



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 PM UTC

PDB ID : 6TO7 / pdb_00006to7
Title : Crystal structure of the Orexin-1 receptor in complex with suvorexant at 2.29 Å resolution
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 : 2.26 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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)

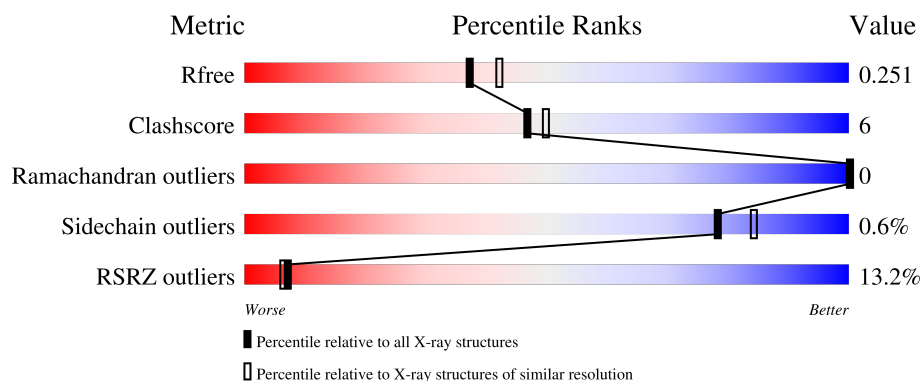
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	12% 80% 8% 11%
1	B	336	12% 82% 10% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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
5	SOG	A	423	-	-	-	X
5	SOG	A	424	-	-	-	X
5	SOG	B	412	-	-	X	-
5	SOG	B	417	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5761 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Orexin receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2377	1576	397	387	17			
1	B	307	Total	C	N	O	S	0	0	0
			2451	1631	404	399	17			

There are 116 discrepancies between the modelled and reference sequences:

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

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

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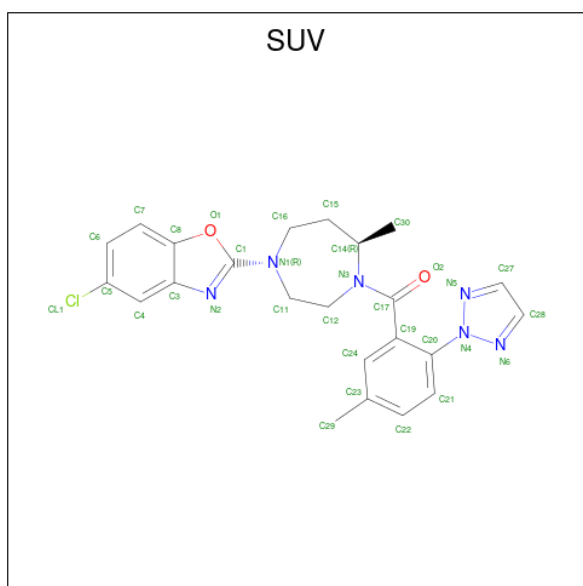
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613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

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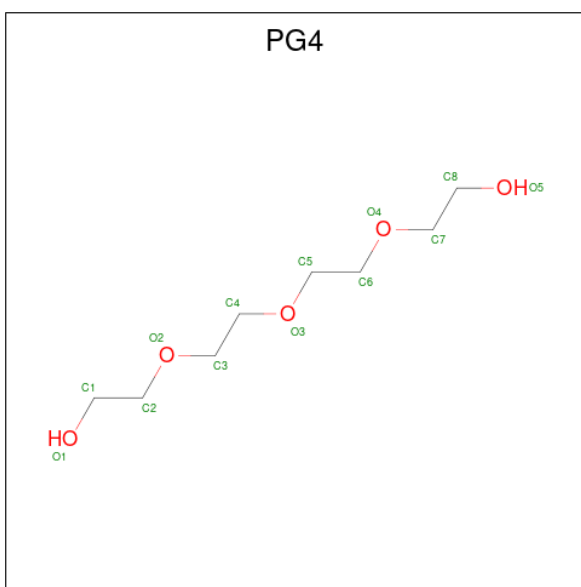
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag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

- Molecule 2 is [(7R)-4-(5-chloro-1,3-benzoxazol-2-yl)-7-methyl-1,4-diazepan-1-yl][5-methyl-2-(2H-1,2,3-triazol-2-yl)phenyl]methanone (CCD ID: SUV) (formula: C₂₃H₂₃ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



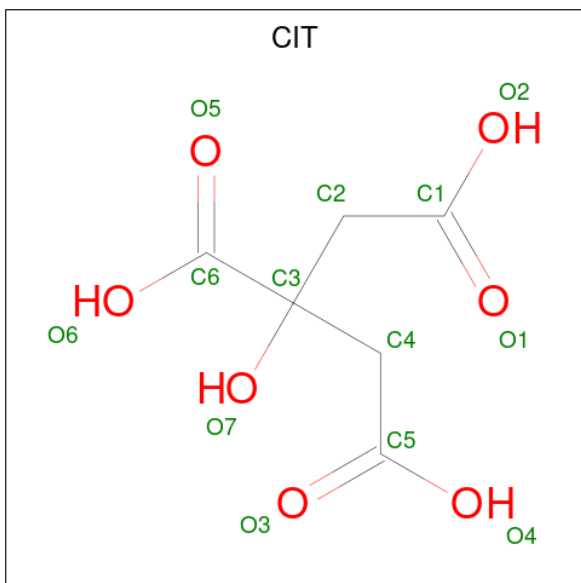
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			32	23	1	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			32	23	1	6	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



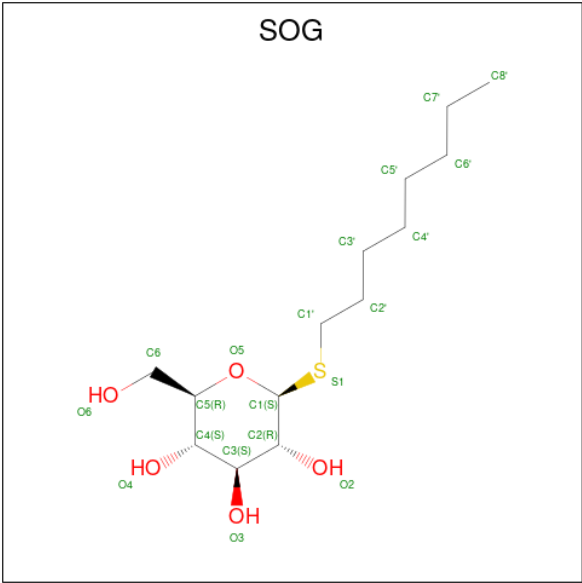
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 5 is octyl 1-thio-beta-D-glucopyranoside (CCD ID: SOG) (formula: C₁₄H₂₈O₅S).



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

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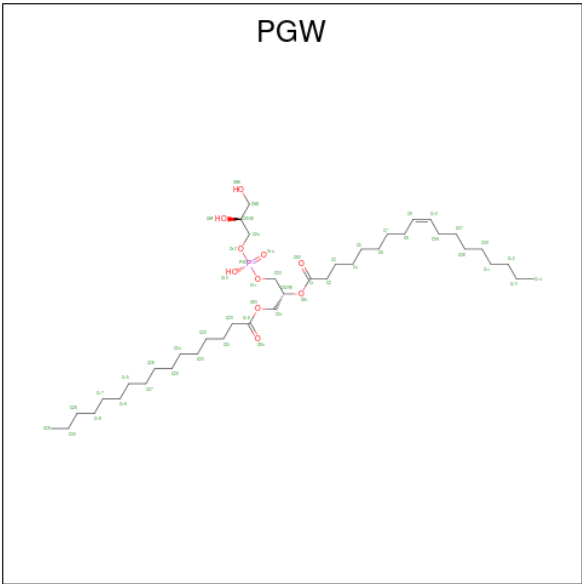
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C S 8 7 1	0	0
5	A	1	Total C 5 5	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 5 5	0	0
5	A	1	Total C S 9 8 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C S 6 5 1	0	0
5	A	1	Total C S 6 5 1	0	0
5	A	1	Total C S 4 3 1	0	0
5	A	1	Total C S 4 3 1	0	0
5	A	1	Total C 4 4	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 16 10 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C S 9 8 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C S 6 5 1	0	0
5	B	1	Total C S 4 3 1	0	0
5	B	1	Total C S 6 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C 6 6	0	0
5	B	1	Total C 5 5	0	0
5	B	1	Total C S 6 5 1	0	0
5	B	1	Total C 6 6	0	0

- Molecule 6 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
6	A	1	Total	C	O	P	0	0
			51	40	10	1		
6	B	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

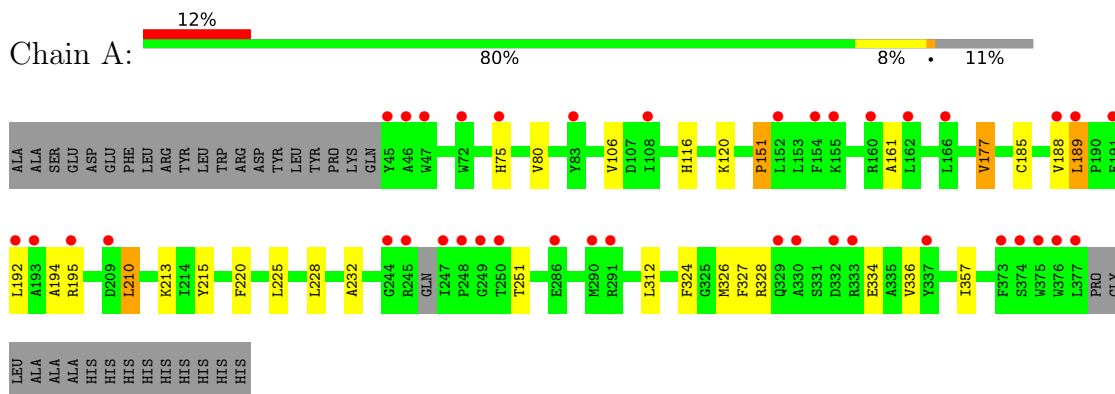
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	84	Total	O	0	0
			84	84		
8	B	64	Total	O	0	0
			64	64		

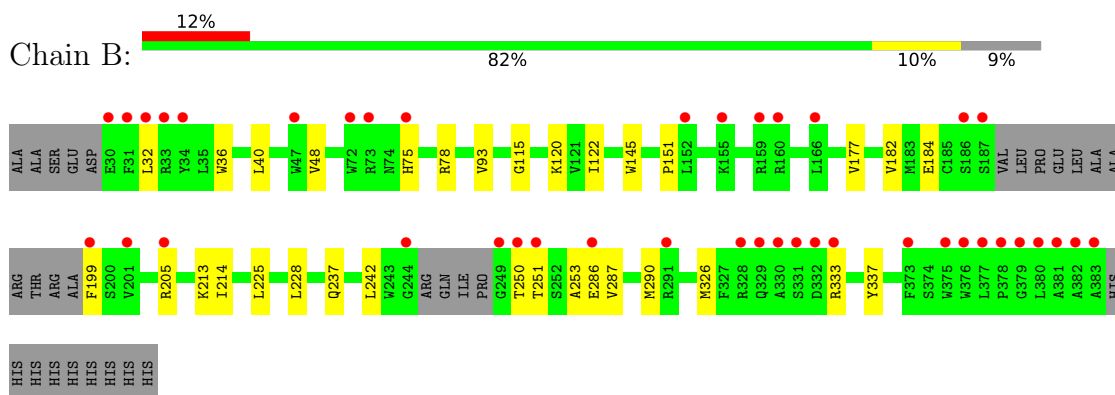
3 Residue-property plots [i](#)

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

• Molecule 1: Orexin receptor type 1



• Molecule 1: Orexin receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.90Å 158.47Å 183.62Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	44.38 – 2.26 44.38 – 2.26	Depositor EDS
% Data completeness (in resolution range)	58.8 (44.38-2.26) 79.3 (44.38-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.16 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.186 , 0.211 0.225 , 0.251	Depositor DCC
R_{free} test set	3882 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.9	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	0.89	EDS
Total number of atoms	5761	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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 [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, CIT, SUV

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	0.88	1/2442 (0.0%)	1.37	12/3330 (0.4%)
1	B	0.89	3/2521 (0.1%)	1.36	15/3436 (0.4%)
All	All	0.89	4/4963 (0.1%)	1.36	27/6766 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	VAL	CA-C	6.32	1.57	1.52
1	B	326	MET	SD-CE	-5.70	1.65	1.79
1	A	177	VAL	CA-C	5.48	1.57	1.52
1	B	122	ILE	CA-C	5.02	1.57	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	VAL	N-CA-C	-7.28	103.69	110.53
1	A	194	ALA	CA-C-N	6.16	128.82	120.44
1	A	194	ALA	C-N-CA	6.16	128.82	120.44
1	B	199	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	287	VAL	N-CA-CB	6.02	118.28	110.57
1	A	251	THR	CA-C-N	6.00	128.64	120.54
1	A	251	THR	C-N-CA	6.00	128.64	120.54
1	B	250	THR	CA-C-N	5.93	130.41	121.40
1	B	250	THR	C-N-CA	5.93	130.41	121.40
1	B	151	PRO	N-CA-C	5.75	121.41	113.65
1	A	106	VAL	N-CA-C	-5.74	105.13	110.53
1	B	48	VAL	CA-C-N	5.56	127.73	120.28
1	B	48	VAL	C-N-CA	5.56	127.73	120.28
1	A	151	PRO	N-CA-C	5.53	121.02	113.84
1	A	225	LEU	N-CA-C	5.50	116.96	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	VAL	N-CA-CB	5.49	117.60	110.57
1	B	120	LYS	CA-C-N	5.46	127.52	120.70
1	B	120	LYS	C-N-CA	5.46	127.52	120.70
1	B	225	LEU	N-CA-C	5.44	116.90	110.97
1	A	177	VAL	N-CA-CB	5.37	113.88	110.50
1	B	177	VAL	N-CA-CB	5.36	113.88	110.50
1	A	120	LYS	CA-C-N	5.34	127.38	120.70
1	A	120	LYS	C-N-CA	5.34	127.38	120.70
1	B	253	ALA	N-CA-C	5.27	117.03	111.28
1	A	334	GLU	N-CA-CB	5.20	117.85	110.16
1	B	115	GLY	CA-C-N	5.16	127.14	120.44
1	B	115	GLY	C-N-CA	5.16	127.14	120.44

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	2377	0	2443	24	0
1	B	2451	0	2498	35	0
2	A	32	0	23	0	0
2	B	32	0	23	0	0
3	A	13	0	18	0	0
3	B	37	0	49	1	0
4	A	13	0	5	0	0
5	A	250	0	348	16	0
5	B	304	0	425	31	0
6	A	51	0	76	1	0
6	B	51	0	76	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	84	0	0	2	0
8	B	64	0	0	0	0
All	All	5761	0	5984	66	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 6.

