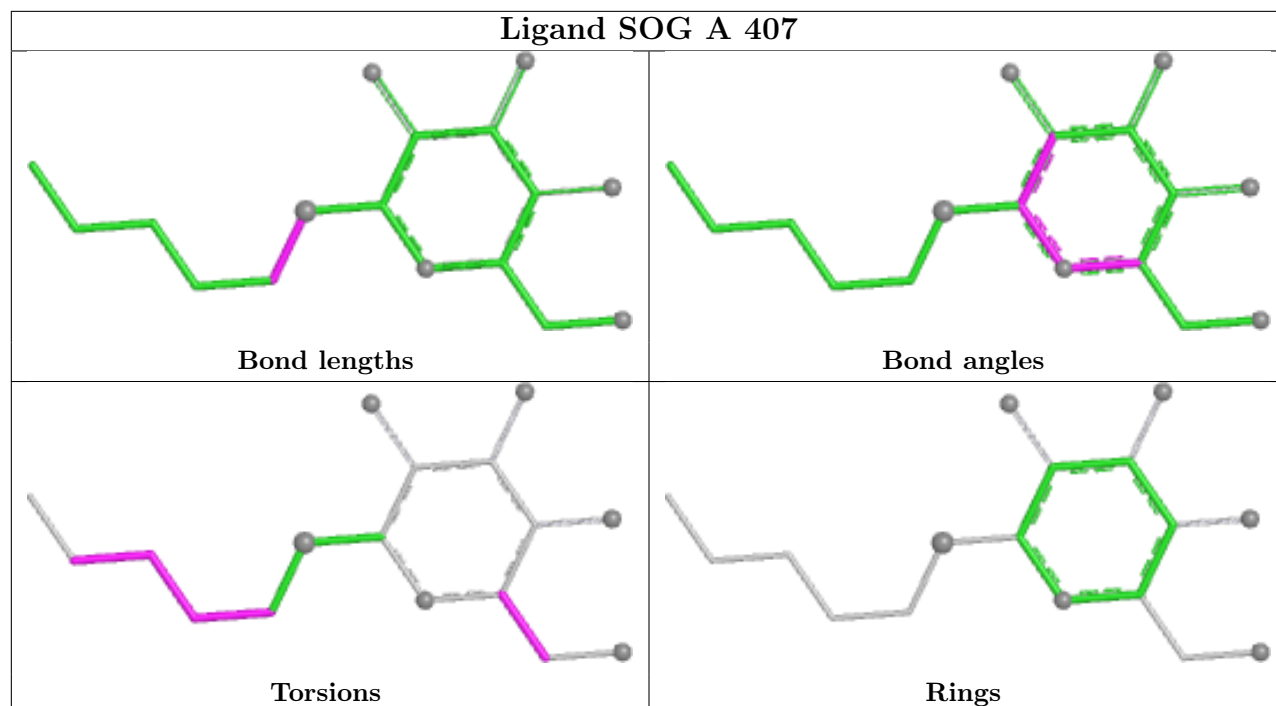


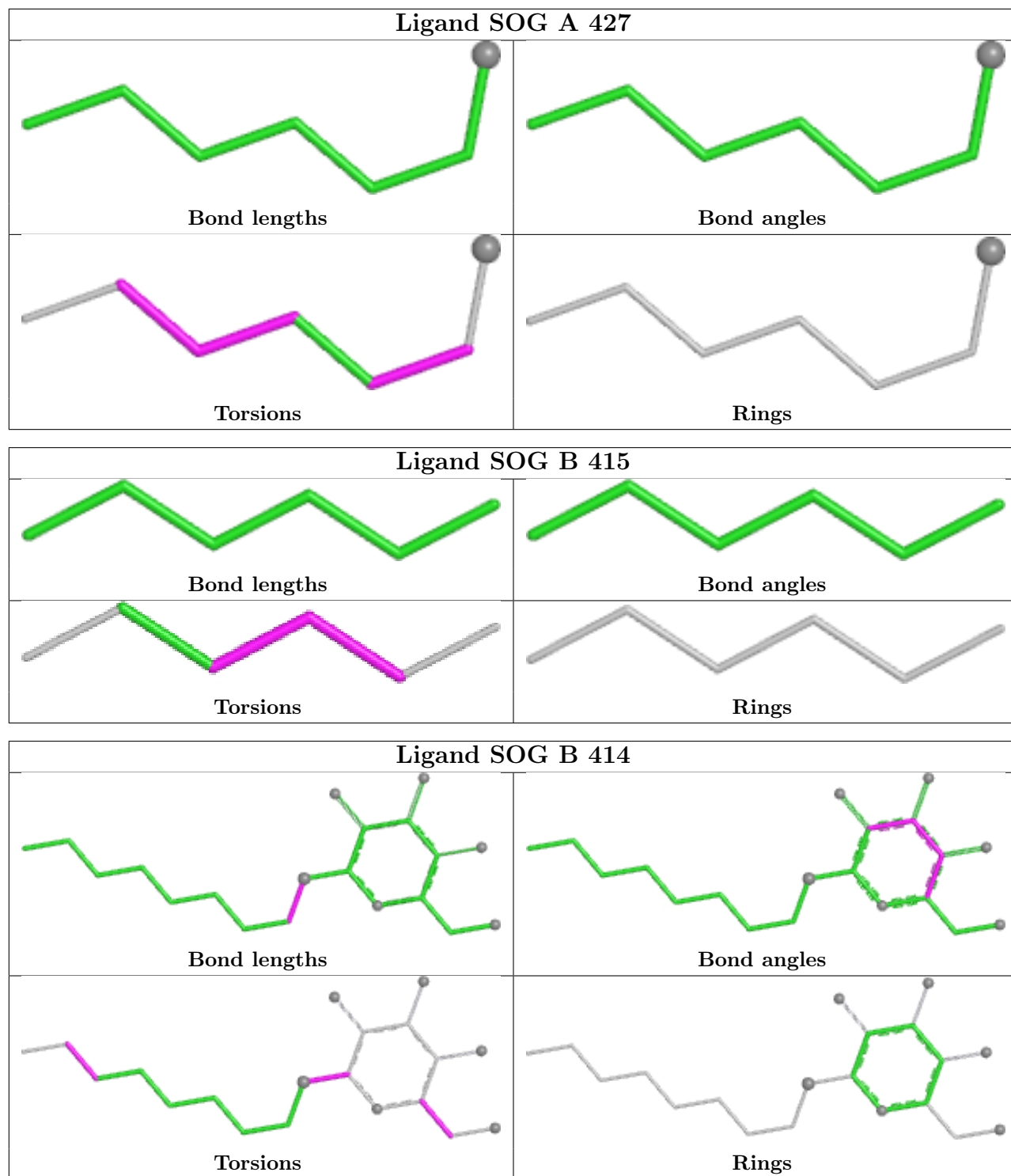


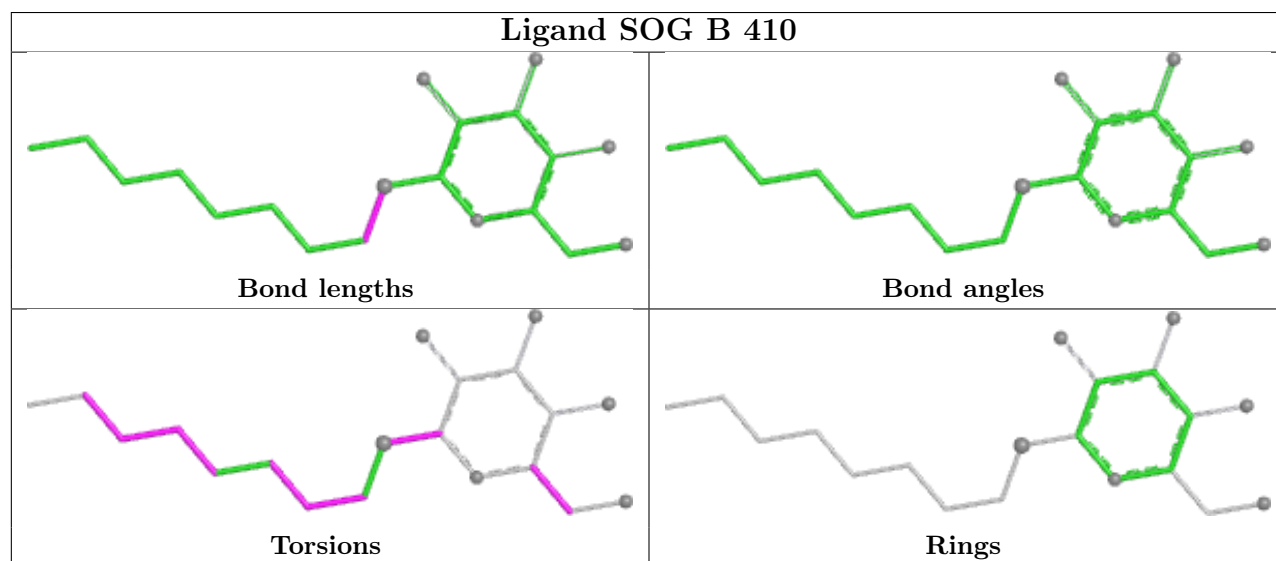
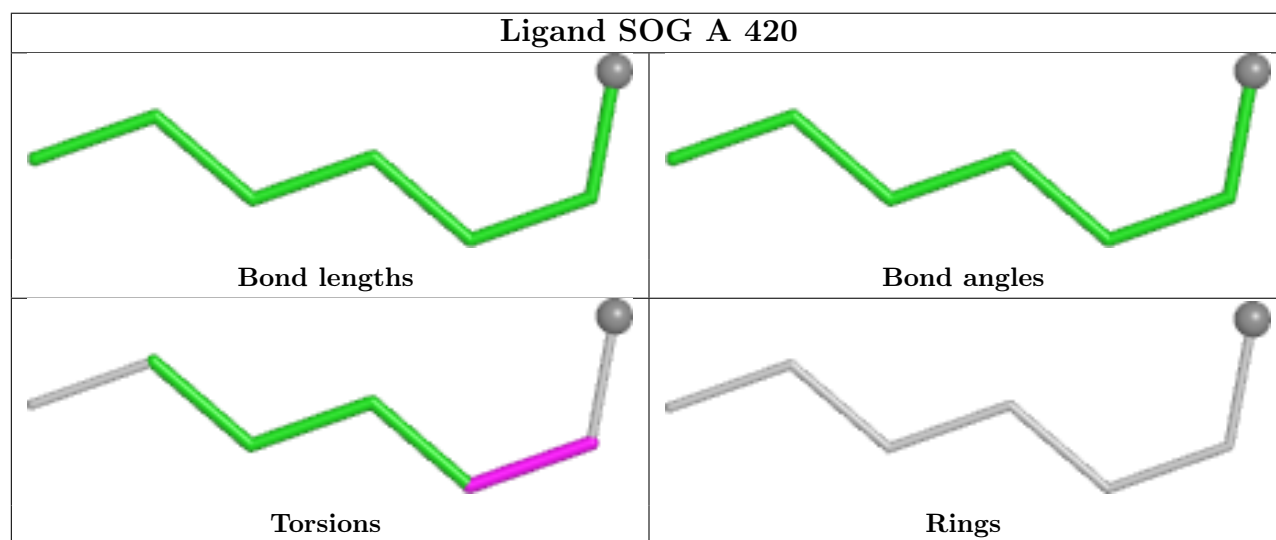
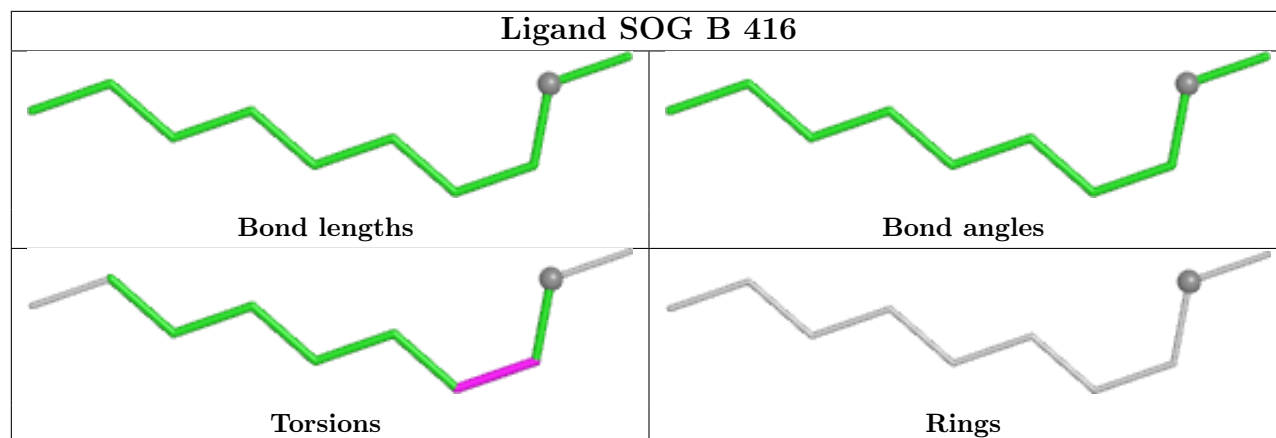