All (66) 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:205:ARG:NH2	5:B:412:SOG:H3'1	1.31	1.43
1:B:205:ARG:NH2	5:B:412:SOG:C3'	2.10	1.14
1:B:205:ARG:HH21	5:B:412:SOG:C3'	1.62	1.12
1:B:205:ARG:NE	5:B:412:SOG:H4'2	1.64	1.12
1:B:205:ARG:HE	5:B:412:SOG:H4'2	0.95	1.09
1:B:184:GLU:OE2	1:B:205:ARG:HD3	1.54	1.08
1:B:205:ARG:HE	5:B:412:SOG:C4'	1.76	0.97
1:B:184:GLU:CD	1:B:205:ARG:HD3	1.99	0.88
1:B:145:TRP:HE1	1:B:237:GLN:HE21	1.20	0.85
1:A:188:VAL:C	1:A:189:LEU:HD12	2.02	0.84
1:B:205:ARG:HH21	5:B:412:SOG:H3'1	0.99	0.82
1:B:184:GLU:OE2	1:B:205:ARG:CD	2.27	0.82
1:B:205:ARG:HH21	5:B:412:SOG:C4'	1.93	0.81
1:B:251:THR:HG22	1:B:286:GLU:OE1	1.83	0.79
1:B:205:ARG:NE	5:B:412:SOG:C4'	2.42	0.78
1:B:205:ARG:CZ	5:B:412:SOG:H4'2	2.15	0.77
1:A:210:LEU:HD12	1:A:210:LEU:O	1.86	0.75
1:B:251:THR:CG2	1:B:286:GLU:OE1	2.37	0.72
1:B:205:ARG:NH2	5:B:412:SOG:C4'	2.54	0.68
1:B:205:ARG:NH2	5:B:412:SOG:H4'2	2.11	0.65
1:B:184:GLU:HG3	5:B:412:SOG:H6'1	1.81	0.62
1:B:205:ARG:HH21	5:B:412:SOG:H4'2	1.65	0.61
5:A:407:SOG:H3	5:B:410:SOG:H2	1.82	0.60
1:A:189:LEU:HD12	1:A:189:LEU:N	2.17	0.59
1:A:151:PRO:HD2	5:A:425:SOG:H8'3	1.85	0.58
6:A:426:PGW:H26	1:B:214:ILE:HG22	1.83	0.58
1:B:36:TRP:HA	1:B:40:LEU:HB2	1.83	0.58
1:A:215:TYR:HB2	6:B:426:PGW:H7	1.85	0.58
1:B:75:HIS:HE1	5:B:417:SOG:H5'1	1.69	0.57
1:A:189:LEU:N	1:A:189:LEU:CD1	2.69	0.55
1:B:205:ARG:CZ	5:B:412:SOG:C4'	2.82	0.54
5:A:410:SOG:H3	5:B:414:SOG:H2	1.89	0.54
1:B:75:HIS:HB3	5:B:417:SOG:O5	2.07	0.54
1:B:182:VAL:HA	5:B:412:SOG:H2'1	1.89	0.53
1:B:75:HIS:CE1	1:B:78:ARG:HH12	2.26	0.53
1:A:192:LEU:HD23	1:A:195:ARG:HD2	1.91	0.52
1:B:93:VAL:HG21	5:B:419:SOG:C1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:CZ	5:B:412:SOG:C3'	2.84	0.50
5:B:406:SOG:H61	5:B:407:SOG:H3	1.94	0.50
1:A:116:HIS:ND1	1:A:185:CYS:HB3	2.27	0.50
1:A:228:LEU:HB3	5:A:413:SOG:H6'2	1.94	0.49
5:A:405:SOG:H3'2	5:B:425:SOG:H6'1	1.94	0.48
1:A:327:PHE:H	5:A:412:SOG:C6	2.26	0.48
1:B:242:LEU:HA	1:B:290:MET:HE2	1.96	0.48
5:A:405:SOG:H3'1	5:B:405:SOG:H6'1	1.95	0.47
5:A:410:SOG:H5'1	5:B:414:SOG:H4'2	1.97	0.46
1:A:210:LEU:HD12	1:A:210:LEU:C	2.37	0.46
1:A:232:ALA:HB2	5:A:413:SOG:H7'1	1.98	0.46
1:B:145:TRP:HE1	1:B:237:GLN:NE2	2.01	0.45
1:A:75:HIS:HB2	8:A:563:HOH:O	2.17	0.45
1:A:357:ILE:HG12	5:A:422:SOG:H2'1	1.98	0.45
1:B:228:LEU:HB3	3:B:403:PG4:H81	1.98	0.45
1:A:177:VAL:HG11	5:B:413:SOG:H61	2.00	0.44
1:A:327:PHE:HB3	1:A:336:VAL:HG21	2.00	0.44
1:B:213:LYS:NZ	5:B:405:SOG:H61	2.32	0.44
1:A:326:MET:HE3	5:A:408:SOG:H62	2.01	0.43
1:A:324:PHE:HB3	5:A:408:SOG:H5	2.01	0.43
1:A:326:MET:HB3	5:A:412:SOG:H61	2.01	0.42
1:A:312:LEU:HD23	5:A:419:SOG:H2'2	2.01	0.42
1:A:213:LYS:HD3	5:A:410:SOG:H2'2	2.02	0.42
1:A:80:VAL:HG13	1:A:161:ALA:HB2	2.02	0.42
1:A:328:ARG:HD2	8:A:502:HOH:O	2.20	0.42
1:B:333:ARG:O	1:B:337:TYR:HD2	2.03	0.41
5:A:405:SOG:H3	5:B:408:SOG:H3	2.02	0.41
1:B:75:HIS:HB3	5:B:417:SOG:C1	2.50	0.41
1:A:220:PHE:HE2	5:B:425:SOG:H8'1	1.84	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	296/336 (88%)	292 (99%)	4 (1%)	0	100	100
1	B	301/336 (90%)	293 (97%)	8 (3%)	0	100	100
All	All	597/672 (89%)	585 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/279 (89%)	247 (99%)	2 (1%)	73	80
1	B	255/279 (91%)	254 (100%)	1 (0%)	84	89
All	All	504/558 (90%)	501 (99%)	3 (1%)	78	84

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

Mol	Chain	Res	Type
1	A	189	LEU
1	A	210	LEU
1	B	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	74	ASN
1	B	64	ASN
1	B	75	HIS
1	B	116	HIS
1	B	150	HIS
1	B	237	GLN
1	B	350	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 54 ligands modelled in this entry, 2 are monoatomic - leaving 52 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
5	SOG	A	414	-	8,8,20	0.20	0	7,7,25	0.38	0
5	SOG	B	409	-	20,20,20	0.93	1 (5%)	24,25,25	0.86	2 (8%)
5	SOG	A	422	-	5,5,20	0.50	0	4,4,25	0.43	0
5	SOG	B	420	-	5,5,20	0.50	0	4,4,25	1.04	0
5	SOG	B	408	-	20,20,20	1.13	2 (10%)	24,25,25	1.26	2 (8%)
5	SOG	B	415	-	20,20,20	0.96	1 (5%)	24,25,25	1.53	4 (16%)
6	PGW	A	426	-	50,50,50	0.95	2 (4%)	53,56,56	1.00	3 (5%)
5	SOG	A	408	-	20,20,20	1.01	2 (10%)	24,25,25	1.72	3 (12%)
3	PG4	B	402	-	12,12,12	0.62	0	11,11,11	0.52	0
5	SOG	A	415	-	7,7,20	0.40	0	6,6,25	0.65	0
3	PG4	A	402	-	12,12,12	0.53	0	11,11,11	0.24	0
5	SOG	A	404	-	20,20,20	0.96	1 (5%)	24,25,25	1.02	1 (4%)
5	SOG	B	407	-	20,20,20	0.89	1 (5%)	24,25,25	0.85	2 (8%)
5	SOG	A	406	-	16,16,20	1.00	1 (6%)	20,21,25	1.33	3 (15%)
5	SOG	B	425	-	5,5,20	0.21	0	4,4,25	0.58	0
5	SOG	A	405	-	20,20,20	0.96	1 (5%)	24,25,25	1.62	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SOG	A	410	-	20,20,20	0.87	1 (5%)	24,25,25	1.09	1 (4%)
5	SOG	A	419	-	8,8,20	0.39	0	7,7,25	0.60	0
4	CIT	A	403	-	12,12,12	1.11	0	17,17,17	1.16	1 (5%)
5	SOG	A	424	-	3,3,20	0.68	0	2,2,25	0.45	0
5	SOG	A	409	-	20,20,20	1.18	2 (10%)	24,25,25	1.36	3 (12%)
5	SOG	B	414	-	20,20,20	0.90	1 (5%)	24,25,25	0.79	0
5	SOG	B	423	-	4,4,20	0.28	0	3,3,25	0.34	0
3	PG4	B	404	-	10,10,12	0.57	0	9,9,11	0.40	0
5	SOG	A	407	-	14,14,20	0.85	1 (7%)	18,19,25	1.13	1 (5%)
5	SOG	A	425	-	3,3,20	0.31	0	2,2,25	0.70	0
5	SOG	B	411	-	20,20,20	1.04	1 (5%)	24,25,25	0.93	1 (4%)
5	SOG	B	413	-	20,20,20	0.97	1 (5%)	24,25,25	1.52	3 (12%)
5	SOG	B	418	-	5,5,20	0.48	0	4,4,25	0.33	0
2	SUV	B	401	-	34,36,36	0.45	0	41,52,52	1.17	4 (9%)
5	SOG	A	418	-	4,4,20	0.27	0	3,3,25	0.43	0
5	SOG	A	413	-	9,9,20	0.39	0	8,8,25	0.43	0
6	PGW	B	426	-	50,50,50	0.97	2 (4%)	53,56,56	0.97	3 (5%)
5	SOG	A	417	-	7,7,20	0.32	0	6,6,25	0.44	0
5	SOG	B	421	-	20,20,20	0.93	1 (5%)	24,25,25	0.97	1 (4%)
5	SOG	B	424	-	5,5,20	0.47	0	4,4,25	0.81	0
5	SOG	B	422	-	5,5,20	0.26	0	4,4,25	0.40	0
2	SUV	A	401	-	34,36,36	0.48	0	41,52,52	1.26	4 (9%)
5	SOG	A	421	-	5,5,20	0.48	0	4,4,25	0.51	0
5	SOG	A	423	-	3,3,20	0.55	0	2,2,25	2.31	1 (50%)
5	SOG	B	406	-	16,16,20	1.15	2 (12%)	20,21,25	0.97	0
5	SOG	A	420	-	20,20,20	0.96	1 (5%)	24,25,25	0.93	1 (4%)
5	SOG	B	405	-	20,20,20	0.92	1 (5%)	24,25,25	1.22	2 (8%)
5	SOG	B	419	-	3,3,20	0.25	0	2,2,25	0.05	0
3	PG4	B	403	-	12,12,12	0.66	0	11,11,11	0.47	0
5	SOG	A	411	-	5,5,20	0.50	0	4,4,25	0.84	0
5	SOG	B	417	-	20,20,20	1.02	2 (10%)	24,25,25	1.40	5 (20%)
5	SOG	B	416	-	8,8,20	0.47	0	7,7,25	0.52	0
5	SOG	B	410	-	20,20,20	0.86	2 (10%)	24,25,25	1.01	2 (8%)
5	SOG	B	412	-	20,20,20	0.96	2 (10%)	24,25,25	1.36	3 (12%)
5	SOG	A	416	-	4,4,20	0.31	0	3,3,25	0.33	0
5	SOG	A	412	-	16,16,20	1.06	1 (6%)	20,21,25	1.40	3 (15%)