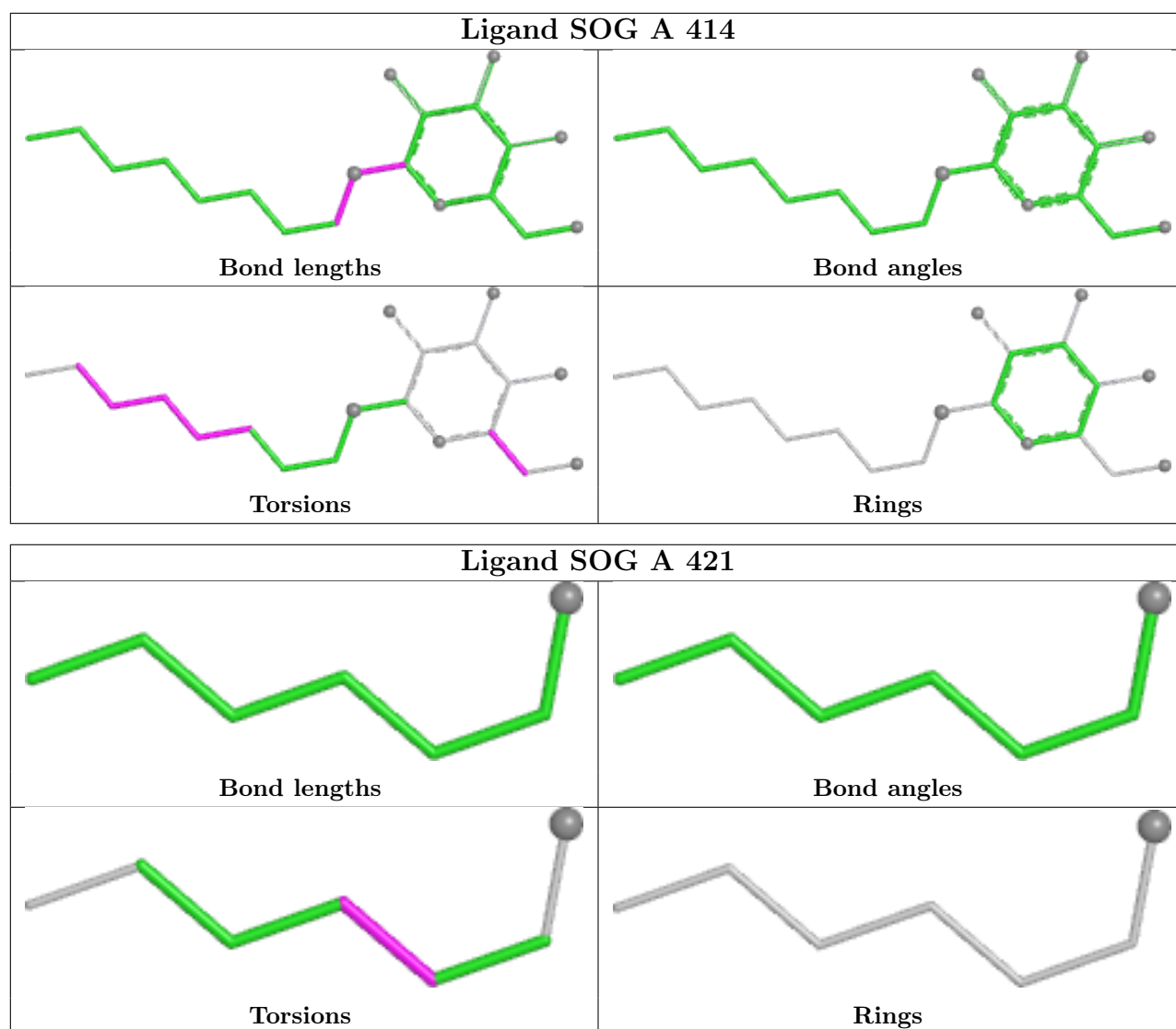












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/336 (89%)	0.57	37 (12%) 8 9	23, 38, 83, 114	0
1	B	311/336 (92%)	0.53	37 (11%) 9 9	22, 35, 78, 122	0
All	All	612/672 (91%)	0.55	74 (12%) 8 9	22, 36, 81, 122	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	THR	9.3
1	A	375	TRP	9.2
1	A	45	TYR	9.0
1	B	188	VAL	7.7
1	B	379	GLY	6.6
1	B	383	ALA	6.0
1	A	376	TRP	5.9
1	A	378	PRO	5.8
1	A	72	TRP	5.8
1	A	249	GLY	5.3
1	A	47	TRP	5.2
1	B	199	PHE	5.0
1	A	377	LEU	4.7
1	B	382	ALA	4.7
1	B	248	PRO	4.6
1	A	244	GLY	4.5
1	A	192	LEU	4.5
1	A	247	ILE	4.4
1	A	337	TYR	4.3
1	B	380	LEU	4.2
1	B	329	GLN	4.2
1	B	378	PRO	4.1
1	B	381	ALA	4.0
1	A	373	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	286	GLU	4.0
1	B	245	ARG	3.9
1	A	191	GLU	3.9
1	B	332	ASP	3.9
1	A	288	LYS	3.7
1	B	288	LYS	3.7
1	A	248	PRO	3.6
1	B	251	THR	3.6
1	B	253	ALA	3.6
1	A	246	GLN	3.5
1	A	250	THR	3.5
1	A	245	ARG	3.4
1	A	188	VAL	3.4
1	B	152	LEU	3.3
1	B	330	ALA	3.2
1	B	159	ARG	3.1
1	B	376	TRP	3.1
1	B	333	ARG	3.0
1	B	249	GLY	3.0
1	B	291	ARG	3.0
1	A	286	GLU	3.0
1	B	72	TRP	2.9
1	A	193	ALA	2.9
1	A	252	SER	2.9
1	A	189	LEU	2.8
1	B	29	ASP	2.8
1	B	32	LEU	2.8
1	B	375	TRP	2.8
1	A	291	ARG	2.6
1	A	46	ALA	2.6
1	A	152	LEU	2.6
1	A	333	ARG	2.6
1	B	377	LEU	2.5
1	A	364	LYS	2.4
1	B	331	SER	2.4
1	A	251	THR	2.4
1	B	290	MET	2.4
1	A	155	LYS	2.4
1	A	108	ILE	2.3
1	B	155	LYS	2.3
1	B	328	ARG	2.2
1	A	195	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	162	LEU	2.1
1	A	374	SER	2.1
1	B	34	TYR	2.1
1	A	75	HIS	2.1
1	A	290	MET	2.1
1	B	37	ARG	2.1
1	B	47	TRP	2.1
1	B	287	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SOG	B	413	16/20	0.34	0.42	106,115,117,117	0
6	SOG	B	422	8/20	0.49	0.53	91,92,95,98	0
6	SOG	B	424	6/20	0.52	0.44	72,76,81,84	0
6	SOG	B	421	16/20	0.59	0.34	121,124,125,126	0
6	SOG	A	415	14/20	0.61	0.32	99,104,106,106	0
6	SOG	B	417	9/20	0.64	0.37	96,99,103,104	0
6	SOG	B	410	20/20	0.65	0.28	100,108,112,113	0
6	SOG	B	427	7/20	0.68	0.35	93,95,101,103	0
6	SOG	B	409	20/20	0.69	0.27	70,99,102,103	0
6	SOG	A	423	7/20	0.70	0.34	78,79,82,84	0
6	SOG	A	407	17/20	0.70	0.31	76,84,88,89	17
6	SOG	A	416	20/20	0.70	0.27	82,98,102,103	0
6	SOG	B	426	7/20	0.71	0.30	76,80,90,93	0
6	SOG	A	426	7/20	0.72	0.33	93,93,97,98	0
6	SOG	A	414	20/20	0.74	0.26	47,65,69,72	20

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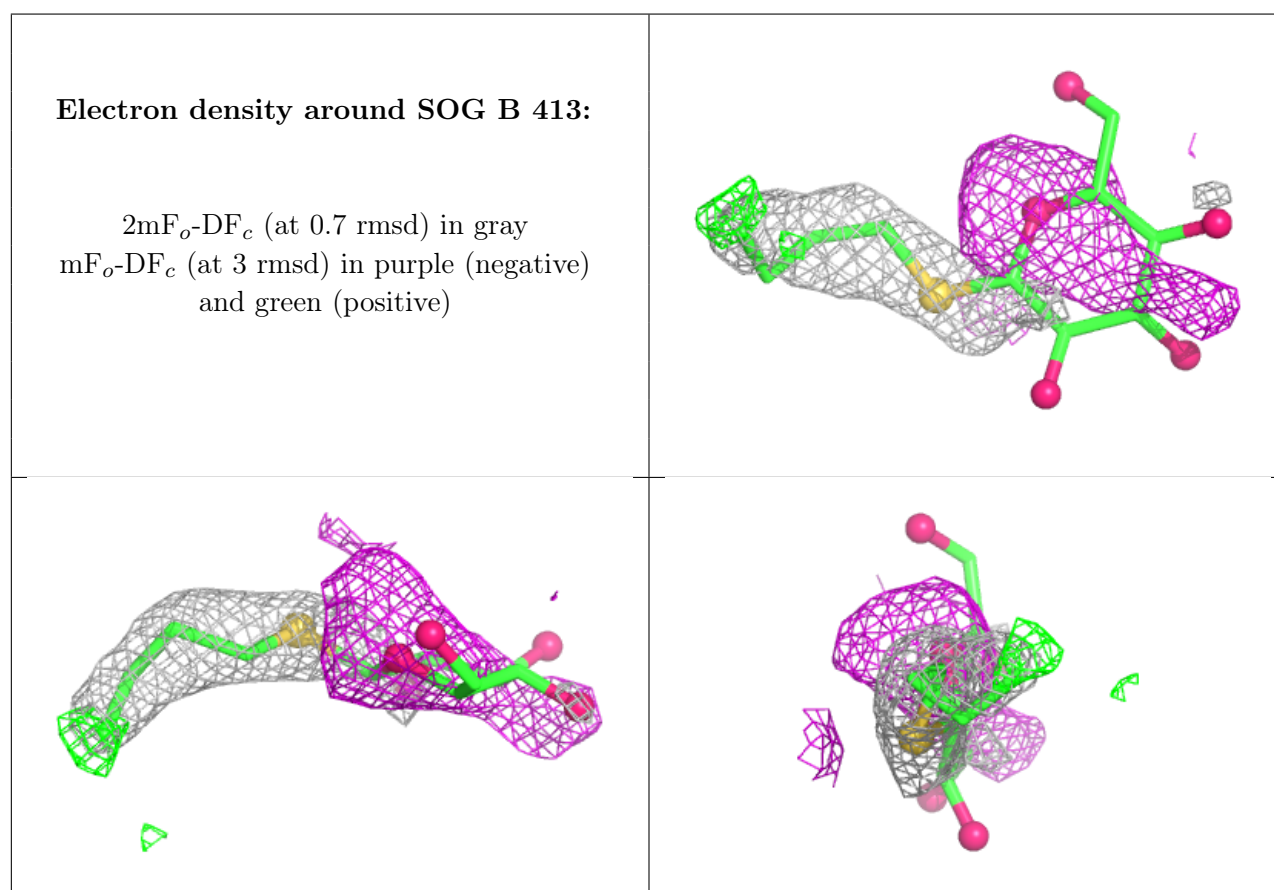
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SOG	B	416	10/20	0.74	0.32	79,84,94,94	0
6	SOG	A	421	7/20	0.74	0.32	83,83,91,95	0
6	SOG	A	412	20/20	0.74	0.23	71,84,86,88	0
6	SOG	A	418	20/20	0.75	0.26	94,110,112,112	0
6	SOG	A	424	7/20	0.76	0.37	91,91,96,99	0
6	SOG	A	410	20/20	0.76	0.20	49,90,98,100	0
6	SOG	A	425	7/20	0.77	0.34	85,86,90,91	0
6	SOG	A	413	20/20	0.77	0.22	31,71,77,79	0
4	PG4	A	405	13/13	0.77	0.23	78,80,83,83	0
6	SOG	B	414	20/20	0.78	0.24	74,99,104,105	0
6	SOG	B	429	7/20	0.78	0.24	54,64,86,92	0
6	SOG	A	419	7/20	0.79	0.27	87,92,103,106	0
6	SOG	B	430	7/20	0.79	0.27	67,68,77,83	0
6	SOG	A	417	20/20	0.80	0.26	85,110,111,111	0
6	SOG	B	428	7/20	0.80	0.30	84,86,96,99	0
6	SOG	B	425	7/20	0.81	0.29	71,72,85,87	0
6	SOG	A	422	7/20	0.81	0.27	66,70,82,86	0
6	SOG	B	419	9/20	0.82	0.23	64,65,68,70	0
3	SO4	B	402	5/5	0.82	0.20	103,105,106,107	0
6	SOG	B	412	20/20	0.82	0.18	63,89,93,95	0
6	SOG	A	409	20/20	0.82	0.20	53,88,91,92	0
6	SOG	B	418	8/20	0.82	0.27	74,76,79,81	0
6	SOG	A	411	20/20	0.83	0.15	34,67,73,77	0
3	SO4	A	402	5/5	0.84	0.16	92,94,95,98	0
6	SOG	A	427	7/20	0.84	0.28	93,94,99,101	0
2	7MA	A	401	32/32	0.85	0.17	31,37,46,60	58
6	SOG	A	420	7/20	0.85	0.22	64,67,81,86	0
6	SOG	B	420	5/20	0.85	0.26	76,77,77,79	0
2	7MA	B	401	32/32	0.86	0.15	32,37,48,62	26
4	PG4	A	404	13/13	0.86	0.20	68,73,75,76	0
6	SOG	B	423	9/20	0.86	0.27	73,77,85,89	0
6	SOG	A	408	16/20	0.86	0.23	119,122,122,123	0
6	SOG	B	411	20/20	0.86	0.16	33,73,82,83	0
3	SO4	B	403	5/5	0.87	0.14	84,84,86,89	0
4	PG4	B	405	13/13	0.87	0.18	64,66,70,70	0
7	PGW	A	429	51/51	0.87	0.16	25,47,99,101	0
7	PGW	B	431	51/51	0.87	0.16	31,43,102,103	0
6	SOG	A	428	7/20	0.88	0.20	65,67,75,77	0
5	CIT	A	406	13/13	0.88	0.14	46,49,56,60	0
6	SOG	B	415	6/20	0.90	0.25	65,67,71,74	0
4	PG4	B	404	13/13	0.90	0.15	48,52,60,63	0
8	NA	B	432	1/1	0.90	0.15	45,45,45,45	0