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
5	SOG	A	414	-	-	1/6/6/31	-
5	SOG	B	409	-	-	5/11/31/31	0/1/1/1
5	SOG	A	422	-	-	3/3/3/31	-
5	SOG	B	420	-	-	2/3/3/31	-
5	SOG	B	408	-	-	4/11/31/31	0/1/1/1
5	SOG	B	415	-	-	7/11/31/31	0/1/1/1
6	PGW	A	426	-	-	29/55/55/55	-
5	SOG	A	408	-	-	9/11/31/31	0/1/1/1
3	PG4	B	402	-	-	3/10/10/10	-
5	SOG	A	415	-	-	3/5/5/31	-
3	PG4	A	402	-	-	6/10/10/10	-
5	SOG	A	404	-	-	4/11/31/31	0/1/1/1
5	SOG	B	407	-	-	6/11/31/31	0/1/1/1
5	SOG	A	406	-	-	3/7/27/31	0/1/1/1
5	SOG	B	425	-	-	3/3/3/31	-
5	SOG	A	405	-	-	7/11/31/31	0/1/1/1
5	SOG	A	410	-	-	4/11/31/31	0/1/1/1
5	SOG	A	419	-	-	3/6/6/31	-
4	CIT	A	403	-	-	1/16/16/16	-
5	SOG	A	424	-	-	0/0/1/31	-
5	SOG	A	409	-	-	8/11/31/31	0/1/1/1
5	SOG	B	414	-	-	7/11/31/31	0/1/1/1
5	SOG	B	423	-	-	2/2/2/31	-
3	PG4	B	404	-	-	4/8/8/10	-
5	SOG	A	407	-	-	2/5/25/31	0/1/1/1
5	SOG	A	425	-	-	0/1/1/31	-
5	SOG	B	411	-	-	6/11/31/31	0/1/1/1
5	SOG	B	413	-	-	3/11/31/31	0/1/1/1
5	SOG	B	418	-	-	2/3/3/31	-
2	SUV	B	401	-	-	0/12/30/30	0/4/5/5
5	SOG	A	418	-	-	1/2/2/31	-
5	SOG	A	413	-	-	4/7/7/31	-
6	PGW	B	426	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	A	417	-	-	4/5/5/31	-
5	SOG	B	421	-	-	8/11/31/31	0/1/1/1
5	SOG	B	424	-	-	2/3/3/31	-
5	SOG	B	422	-	-	1/3/3/31	-
2	SUV	A	401	-	-	0/12/30/30	0/4/5/5
5	SOG	A	421	-	-	3/3/3/31	-
5	SOG	A	423	-	-	1/1/1/31	-
5	SOG	B	406	-	-	3/7/27/31	0/1/1/1
5	SOG	A	420	-	-	4/11/31/31	0/1/1/1
5	SOG	B	405	-	-	1/11/31/31	0/1/1/1
5	SOG	B	419	-	-	0/0/1/31	-
3	PG4	B	403	-	-	8/10/10/10	-
5	SOG	A	411	-	-	0/3/3/31	-
5	SOG	B	417	-	-	9/11/31/31	0/1/1/1
5	SOG	B	416	-	-	3/6/6/31	-
5	SOG	B	410	-	-	4/11/31/31	0/1/1/1
5	SOG	B	412	-	-	6/11/31/31	0/1/1/1
5	SOG	A	416	-	-	1/2/2/31	-
5	SOG	A	412	-	-	4/7/27/31	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	426	PGW	O03-C19	4.57	1.46	1.33
6	B	426	PGW	O03-C19	4.39	1.46	1.33
6	B	426	PGW	O01-C1	4.34	1.46	1.34
6	A	426	PGW	O01-C1	3.79	1.45	1.34
5	A	409	SOG	C1'-S1	-3.75	1.76	1.81
5	B	408	SOG	C1'-S1	-3.73	1.76	1.81
5	B	406	SOG	C1'-S1	-3.51	1.76	1.81
5	A	408	SOG	C1'-S1	-3.47	1.76	1.81
5	B	411	SOG	C1'-S1	-3.46	1.76	1.81
5	A	412	SOG	C1'-S1	-3.37	1.76	1.81
5	A	405	SOG	C1'-S1	-3.32	1.76	1.81
5	B	412	SOG	C1'-S1	-3.21	1.76	1.81
5	A	420	SOG	C1'-S1	-3.20	1.76	1.81
5	B	413	SOG	C1'-S1	-3.16	1.77	1.81
5	B	415	SOG	C1'-S1	-3.13	1.77	1.81
5	A	406	SOG	C1'-S1	-3.12	1.77	1.81
5	B	417	SOG	C1'-S1	-3.09	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	409	SOG	C1'-S1	-3.05	1.77	1.81
5	A	404	SOG	C1'-S1	-3.02	1.77	1.81
5	B	421	SOG	C1'-S1	-3.01	1.77	1.81
5	B	405	SOG	C1'-S1	-2.98	1.77	1.81
5	A	410	SOG	C1'-S1	-2.86	1.77	1.81
5	B	414	SOG	C1'-S1	-2.85	1.77	1.81
5	B	407	SOG	C1'-S1	-2.81	1.77	1.81
5	A	409	SOG	C1-S1	-2.79	1.76	1.80
5	B	410	SOG	C1-S1	-2.40	1.76	1.80
5	B	417	SOG	C1-S1	-2.38	1.76	1.80
5	B	406	SOG	C1-S1	-2.28	1.76	1.80
5	A	407	SOG	C1-S1	-2.18	1.77	1.80
5	B	408	SOG	C1-S1	-2.18	1.77	1.80
5	B	410	SOG	C1'-S1	-2.12	1.78	1.81
5	B	412	SOG	C1-S1	-2.11	1.77	1.80
5	A	408	SOG	C1-S1	-2.03	1.77	1.80

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	SOG	C1-O5-C5	6.38	124.02	112.56
5	B	413	SOG	C1-O5-C5	4.24	120.16	112.56
5	A	404	SOG	C1-O5-C5	4.14	119.99	112.56
5	B	415	SOG	C1-C2-C3	4.04	118.44	110.55
5	A	409	SOG	C4-C3-C2	3.98	117.81	110.83
5	B	415	SOG	C4-C3-C2	3.94	117.74	110.83
2	A	401	SUV	O1-C1-N2	-3.80	112.96	116.47
5	A	412	SOG	C4-C3-C2	3.79	117.49	110.83
6	A	426	PGW	O01-C1-C2	3.70	119.49	111.48
5	B	405	SOG	C1'-S1-C1	3.67	108.38	100.45
5	A	405	SOG	C1-O5-C5	3.65	119.11	112.56
6	B	426	PGW	O01-C1-C2	3.54	119.13	111.48
5	B	413	SOG	O5-C5-C4	3.51	116.02	109.70
5	A	405	SOG	C4-C3-C2	3.43	116.85	110.83
5	B	412	SOG	C1-O5-C5	3.39	118.64	112.56
5	A	405	SOG	C1-C2-C3	3.38	117.15	110.55
5	B	413	SOG	C3-C4-C5	3.33	116.28	110.23
2	A	401	SUV	C3-N2-C1	3.33	106.05	103.42
5	B	412	SOG	O5-C5-C4	3.32	115.67	109.70
5	A	423	SOG	C2'-C1'-S1	-3.27	110.34	113.74
2	B	401	SUV	O1-C1-N2	-3.23	113.49	116.47
6	B	426	PGW	O03-C19-C20	3.18	121.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	SOG	O5-C5-C4	3.15	115.38	109.70
5	B	408	SOG	C3-C4-C5	3.12	115.90	110.23
2	B	401	SUV	C3-N2-C1	3.12	105.88	103.42
5	A	412	SOG	C3-C4-C5	3.10	115.85	110.23
4	A	403	CIT	O6-C6-C3	3.08	119.04	113.14
5	B	417	SOG	C4-C3-C2	3.07	116.22	110.83
5	A	410	SOG	C4-C3-C2	3.04	116.17	110.83
5	B	412	SOG	C3-C4-C5	2.98	115.63	110.23
5	B	417	SOG	O5-C5-C6	2.95	113.75	106.44
5	B	417	SOG	C1-O5-C5	2.79	117.56	112.56
2	A	401	SUV	O1-C8-C7	2.73	132.23	126.49
5	A	406	SOG	C1-O5-C5	2.72	117.44	112.56
5	A	409	SOG	C1-C2-C3	2.68	115.78	110.55
5	A	406	SOG	C3-C4-C5	2.65	115.04	110.23
5	B	408	SOG	O5-C5-C4	2.64	114.47	109.70
5	A	406	SOG	C4-C3-C2	2.64	115.46	110.83
5	B	405	SOG	O5-C5-C6	2.63	112.96	106.44
2	B	401	SUV	O1-C8-C7	2.61	131.98	126.49
5	B	411	SOG	C4-C3-C2	2.58	115.36	110.83
5	B	415	SOG	C3-C4-C5	2.54	114.83	110.23
5	A	407	SOG	C6-C5-C4	2.52	119.19	113.02
5	B	421	SOG	C1'-S1-C1	2.49	105.84	100.45
5	B	410	SOG	C3-C4-C5	2.49	114.75	110.23
6	A	426	PGW	C4-C3-C2	-2.44	104.18	113.13
5	B	417	SOG	C3-C4-C5	2.37	114.53	110.23
5	B	407	SOG	C1-O5-C5	2.36	116.79	112.56
6	A	426	PGW	O03-C19-C20	2.36	119.03	111.83
6	B	426	PGW	O03-C19-O04	-2.35	117.75	123.63
5	A	405	SOG	O2-C2-C1	-2.31	106.18	110.30
5	A	408	SOG	C3-C4-C5	2.31	114.42	110.23
5	B	410	SOG	C4-C3-C2	2.30	114.88	110.83
2	B	401	SUV	C7-C8-C3	-2.30	120.83	123.62
5	B	409	SOG	C1'-S1-C1	2.28	105.37	100.45
2	A	401	SUV	C7-C8-C3	-2.26	120.87	123.62
5	A	405	SOG	O5-C1-C2	2.19	113.34	110.32
5	A	409	SOG	C1-O5-C5	-2.16	108.69	112.56
5	B	409	SOG	C1-O5-C5	2.15	116.42	112.56
5	B	415	SOG	O5-C5-C6	2.11	111.67	106.44
5	A	405	SOG	C3-C4-C5	2.10	114.04	110.23
5	B	417	SOG	O5-C1-C2	2.06	113.16	110.32
5	B	407	SOG	C1'-S1-C1	2.05	104.88	100.45
5	A	412	SOG	C1-C2-C3	2.03	114.52	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	420	SOG	C4-C3-C2	2.01	114.36	110.83

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	SOG	O5-C1-S1-C1'
5	A	408	SOG	O5-C1-S1-C1'
5	A	414	SOG	S1-C1'-C2'-C3'
5	A	419	SOG	S1-C1'-C2'-C3'
5	B	407	SOG	O5-C1-S1-C1'
5	B	414	SOG	O5-C1-S1-C1'
5	B	417	SOG	O5-C1-S1-C1'
5	B	424	SOG	S1-C1'-C2'-C3'
6	A	426	PGW	OAF-C05-CAD-OAE
6	A	426	PGW	C04-C05-CAD-OAE
6	A	426	PGW	C03-O11-P-O12
6	A	426	PGW	C03-O11-P-O13
6	A	426	PGW	C04-O12-P-O13
6	A	426	PGW	C04-O12-P-O14
6	B	426	PGW	C03-O11-P-O14
6	B	426	PGW	C04-O12-P-O14
5	A	412	SOG	C4-C5-C6-O6
5	B	408	SOG	S1-C1'-C2'-C3'
5	B	415	SOG	O5-C5-C6-O6
5	A	409	SOG	O5-C5-C6-O6
5	A	420	SOG	O5-C5-C6-O6
5	A	407	SOG	C4-C5-C6-O6
5	B	417	SOG	C4-C5-C6-O6
5	A	407	SOG	O5-C5-C6-O6
5	B	421	SOG	O5-C5-C6-O6
5	A	405	SOG	S1-C1'-C2'-C3'
5	A	406	SOG	S1-C1'-C2'-C3'
5	A	408	SOG	O5-C5-C6-O6
3	A	402	PG4	O2-C3-C4-O3
3	B	404	PG4	O2-C3-C4-O3
5	A	412	SOG	O5-C5-C6-O6
5	B	411	SOG	O5-C5-C6-O6
5	B	414	SOG	O5-C5-C6-O6
5	B	407	SOG	S1-C1'-C2'-C3'
5	B	412	SOG	C4-C5-C6-O6
5	B	411	SOG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	412	SOG	O5-C5-C6-O6
5	B	417	SOG	O5-C5-C6-O6
5	A	409	SOG	C4-C5-C6-O6
5	B	414	SOG	C4-C5-C6-O6
3	B	404	PG4	O3-C5-C6-O4
5	B	415	SOG	C4-C5-C6-O6
6	B	426	PGW	OAF-C05-CAD-OAE
3	B	403	PG4	O2-C3-C4-O3
5	A	406	SOG	C4-C5-C6-O6
5	A	420	SOG	C4-C5-C6-O6
5	B	408	SOG	O5-C5-C6-O6
5	A	412	SOG	S1-C1'-C2'-C3'
3	A	402	PG4	O4-C7-C8-O5
3	B	402	PG4	O1-C1-C2-O2
5	A	419	SOG	C1'-C2'-C3'-C4'
5	A	406	SOG	O5-C5-C6-O6
5	B	413	SOG	C1'-C2'-C3'-C4'
5	B	420	SOG	C1'-C2'-C3'-C4'
6	A	426	PGW	C19-C20-C21-C22
5	A	413	SOG	S1-C1'-C2'-C3'
6	B	426	PGW	C04-C05-CAD-OAE
5	A	410	SOG	C1'-C2'-C3'-C4'
5	A	413	SOG	C1'-C2'-C3'-C4'
5	B	417	SOG	C1'-C2'-C3'-C4'
3	B	403	PG4	O3-C5-C6-O4
5	A	409	SOG	S1-C1'-C2'-C3'
3	B	402	PG4	O3-C5-C6-O4
5	A	413	SOG	C2'-C3'-C4'-C5'
5	B	411	SOG	C4'-C5'-C6'-C7'
5	B	407	SOG	C3'-C4'-C5'-C6'
6	B	426	PGW	C25-C26-C27-C15
5	B	409	SOG	C1'-C2'-C3'-C4'
5	A	404	SOG	C4'-C5'-C6'-C7'
6	A	426	PGW	C23-C24-C25-C26
5	A	417	SOG	C3'-C4'-C5'-C6'
5	B	412	SOG	C3'-C4'-C5'-C6'
3	B	403	PG4	O1-C1-C2-O2
5	B	406	SOG	C4-C5-C6-O6
5	B	407	SOG	C1'-C2'-C3'-C4'
5	B	413	SOG	C2'-C3'-C4'-C5'
5	B	413	SOG	C4'-C5'-C6'-C7'
6	A	426	PGW	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
5	A	410	SOG	S1-C1'-C2'-C3'
5	B	412	SOG	S1-C1'-C2'-C3'
5	B	418	SOG	S1-C1'-C2'-C3'
5	B	421	SOG	C4'-C5'-C6'-C7'
5	A	408	SOG	C3'-C4'-C5'-C6'
6	A	426	PGW	C24-C25-C26-C27
5	A	408	SOG	C1'-C2'-C3'-C4'
5	A	409	SOG	C1'-C2'-C3'-C4'
6	A	426	PGW	C07-C08-C09-C11
5	B	410	SOG	C4'-C5'-C6'-C7'
6	B	426	PGW	C06-C07-C08-C09
5	B	409	SOG	C2'-C3'-C4'-C5'
5	B	417	SOG	C2'-C3'-C4'-C5'
6	A	426	PGW	C21-C22-C23-C24
5	A	404	SOG	C3'-C4'-C5'-C6'
3	A	402	PG4	O1-C1-C2-O2
5	B	421	SOG	C2'-C3'-C4'-C5'
5	A	404	SOG	S1-C1'-C2'-C3'
3	A	402	PG4	O3-C5-C6-O4
5	A	415	SOG	C2'-C3'-C4'-C5'
5	B	406	SOG	O5-C5-C6-O6
5	B	414	SOG	C3'-C4'-C5'-C6'
6	A	426	PGW	C10-C06-C07-C08
6	B	426	PGW	C10-C06-C07-C08
5	B	406	SOG	C1'-C2'-C3'-C4'
5	A	408	SOG	C4-C5-C6-O6
5	B	409	SOG	O5-C5-C6-O6
5	B	411	SOG	C3'-C4'-C5'-C6'
5	B	405	SOG	O5-C5-C6-O6
5	A	417	SOG	C2'-C3'-C4'-C5'
5	A	413	SOG	C3'-C4'-C5'-C6'
5	B	425	SOG	C4'-C5'-C6'-C7'
5	A	404	SOG	O5-C5-C6-O6
6	B	426	PGW	C21-C22-C23-C24
5	B	414	SOG	C4'-C5'-C6'-C7'
5	B	412	SOG	C2'-C3'-C4'-C5'
5	A	409	SOG	C2'-C3'-C4'-C5'
5	B	407	SOG	C5'-C6'-C7'-C8'
6	A	426	PGW	C08-C09-C11-C12
5	B	416	SOG	C3'-C4'-C5'-C6'
5	A	421	SOG	C2'-C3'-C4'-C5'
5	B	421	SOG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	412	SOG	C5'-C6'-C7'-C8'
5	B	416	SOG	C5'-C6'-C7'-C8'
5	A	408	SOG	C5'-C6'-C7'-C8'
5	A	410	SOG	C3'-C4'-C5'-C6'
5	B	414	SOG	C1'-C2'-C3'-C4'
5	B	417	SOG	C5'-C6'-C7'-C8'
5	B	418	SOG	C1'-C2'-C3'-C4'
5	A	405	SOG	C4'-C5'-C6'-C7'
6	B	426	PGW	C16-C17-C18-C28
6	B	426	PGW	C1-C2-C3-C4
5	A	409	SOG	C5'-C6'-C7'-C8'
5	B	410	SOG	C5'-C6'-C7'-C8'
5	B	414	SOG	C5'-C6'-C7'-C8'
5	B	411	SOG	S1-C1'-C2'-C3'
5	A	410	SOG	C4'-C5'-C6'-C7'
5	A	412	SOG	C1'-C2'-C3'-C4'
5	B	421	SOG	C5'-C6'-C7'-C8'
5	B	423	SOG	C4'-C5'-C6'-C7'
5	A	420	SOG	C5'-C6'-C7'-C8'
6	A	426	PGW	C11-C12-C13-C14
5	B	415	SOG	C4'-C5'-C6'-C7'
3	B	403	PG4	C3-C4-O3-C5
3	B	403	PG4	C5-C6-O4-C7
5	B	415	SOG	C3'-C4'-C5'-C6'
3	B	404	PG4	C3-C4-O3-C5
5	B	415	SOG	S1-C1'-C2'-C3'
3	B	403	PG4	C1-C2-O2-C3
6	A	426	PGW	C6-C7-C8-C9
6	B	426	PGW	O01-C02-C03-O11
5	A	405	SOG	C2-C1-S1-C1'
5	A	422	SOG	S1-C1'-C2'-C3'
5	B	416	SOG	S1-C1'-C2'-C3'
5	B	417	SOG	C2-C1-S1-C1'
3	A	402	PG4	C8-C7-O4-C6
5	B	421	SOG	S1-C1'-C2'-C3'
5	A	405	SOG	C1'-C2'-C3'-C4'
5	B	425	SOG	C3'-C4'-C5'-C6'
5	B	410	SOG	C3'-C4'-C5'-C6'
6	B	426	PGW	C01-C02-C03-O11
3	B	404	PG4	C6-C5-O3-C4
6	A	426	PGW	C20-C21-C22-C23
3	B	403	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
6	B	426	PGW	O03-C01-C02-C03
6	A	426	PGW	C03-O11-P-O14
6	A	426	PGW	C04-O12-P-O11
6	B	426	PGW	C04-O12-P-O11
6	B	426	PGW	C04-O12-P-O13
5	B	417	SOG	C3'-C4'-C5'-C6'
6	B	426	PGW	C05-C04-O12-P
5	A	418	SOG	C5'-C6'-C7'-C8'
5	A	420	SOG	C3'-C4'-C5'-C6'
5	A	423	SOG	S1-C1'-C2'-C3'
6	B	426	PGW	C27-C15-C16-C17
5	A	408	SOG	S1-C1'-C2'-C3'
3	B	402	PG4	C3-C4-O3-C5
6	A	426	PGW	O02-C1-O01-C02
6	B	426	PGW	O03-C01-C02-O01
6	A	426	PGW	C2-C1-O01-C02
5	A	417	SOG	C4'-C5'-C6'-C7'
5	A	417	SOG	C1'-C2'-C3'-C4'
5	A	421	SOG	C1'-C2'-C3'-C4'
5	B	424	SOG	C1'-C2'-C3'-C4'
5	B	408	SOG	C5'-C6'-C7'-C8'
5	B	411	SOG	C2'-C3'-C4'-C5'
5	A	409	SOG	C4'-C5'-C6'-C7'
6	A	426	PGW	C09-C11-C12-C13
5	A	405	SOG	C2'-C3'-C4'-C5'
5	A	422	SOG	C2'-C3'-C4'-C5'
3	B	403	PG4	C4-C3-O2-C2
5	B	417	SOG	C4'-C5'-C6'-C7'
5	A	416	SOG	C5'-C6'-C7'-C8'
5	B	421	SOG	C1'-C2'-C3'-C4'
5	A	422	SOG	C1'-C2'-C3'-C4'
5	A	419	SOG	C2'-C3'-C4'-C5'
5	B	421	SOG	O5-C1-S1-C1'
5	B	420	SOG	C2'-C3'-C4'-C5'
6	A	426	PGW	C16-C17-C18-C28
5	B	425	SOG	C5'-C6'-C7'-C8'
5	B	415	SOG	C1'-C2'-C3'-C4'
5	B	407	SOG	C4'-C5'-C6'-C7'
5	A	415	SOG	C1'-C2'-C3'-C4'
5	A	408	SOG	C2'-C3'-C4'-C5'
5	A	415	SOG	S1-C1'-C2'-C3'
5	A	421	SOG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
5	B	423	SOG	C5'-C6'-C7'-C8'
5	B	422	SOG	C3'-C4'-C5'-C6'
5	A	405	SOG	C2'-C1'-S1-C1
5	A	408	SOG	C2'-C1'-S1-C1
5	A	409	SOG	C2'-C1'-S1-C1
5	B	408	SOG	C2'-C1'-S1-C1
5	B	409	SOG	C2'-C1'-S1-C1
5	B	410	SOG	C2'-C1'-S1-C1
5	B	415	SOG	C2'-C1'-S1-C1
6	A	426	PGW	C18-C28-C30-C29
6	B	426	PGW	O01-C1-C2-C3
3	A	402	PG4	C1-C2-O2-C3
6	A	426	PGW	O03-C19-C20-C21
6	B	426	PGW	C23-C24-C25-C26
6	B	426	PGW	C15-C16-C17-C18
6	A	426	PGW	C05-C04-O12-P
6	A	426	PGW	C22-C23-C24-C25
6	A	426	PGW	O04-C19-C20-C21
5	B	409	SOG	S1-C1'-C2'-C3'
6	B	426	PGW	O02-C1-C2-C3
4	A	403	CIT	O7-C3-C4-C5
6	A	426	PGW	O01-C1-C2-C3

There are no ring outliers.