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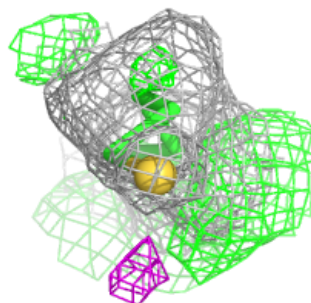
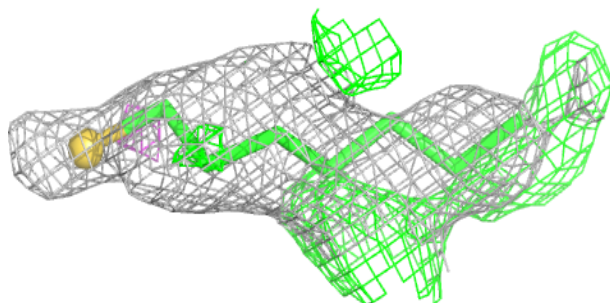
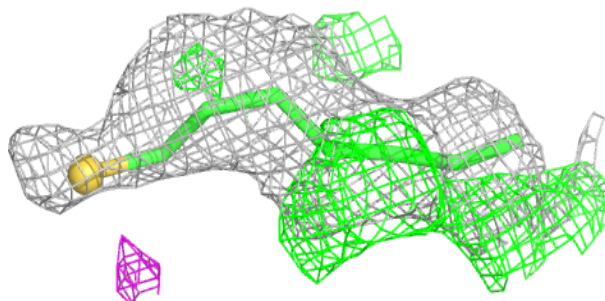
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SOG	B	406	20/20	0.91	0.11	30,47,52,55	0
6	SOG	B	408	20/20	0.91	0.18	67,74,76,77	0
4	PG4	A	403	13/13	0.91	0.13	49,53,60,60	0
6	SOG	B	407	20/20	0.94	0.13	42,47,67,68	0
8	NA	A	430	1/1	0.95	0.09	52,52,52,52	0

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.

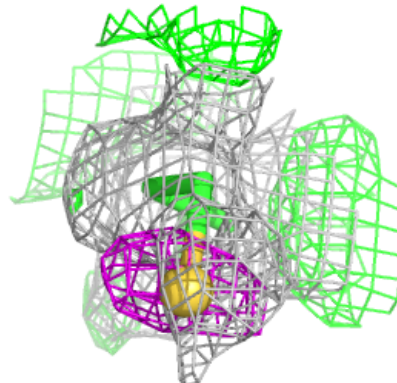
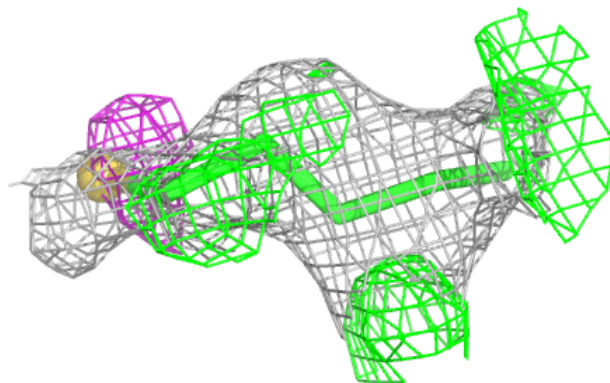
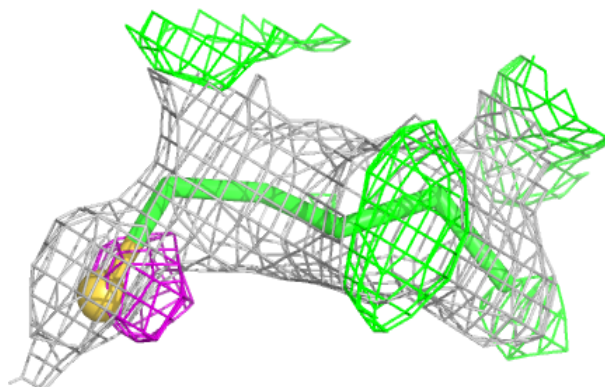


Electron density around SOG B 422:

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

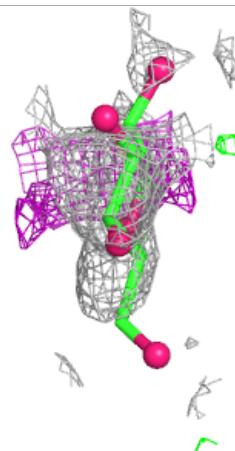
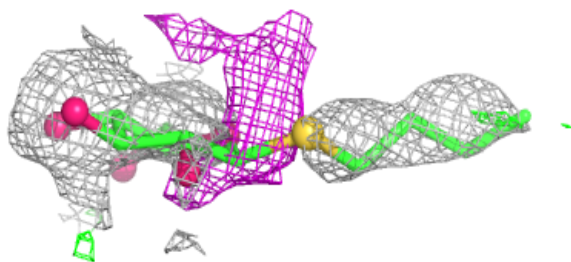
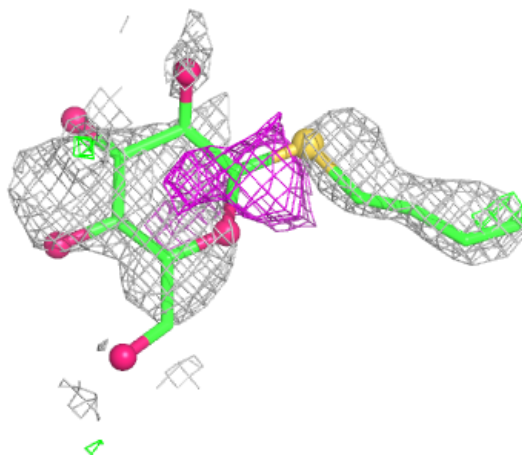
**Electron density around SOG B 424:**

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



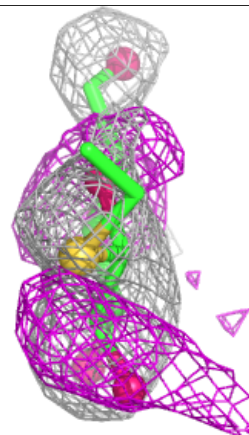
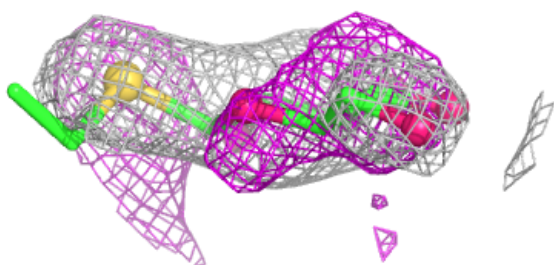
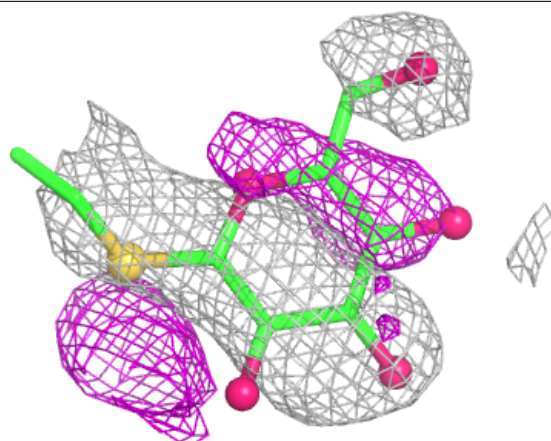
Electron density around SOG B 421:

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



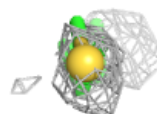
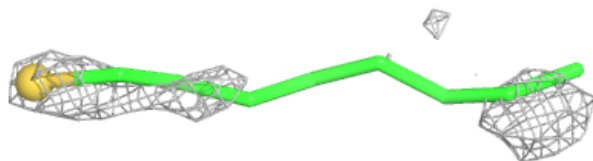
Electron density around SOG A 415:

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

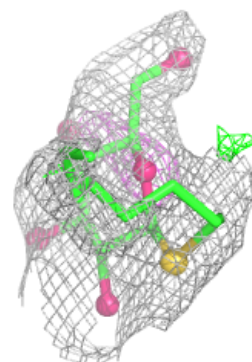
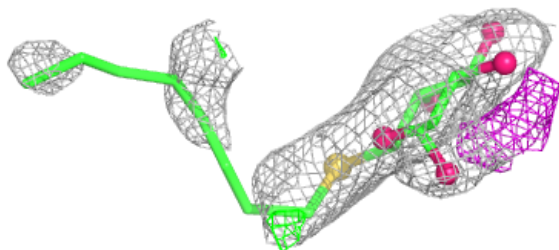
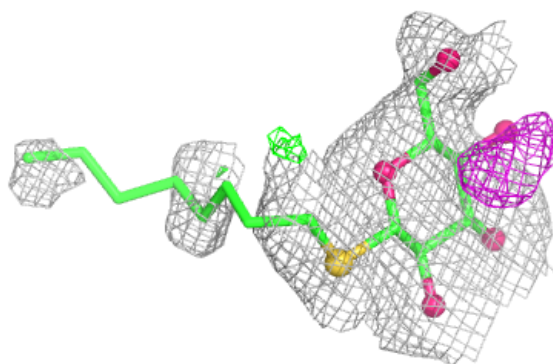