23 monomers are involved in 44 short contacts:

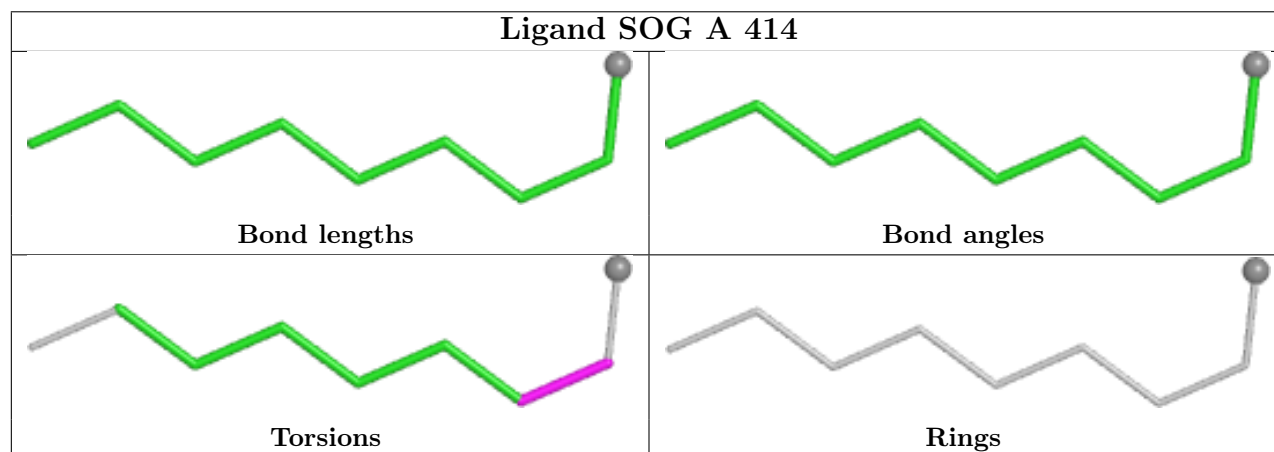
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	422	SOG	1	0
5	B	408	SOG	1	0
6	A	426	PGW	1	0
5	A	408	SOG	2	0
5	B	407	SOG	1	0
5	B	425	SOG	2	0
5	A	405	SOG	3	0
5	A	410	SOG	3	0
5	A	419	SOG	1	0
5	B	414	SOG	2	0
5	A	407	SOG	1	0
5	A	425	SOG	1	0
5	B	413	SOG	1	0
5	A	413	SOG	2	0
6	B	426	PGW	1	0

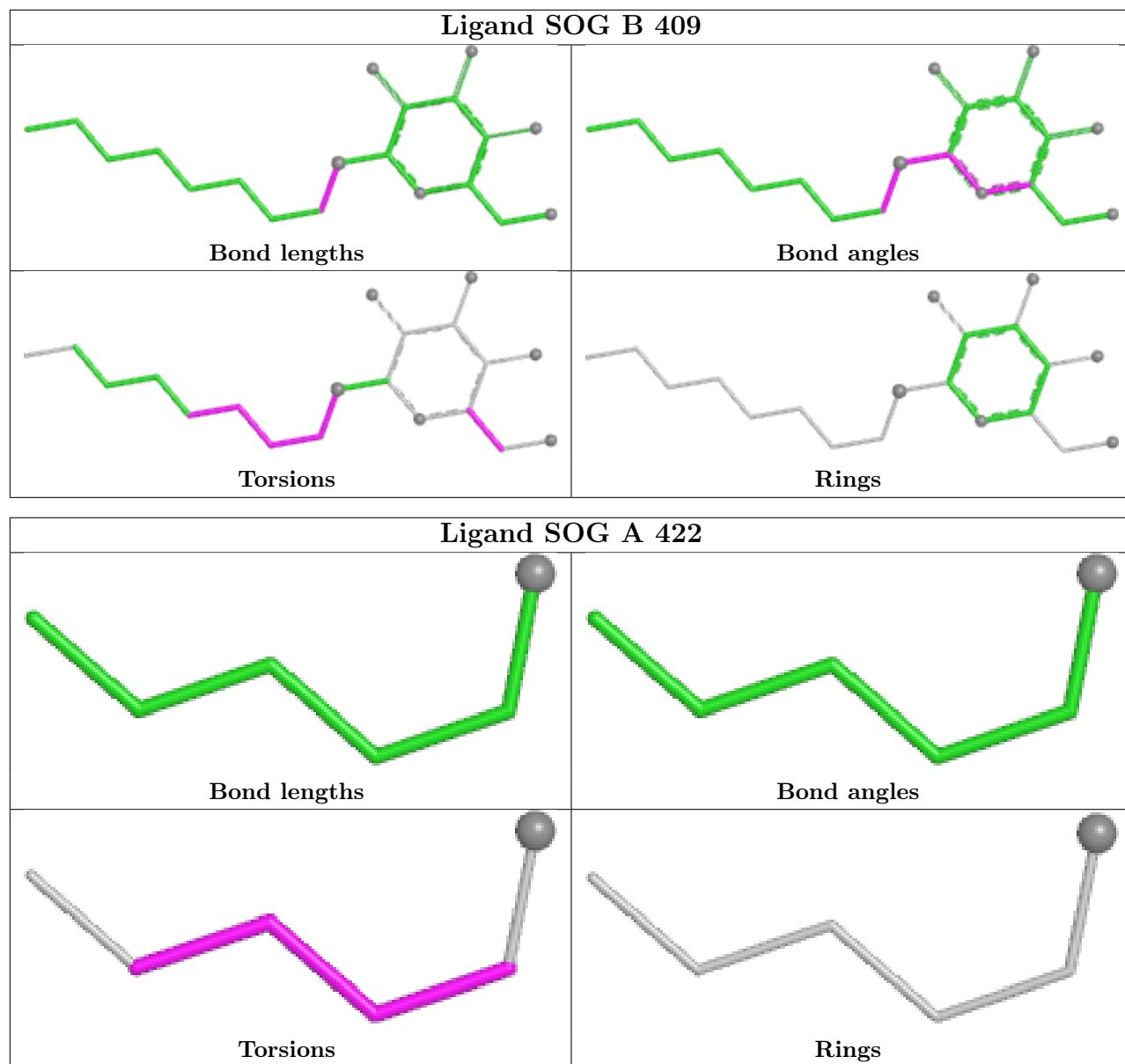
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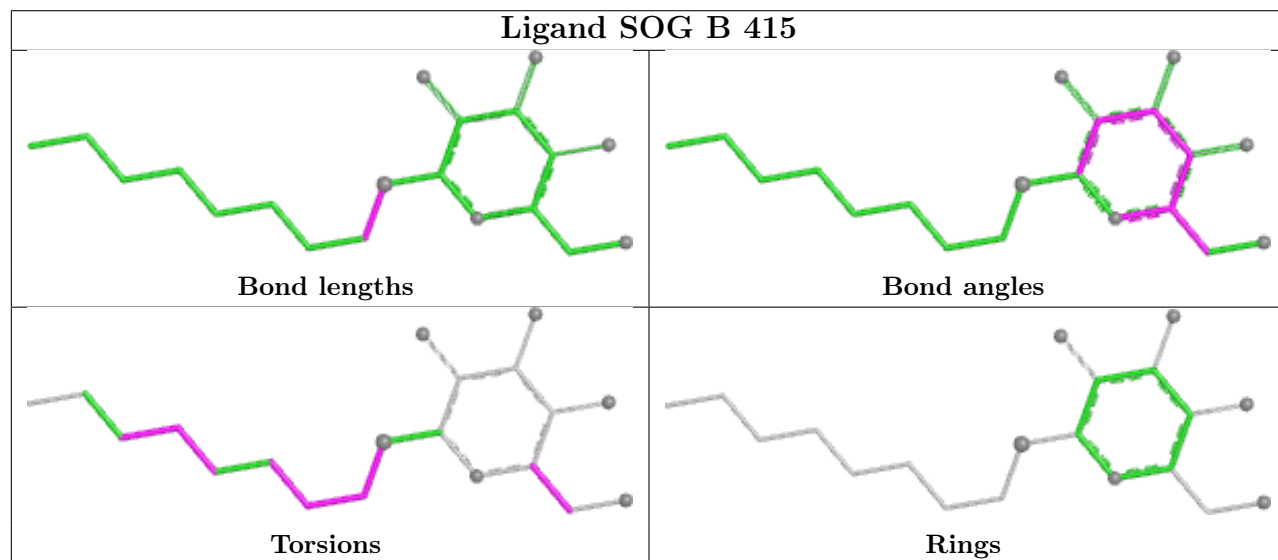
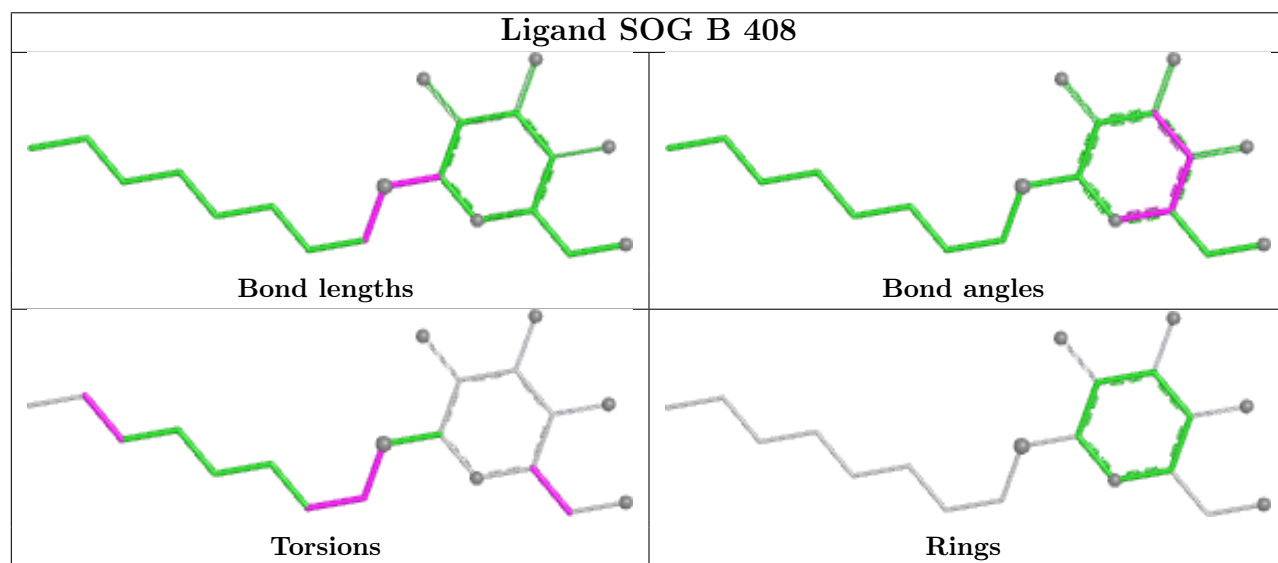
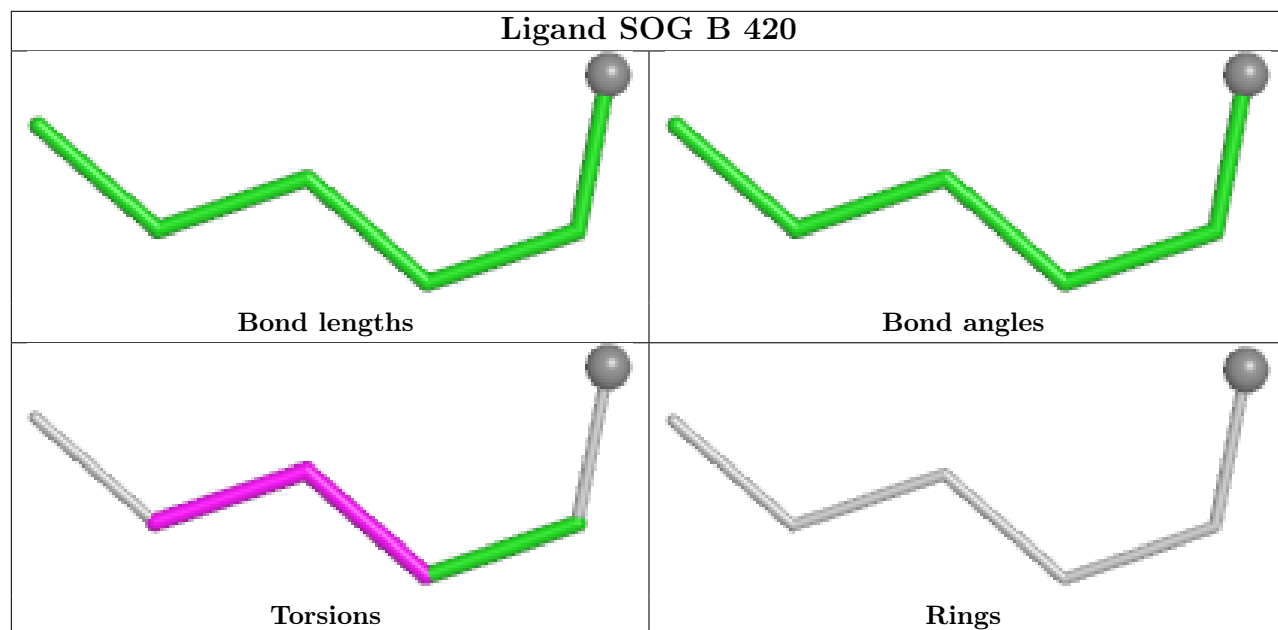
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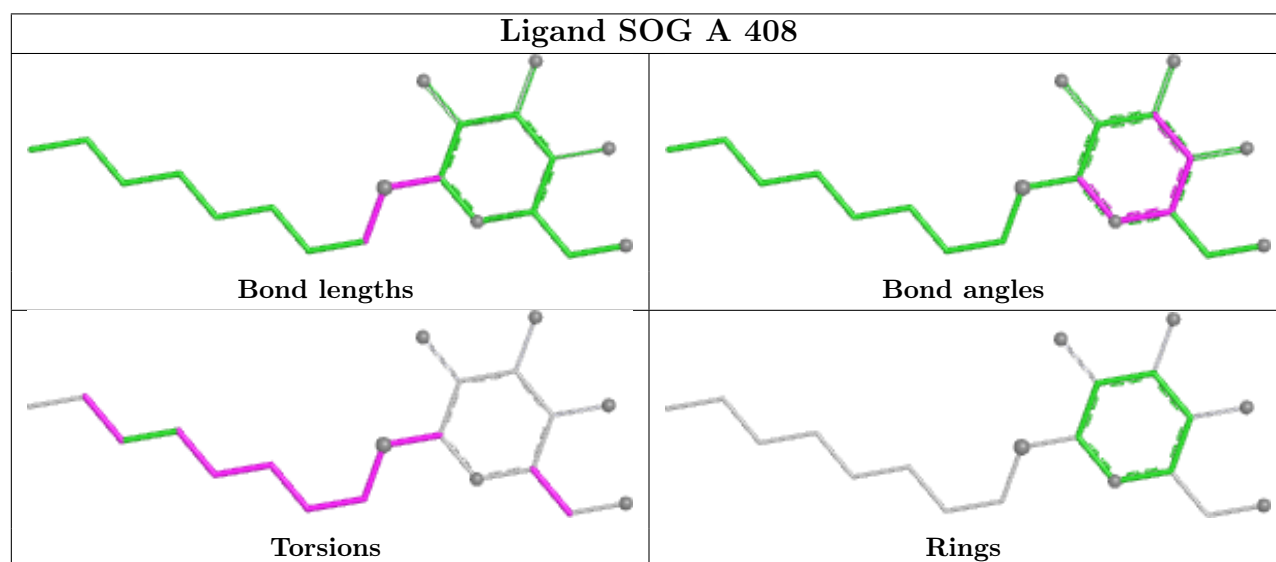
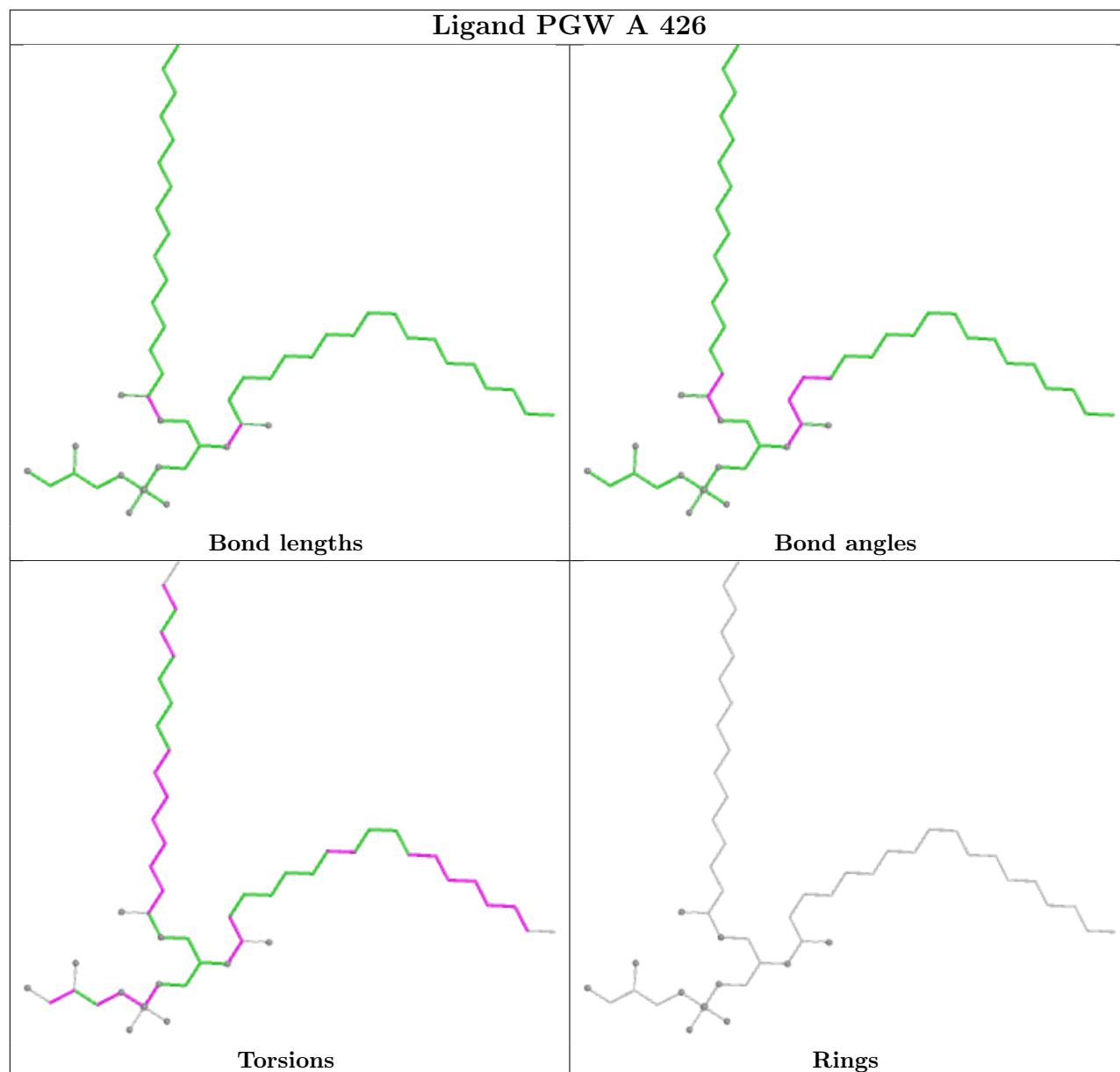
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	SOG	1	0
5	B	405	SOG	2	0
5	B	419	SOG	1	0
3	B	403	PG4	1	0
5	B	417	SOG	3	0
5	B	410	SOG	1	0
5	B	412	SOG	17	0
5	A	412	SOG	2	0