Electron density around SOG B 417:

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

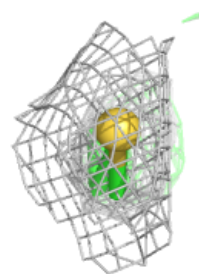
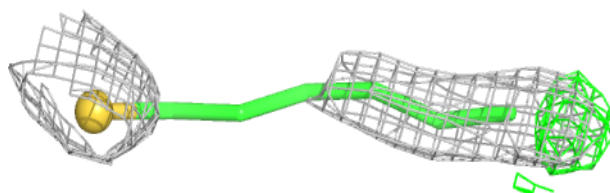
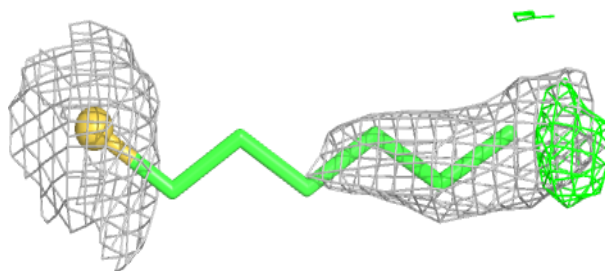
**Electron density around SOG B 410:**

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

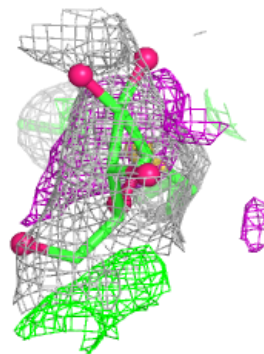
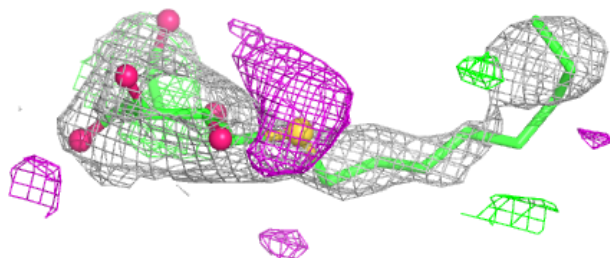
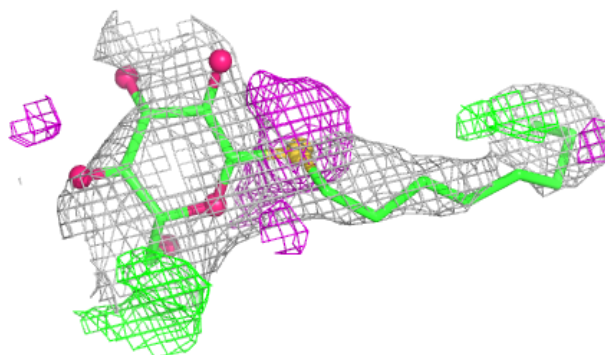


Electron density around SOG B 427:

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

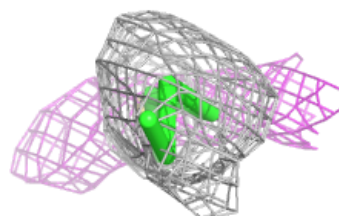
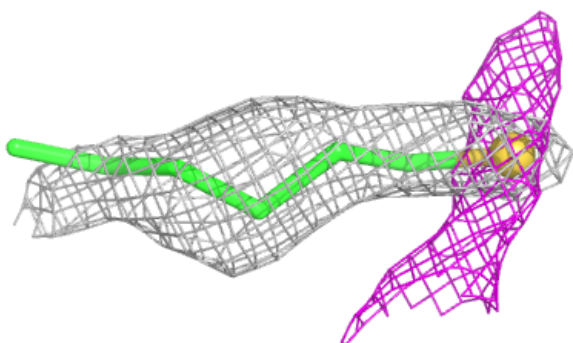
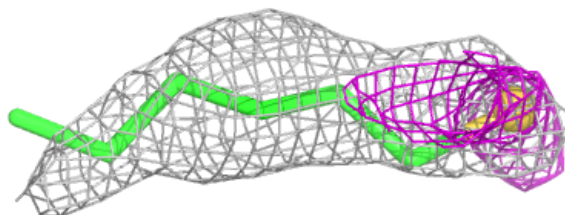
**Electron density around SOG B 409:**

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

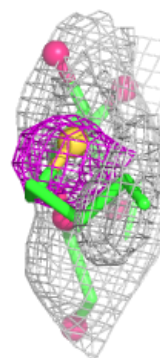
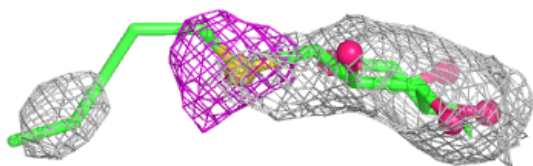
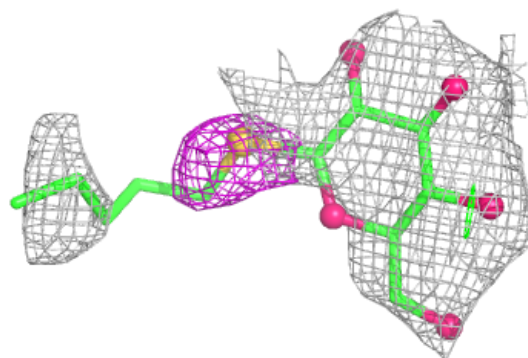


Electron density around SOG A 423:

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

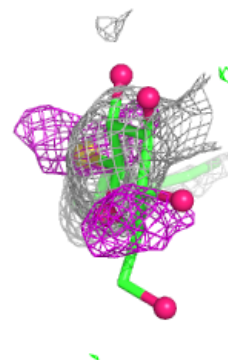
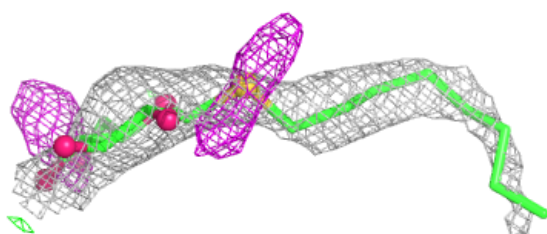
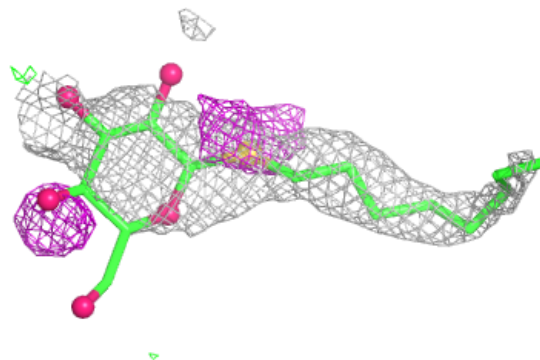
**Electron density around SOG A 407:**

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

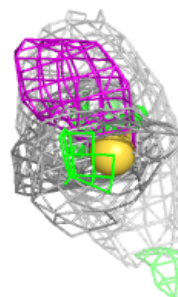
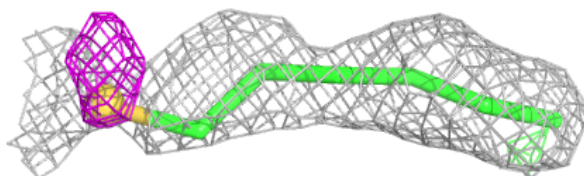
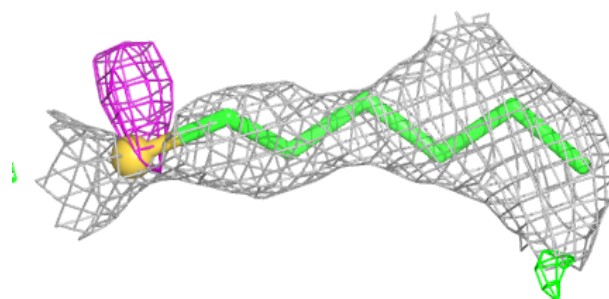


Electron density around SOG A 416:

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

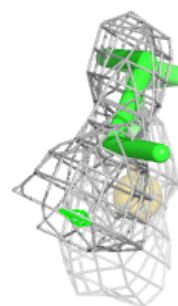
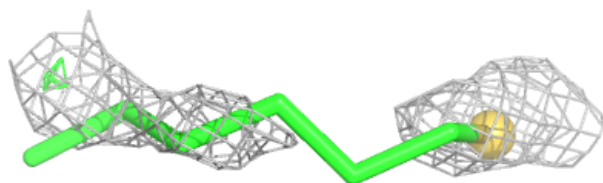
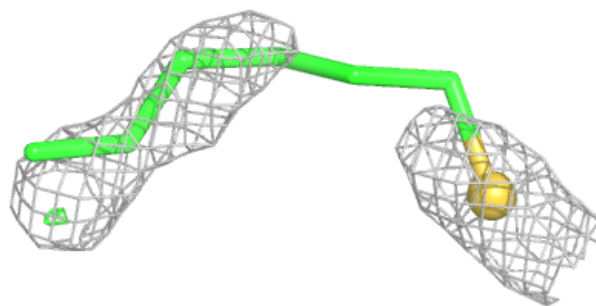
**Electron density around SOG B 426:**

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

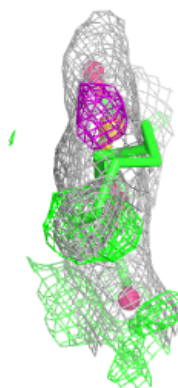
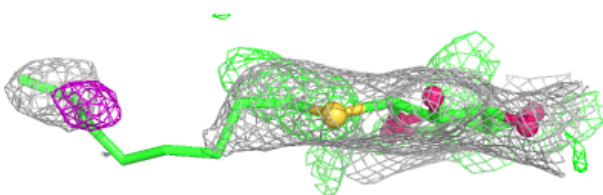
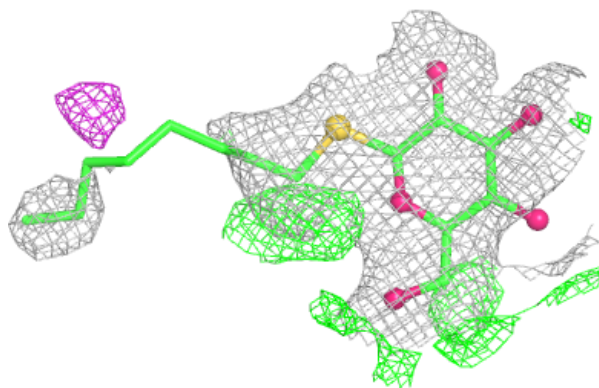


Electron density around SOG A 426:

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

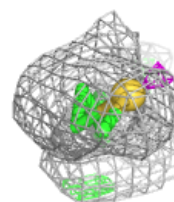
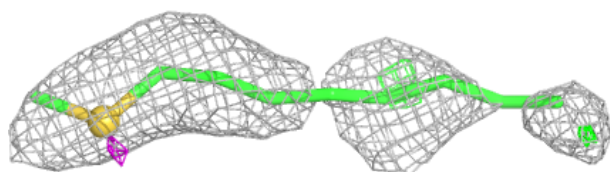
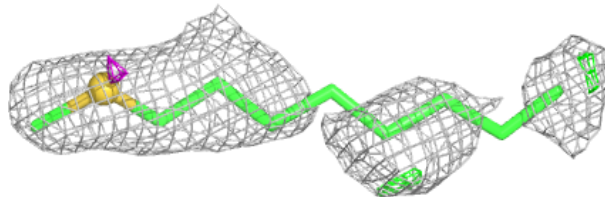
**Electron density around SOG A 414:**