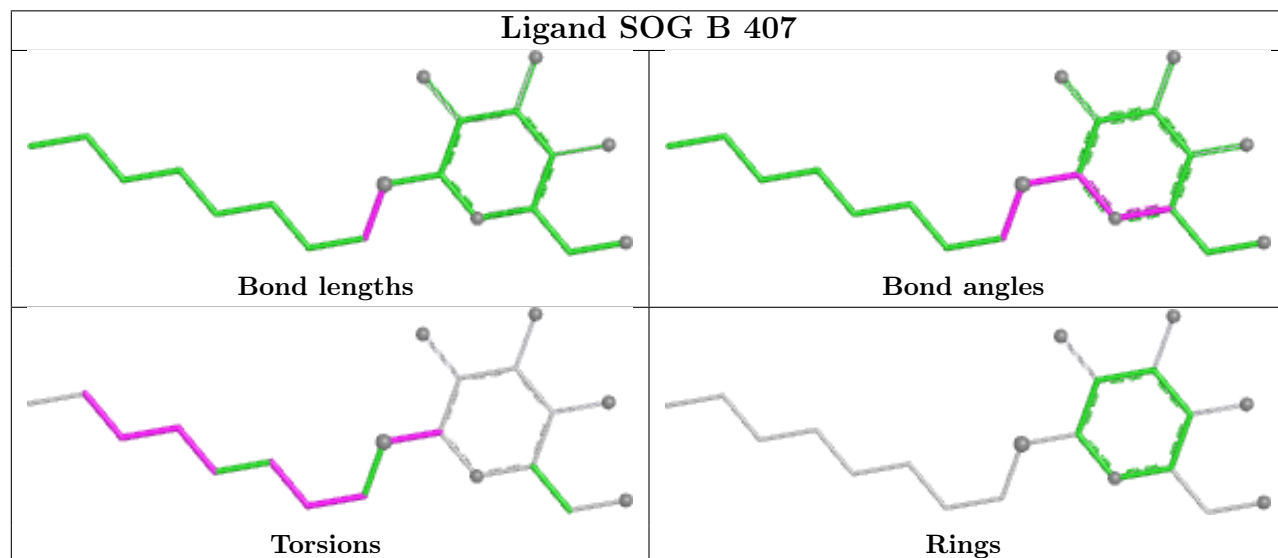
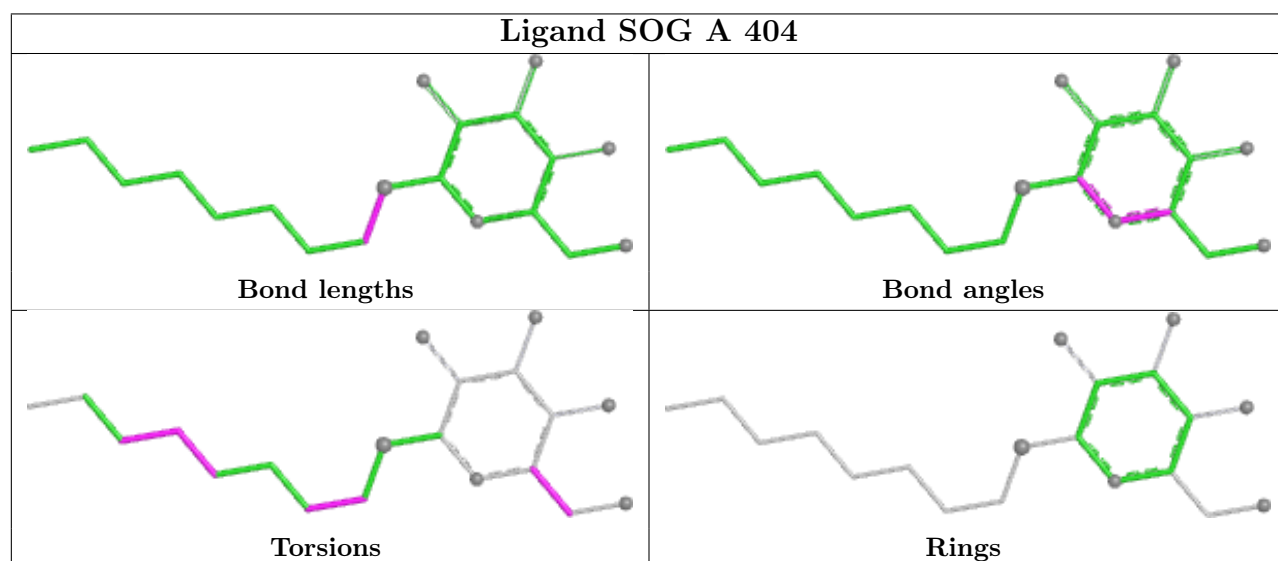
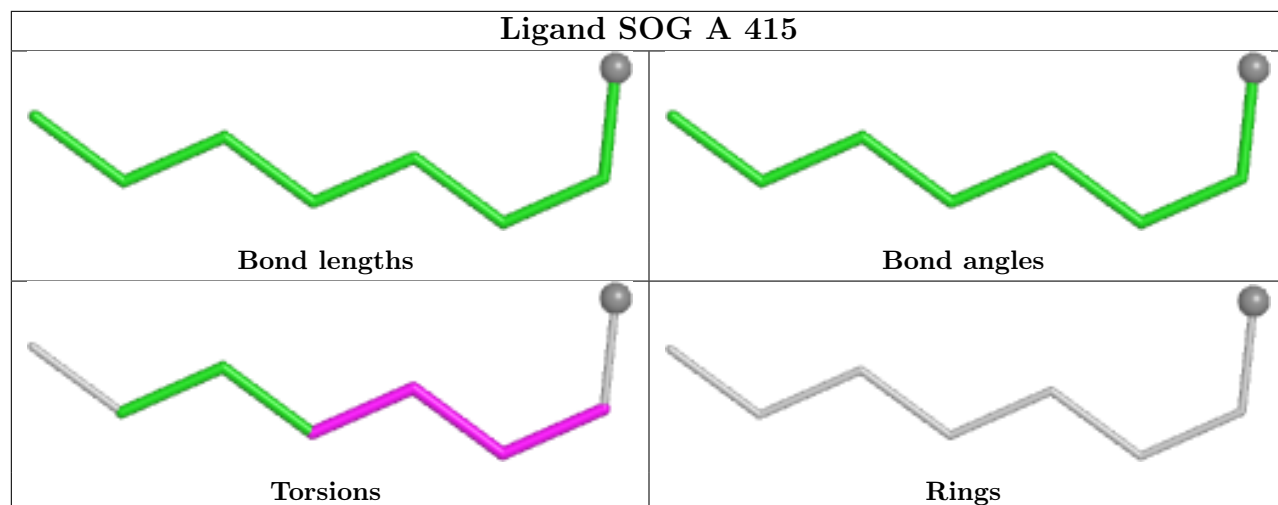
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