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

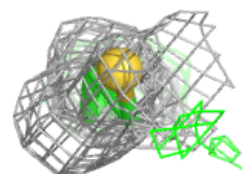
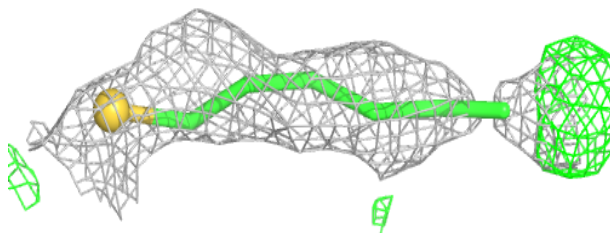
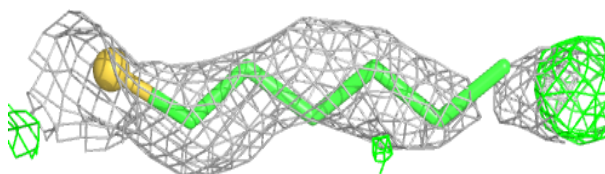


Electron density around SOG B 416:

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

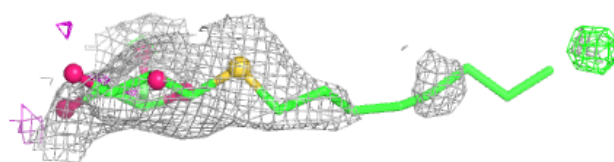
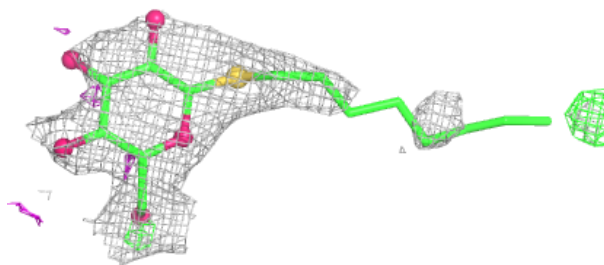
**Electron density around SOG A 421:**

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and green (positive)

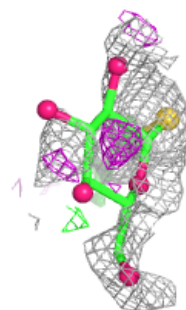
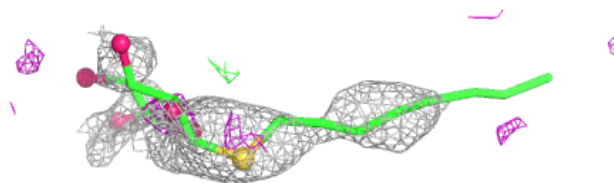
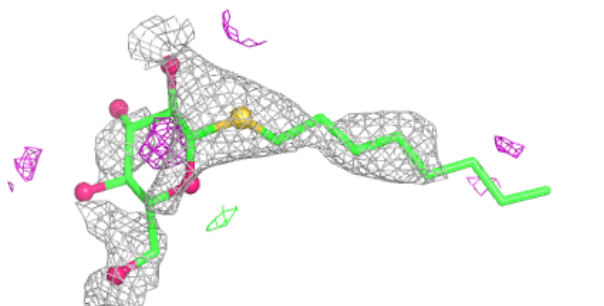


Electron density around SOG A 412:

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and green (positive)

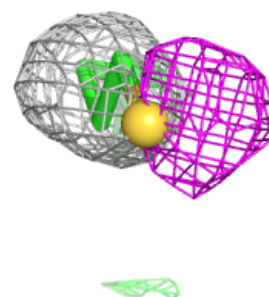
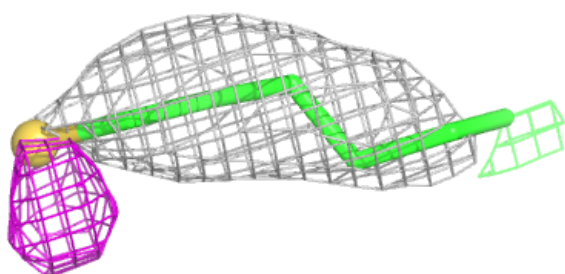
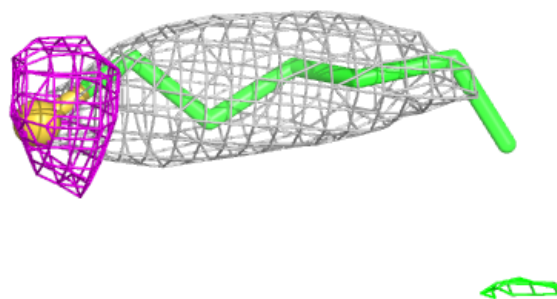
**Electron density around SOG A 418:**

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and green (positive)

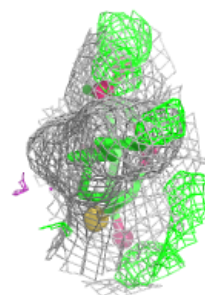
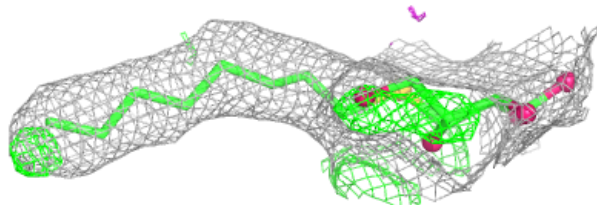
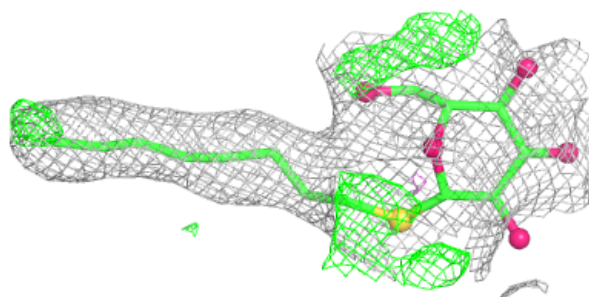


Electron density around SOG A 424:

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and green (positive)

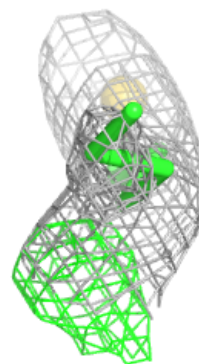
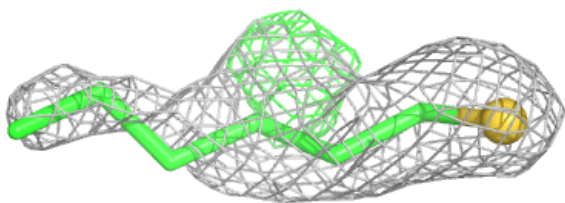
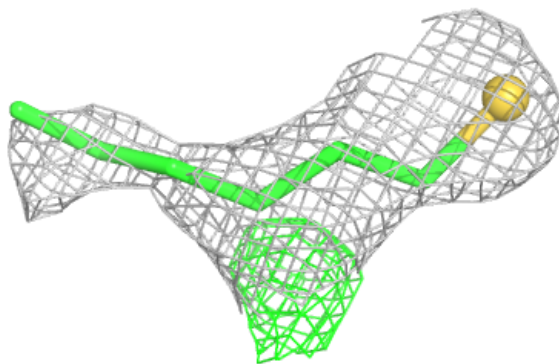
**Electron density around SOG A 410:**

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

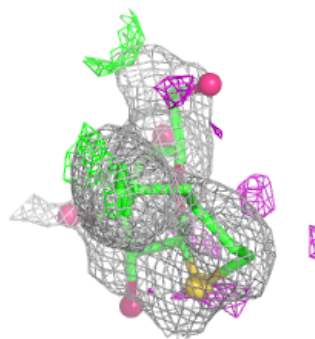
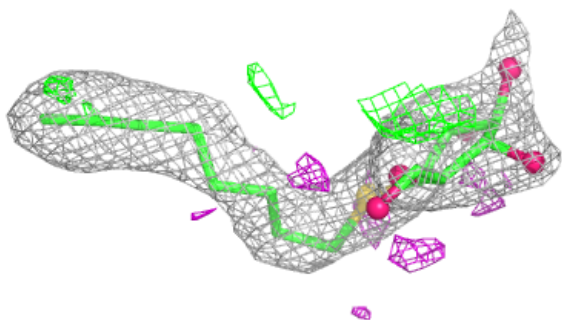
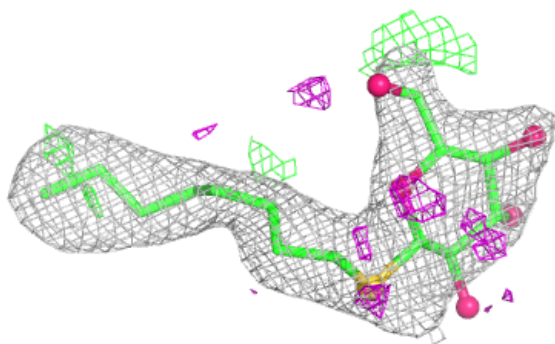


Electron density around SOG A 425:

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

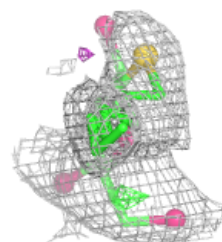
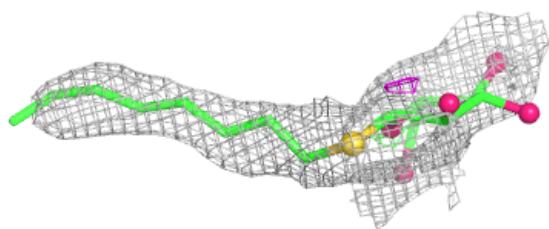
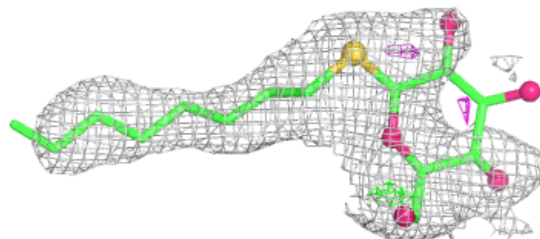
**Electron density around SOG A 413:**

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

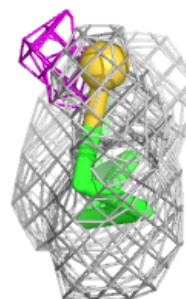
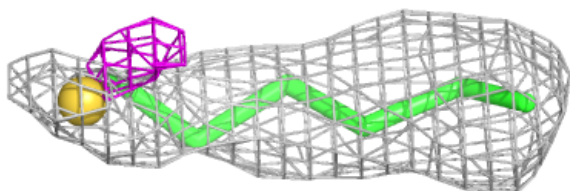
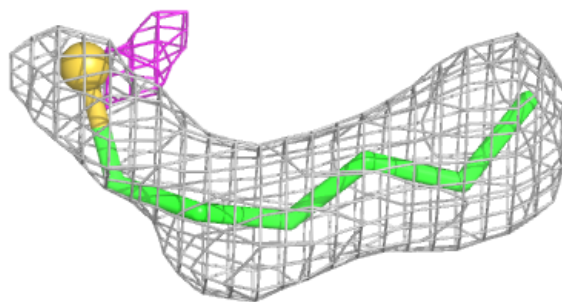


Electron density around SOG B 414:

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

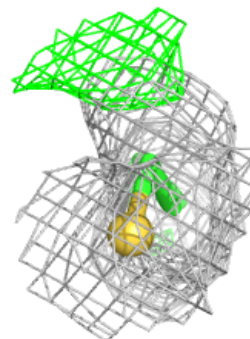
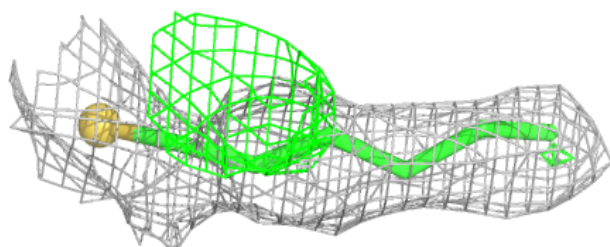
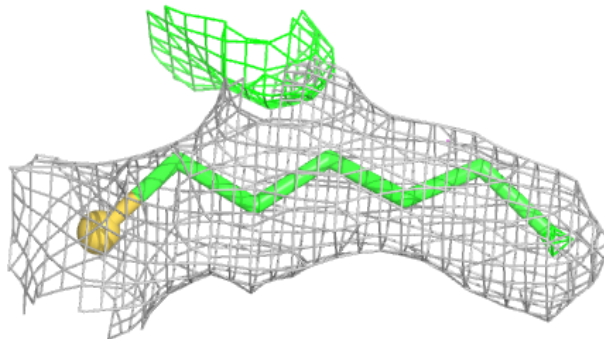
**Electron density around SOG B 429:**

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

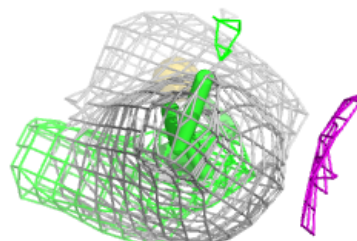
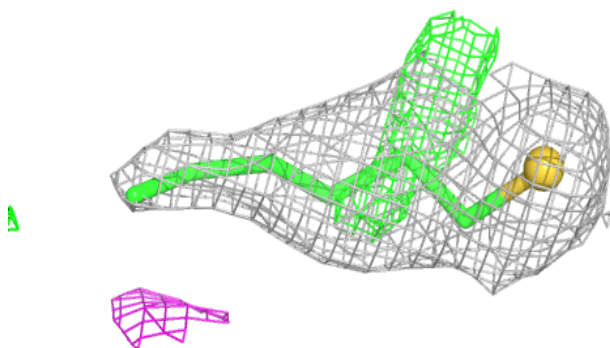
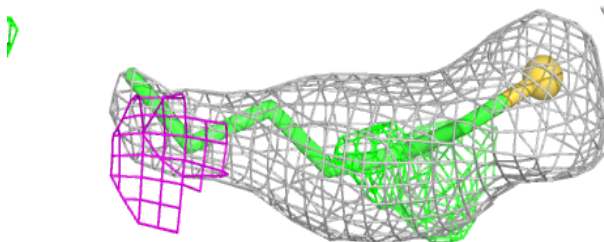


Electron density around SOG A 419:

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

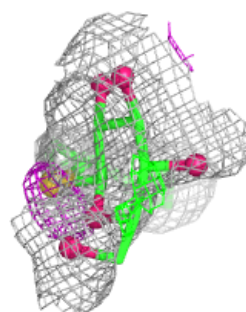
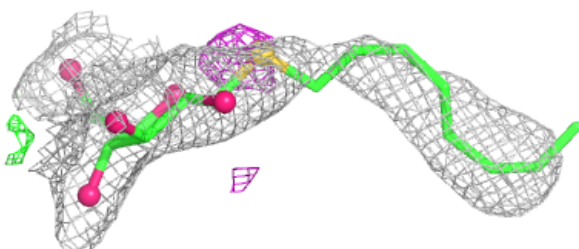
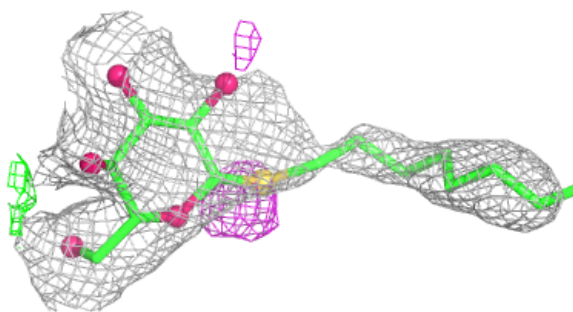
**Electron density around SOG B 430:**

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

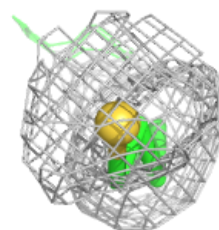
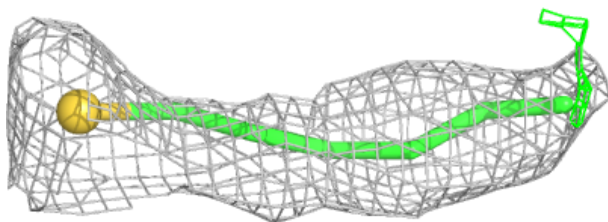
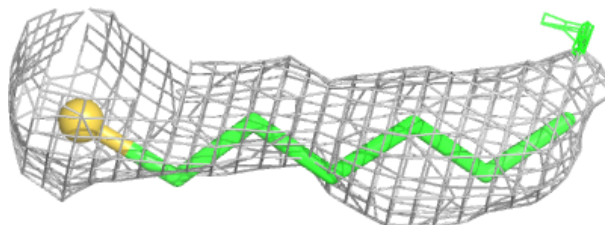


Electron density around SOG A 417:

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

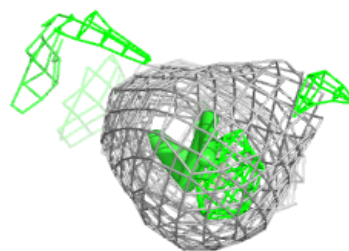
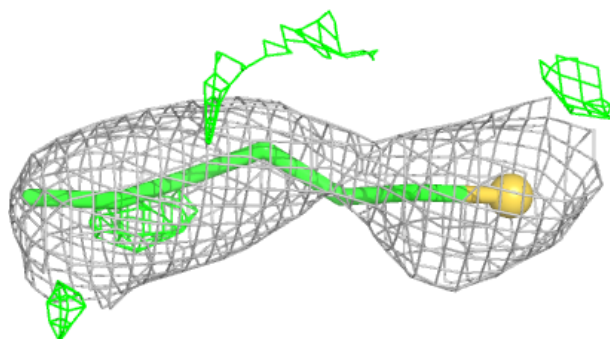
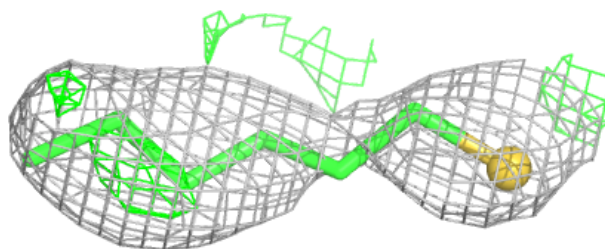
**Electron density around SOG B 428:**

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

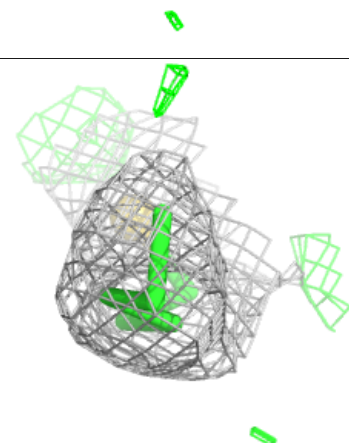
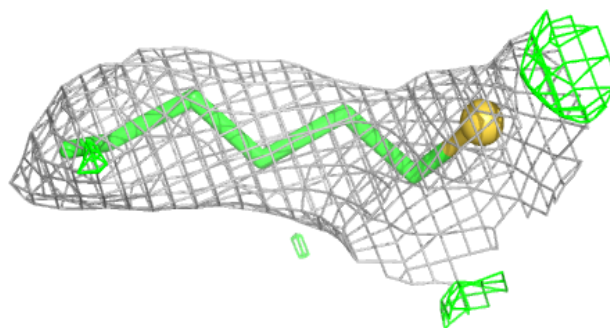
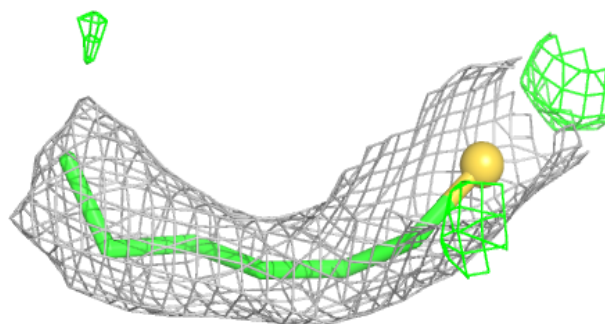


Electron density around SOG B 425:

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

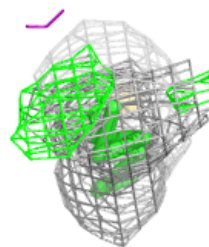
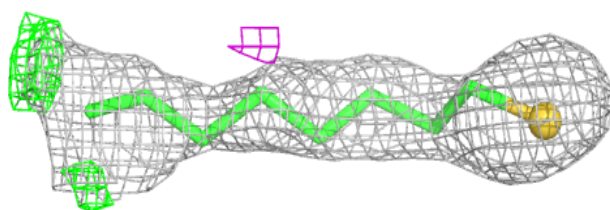
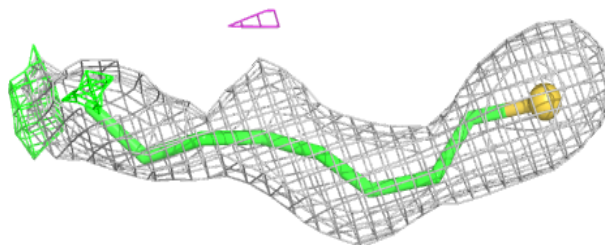
**Electron density around SOG A 422:**

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

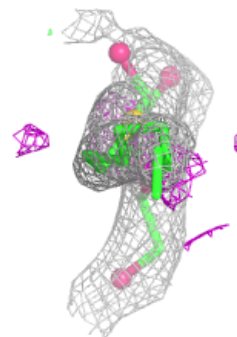
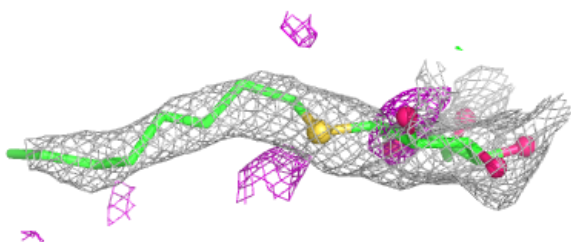
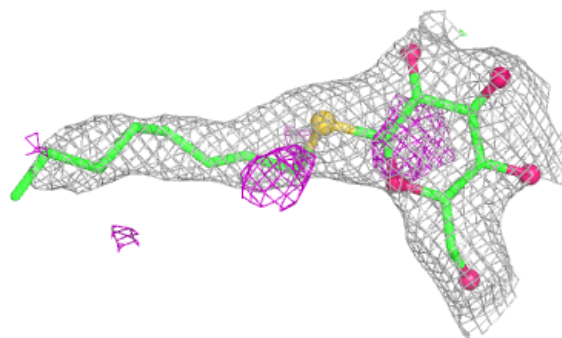


Electron density around SOG B 419:

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

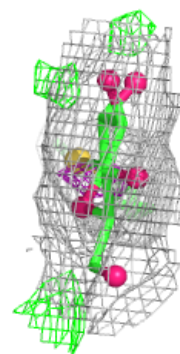
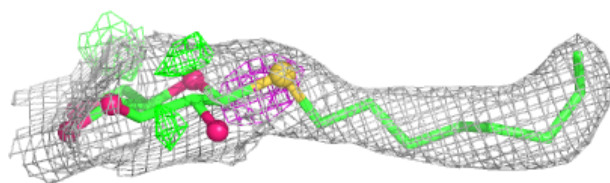
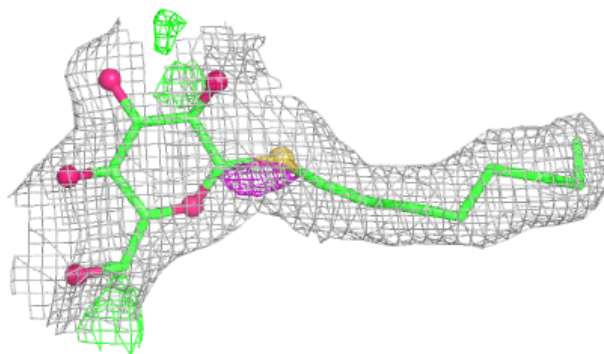
**Electron density around SOG B 412:**