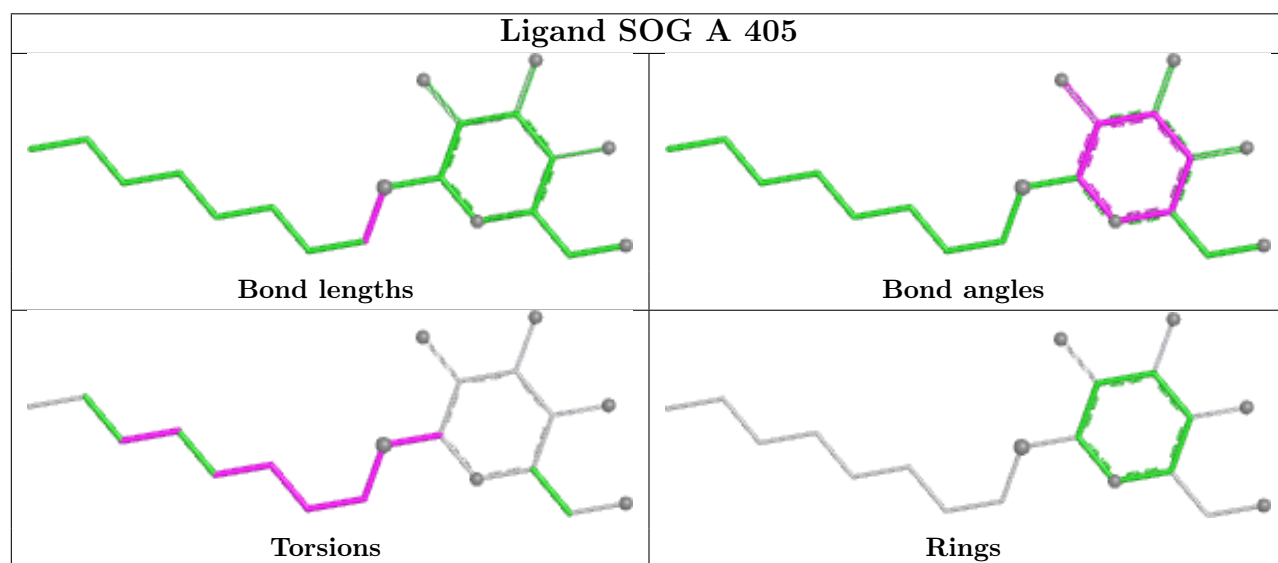
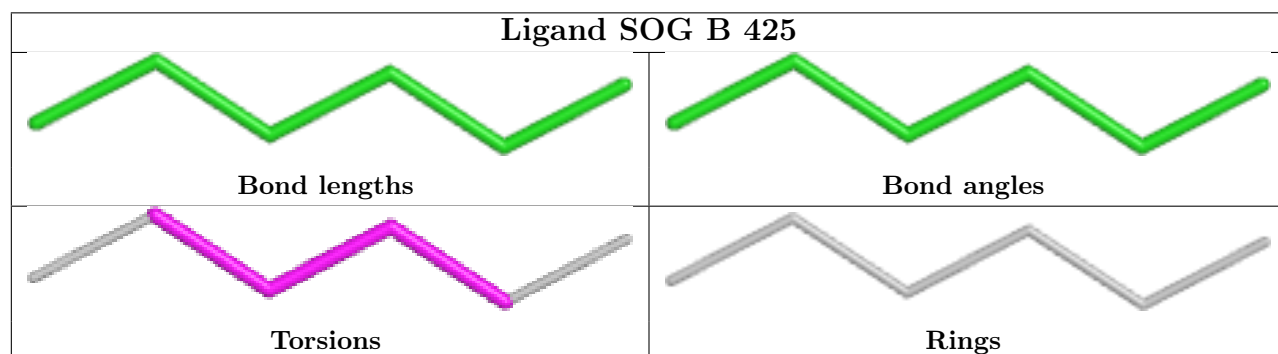
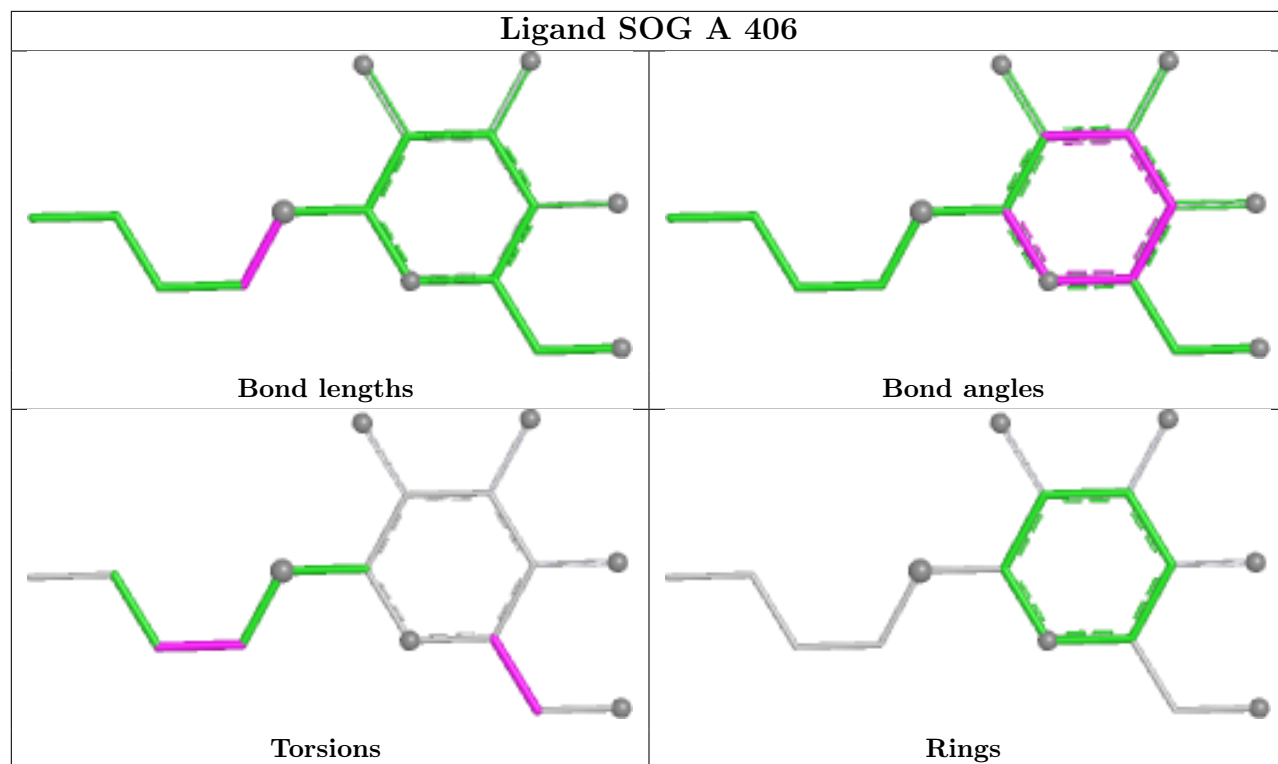