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

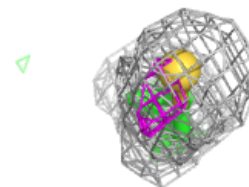
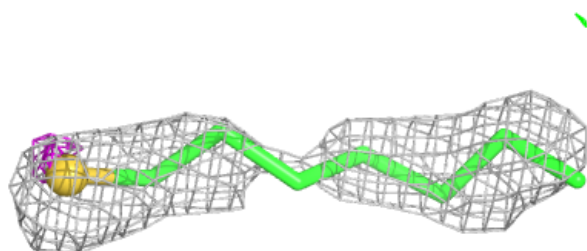
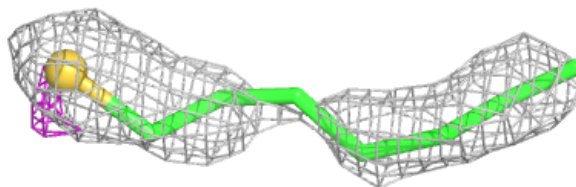


Electron density around SOG A 409:

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

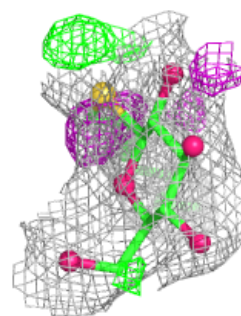
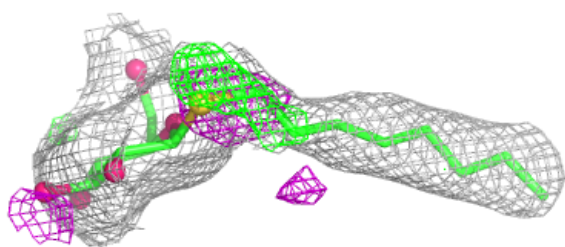
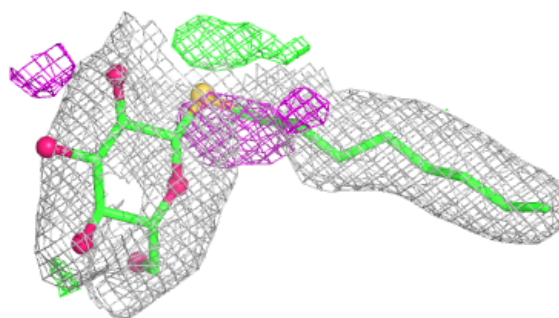
**Electron density around SOG B 418:**

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

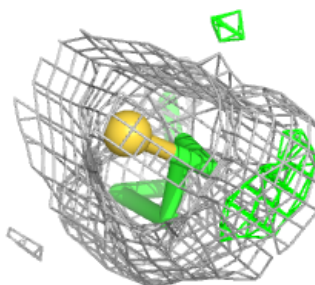
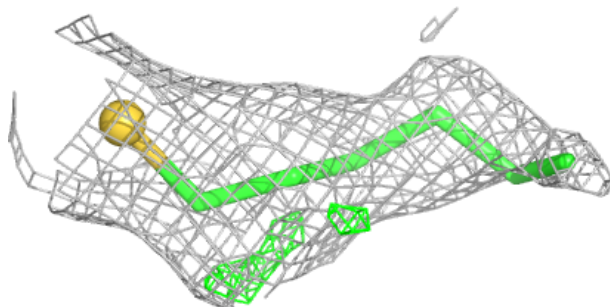
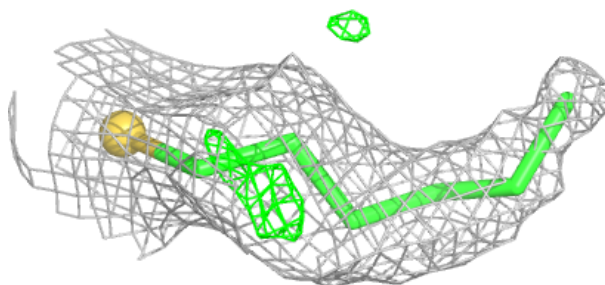


Electron density around SOG A 411:

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

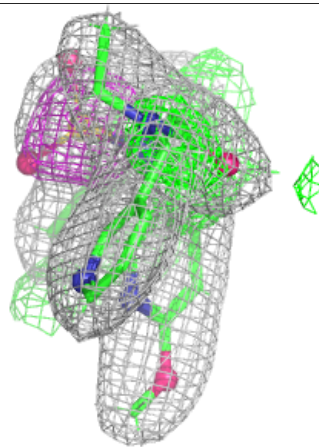
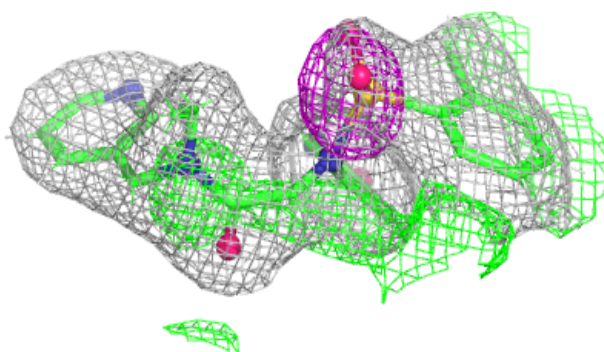
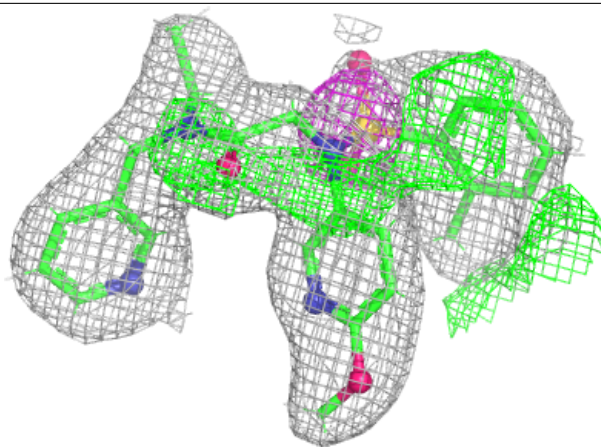
**Electron density around SOG A 427:**

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

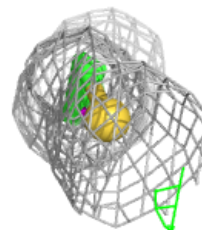
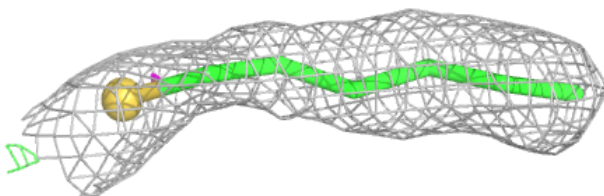
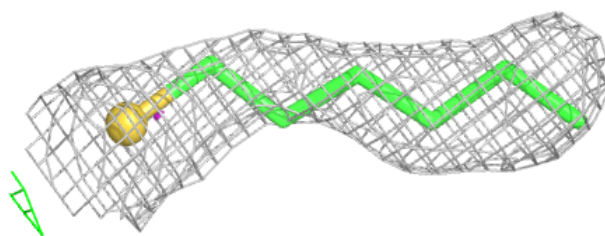


Electron density around 7MA A 401:

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

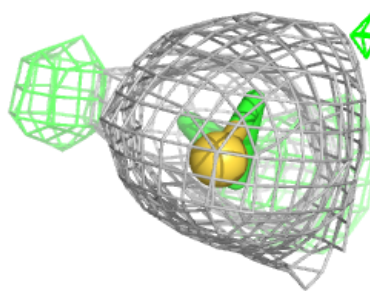
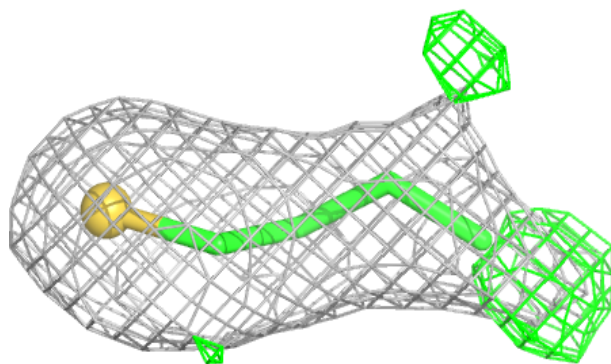
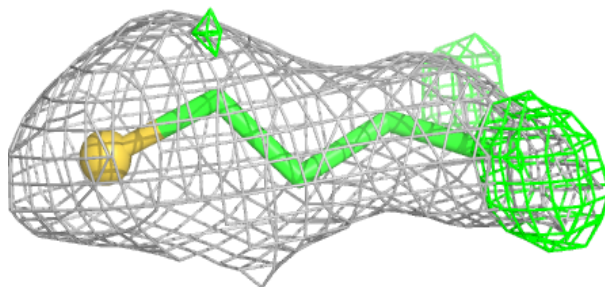
**Electron density around SOG A 420:**

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



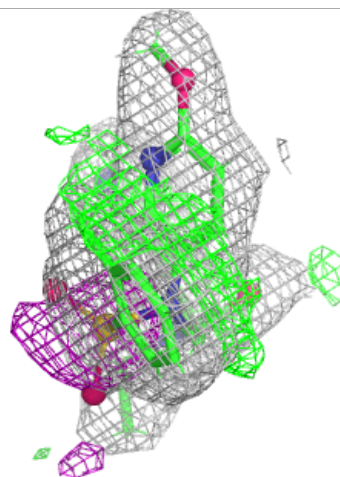
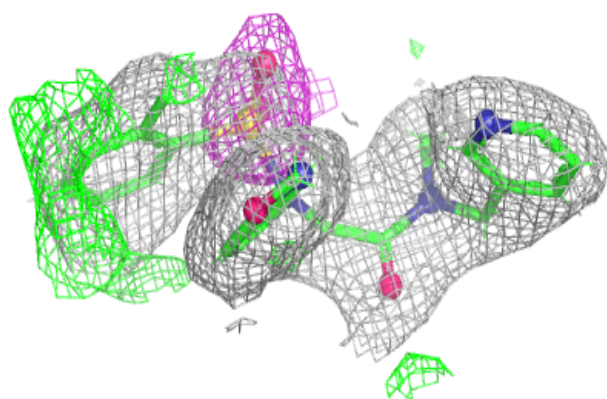
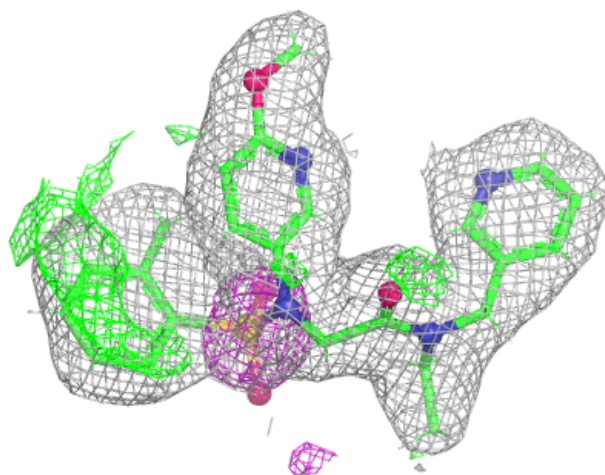
Electron density around SOG B 420:

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



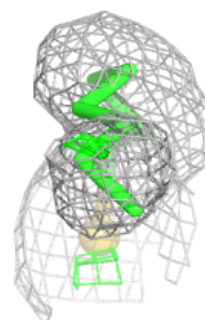
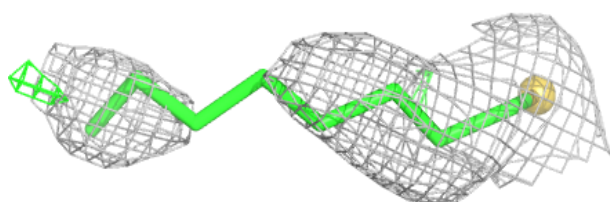
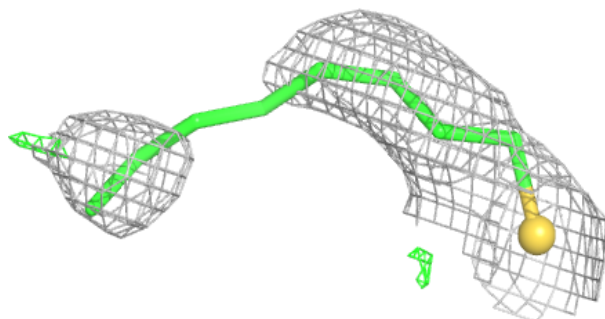
Electron density around 7MA B 401:

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

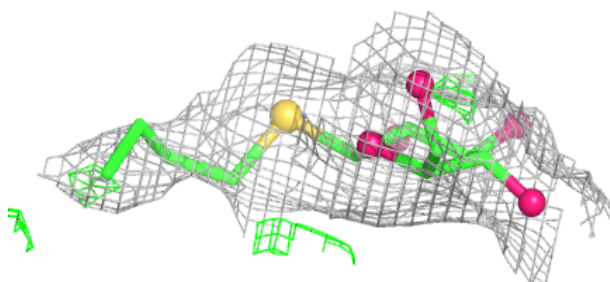


Electron density around SOG B 423:

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

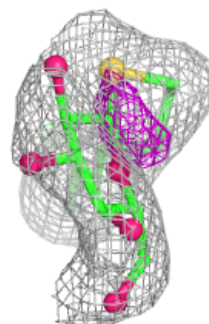
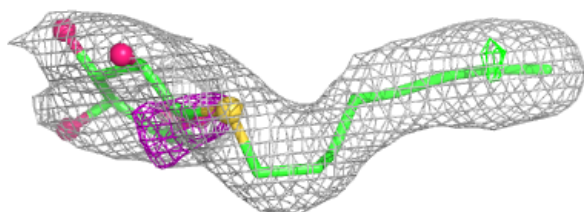
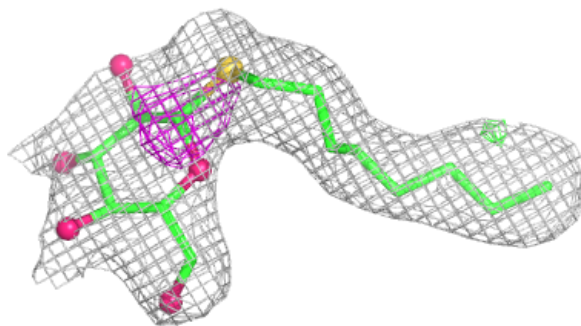
**Electron density around SOG A 408:**

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

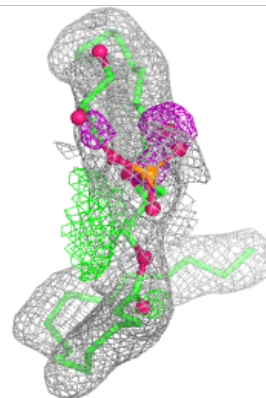
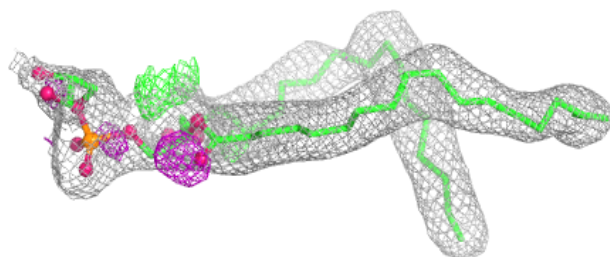
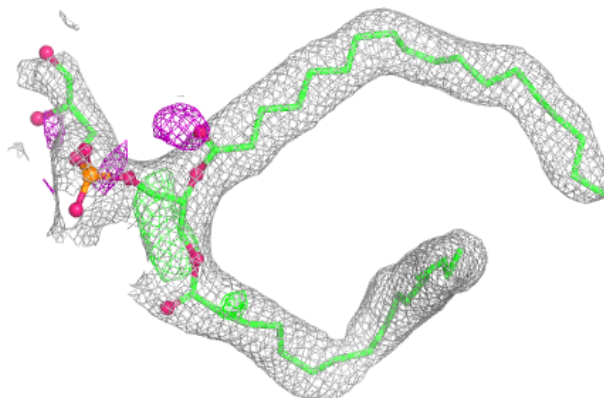


Electron density around SOG B 411:

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

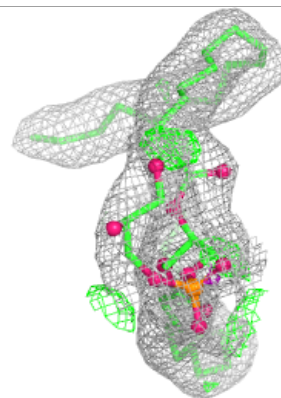
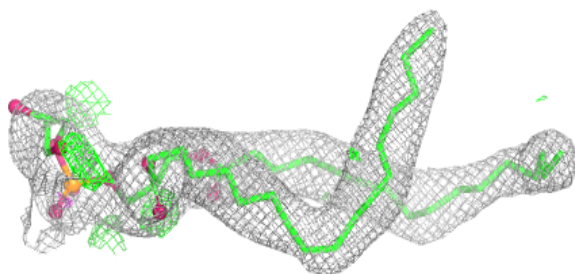
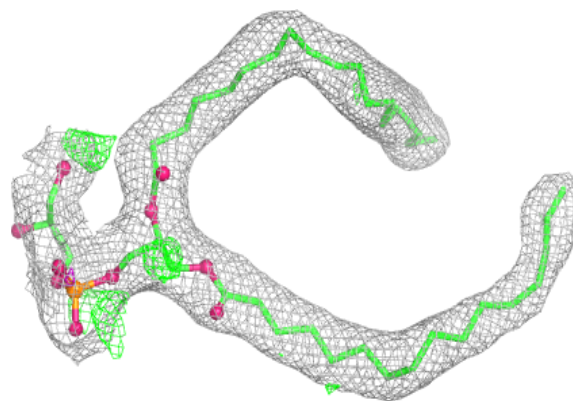
**Electron density around PGW A 429:**

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

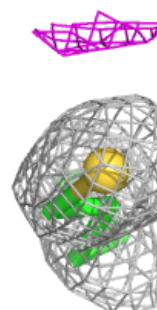
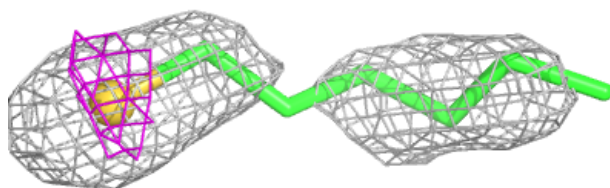
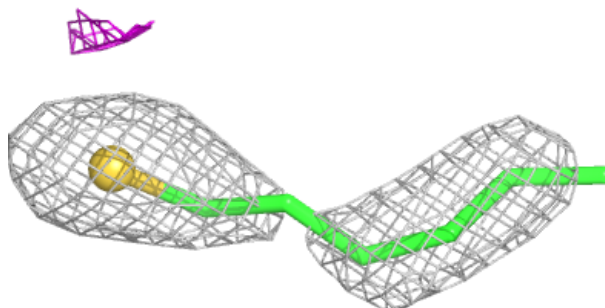


Electron density around PGW B 431:

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

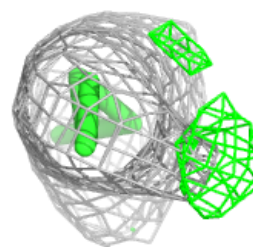
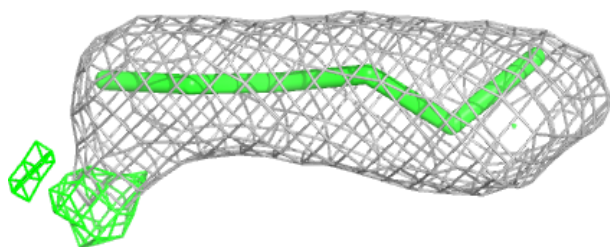
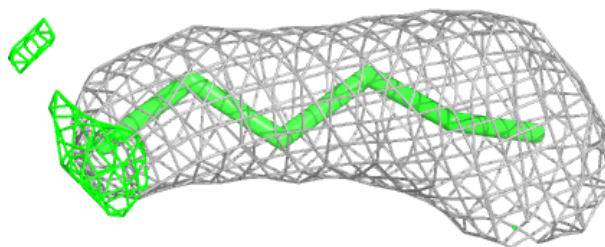
**Electron density around SOG A 428:**

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

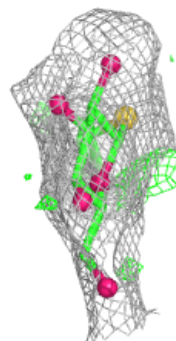
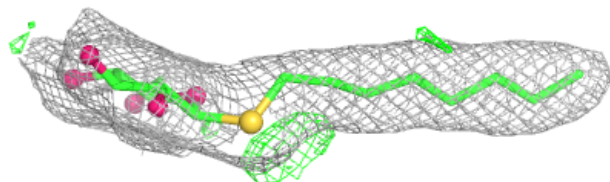
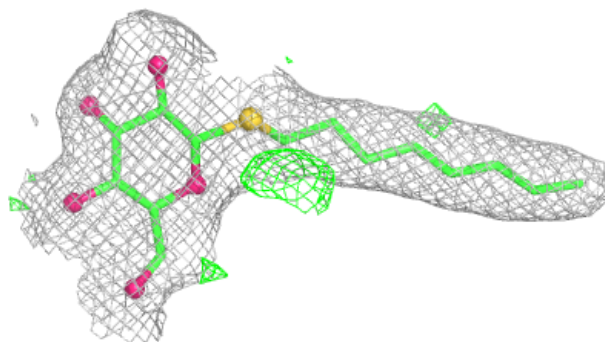


Electron density around SOG B 415:

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

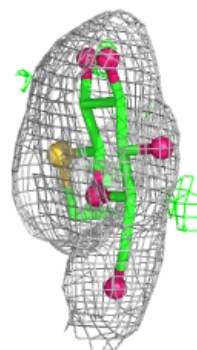
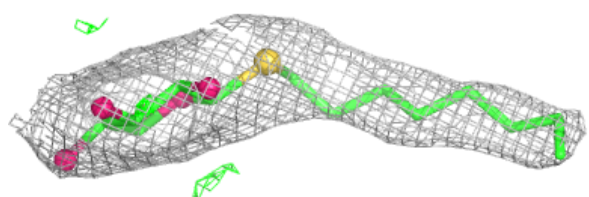
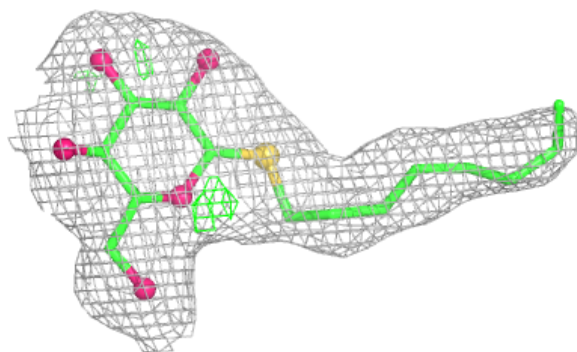
**Electron density around SOG B 406:**

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

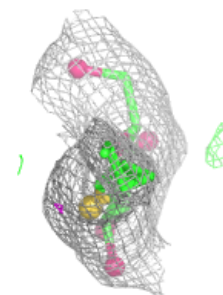
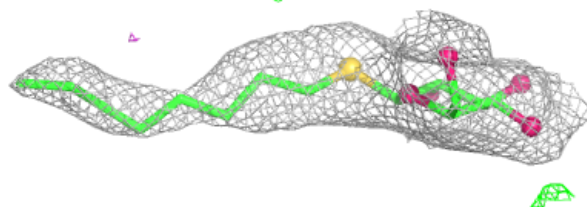
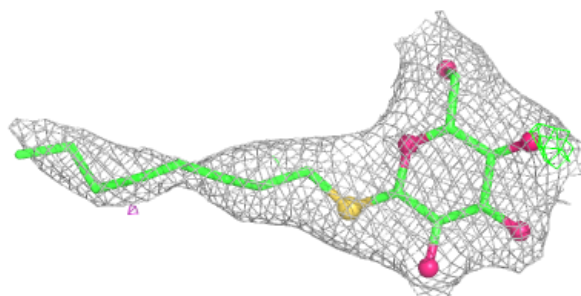


Electron density around SOG B 408:

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

**Electron density around SOG B 407:**

$2mF_o-DF_c$ (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.