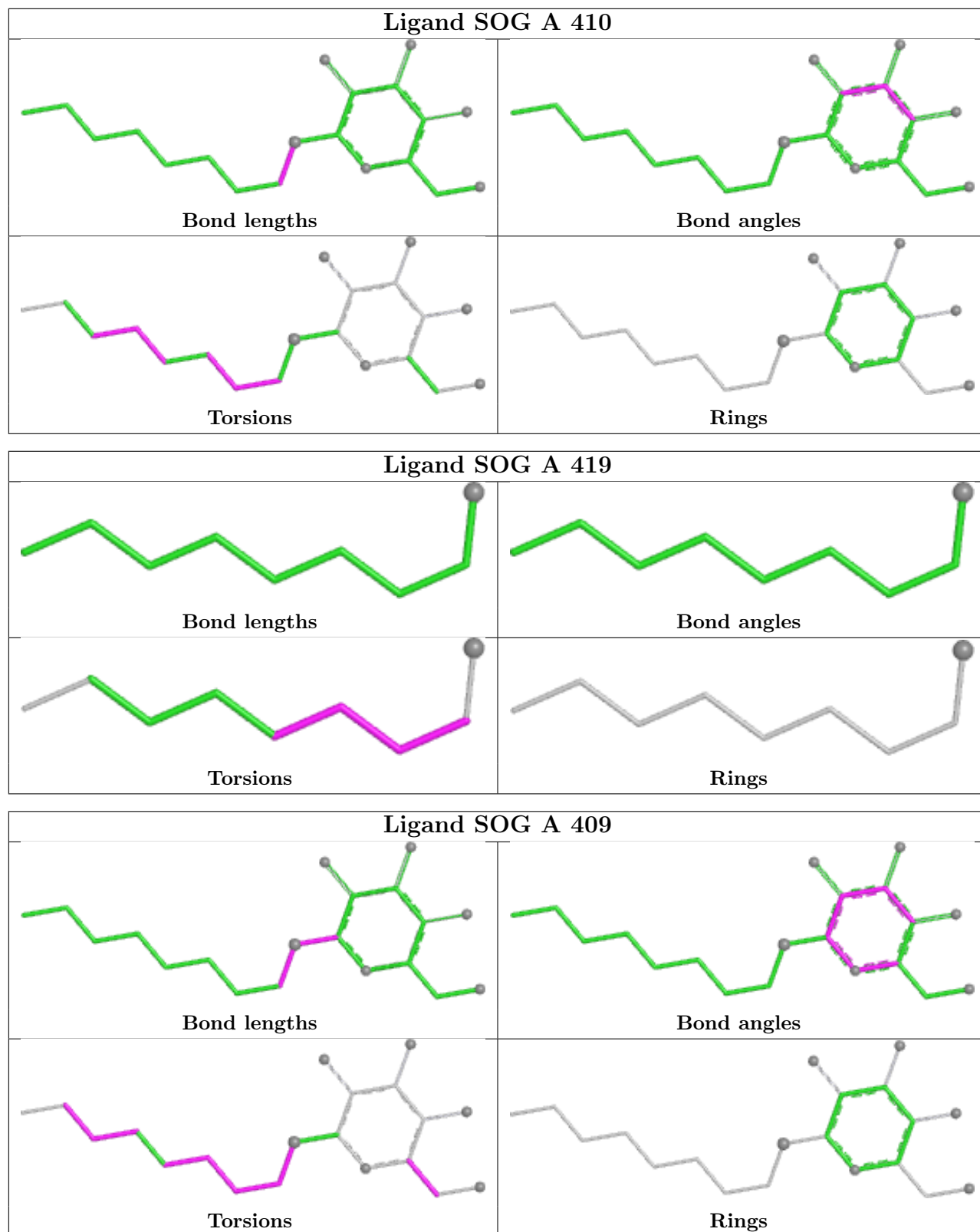


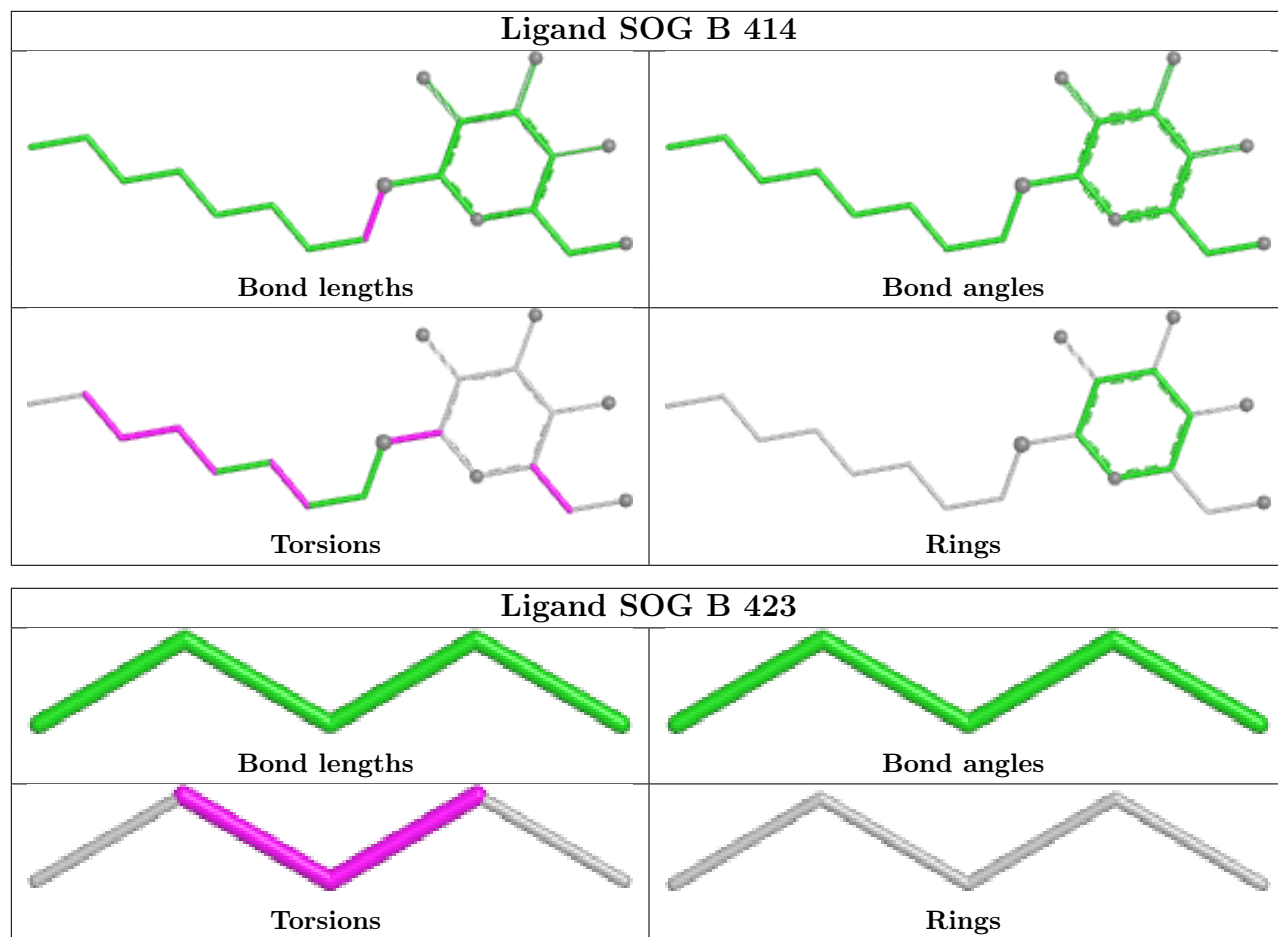


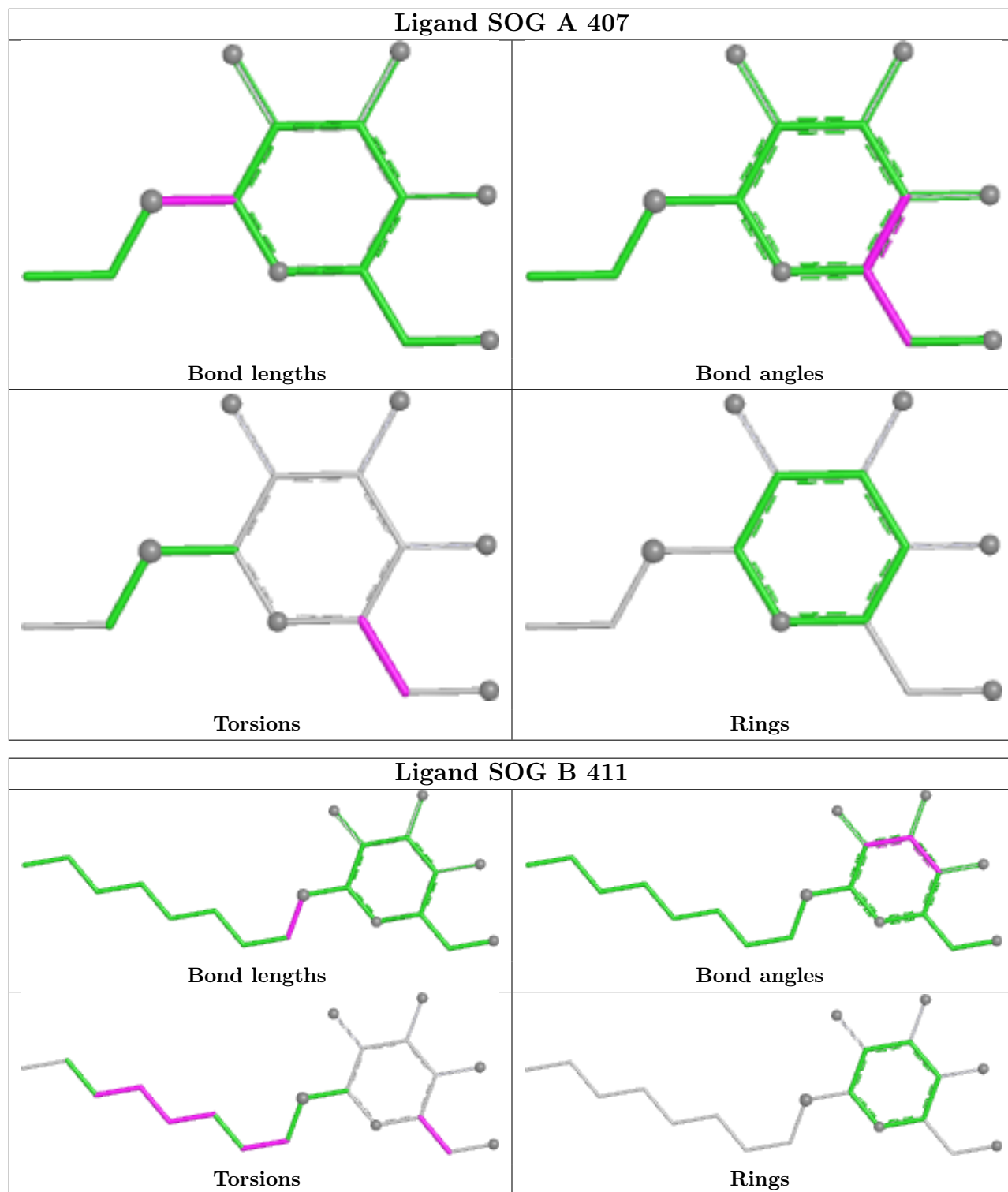


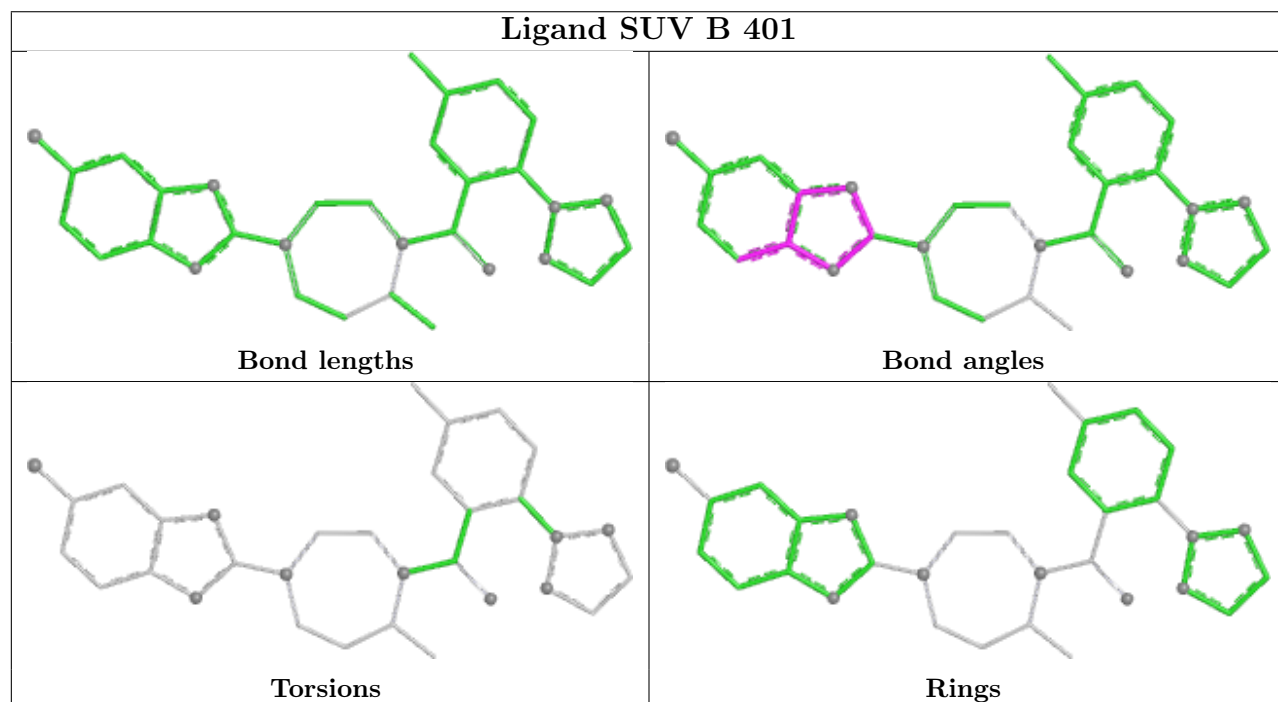
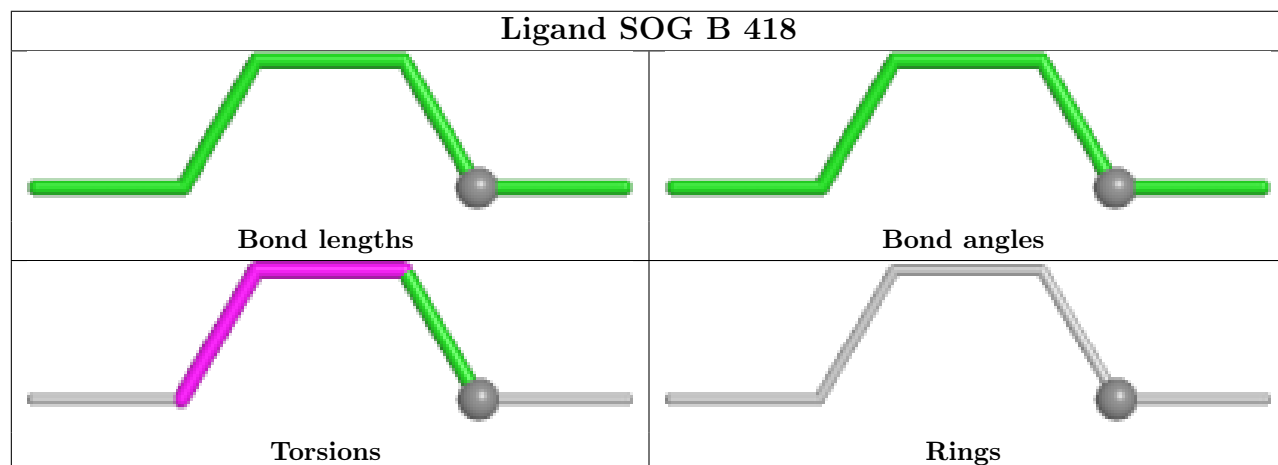
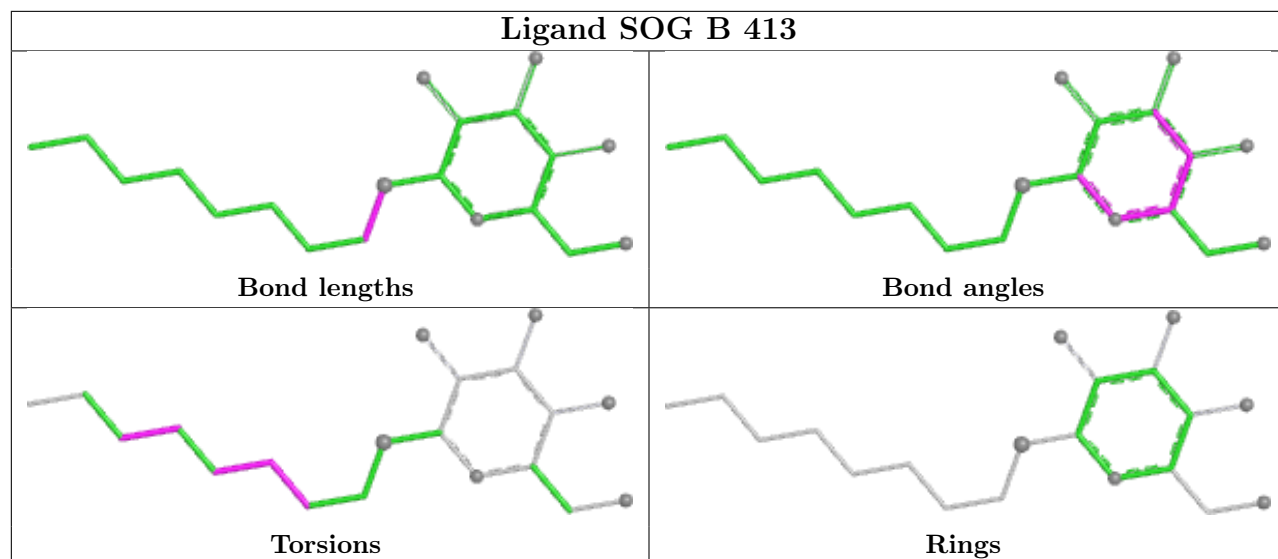


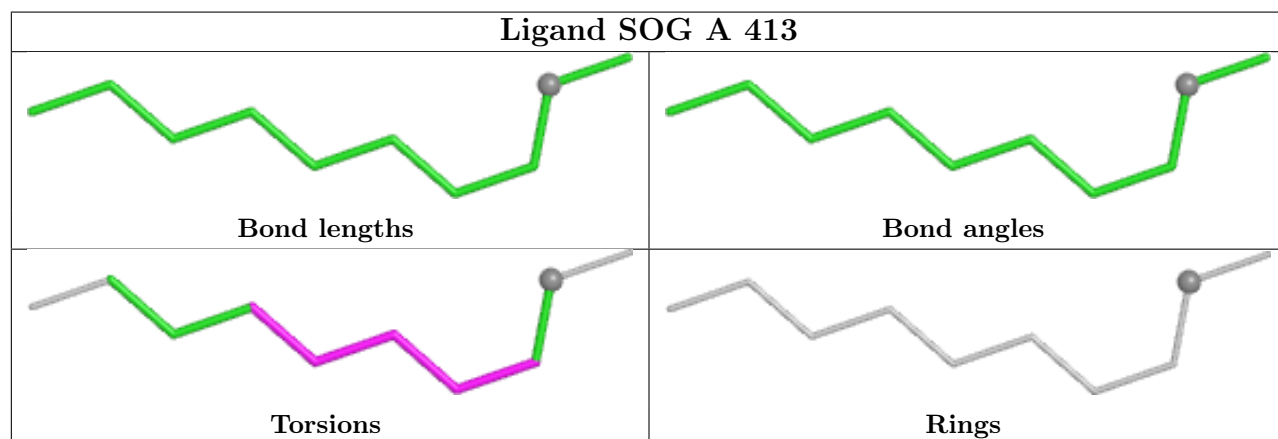
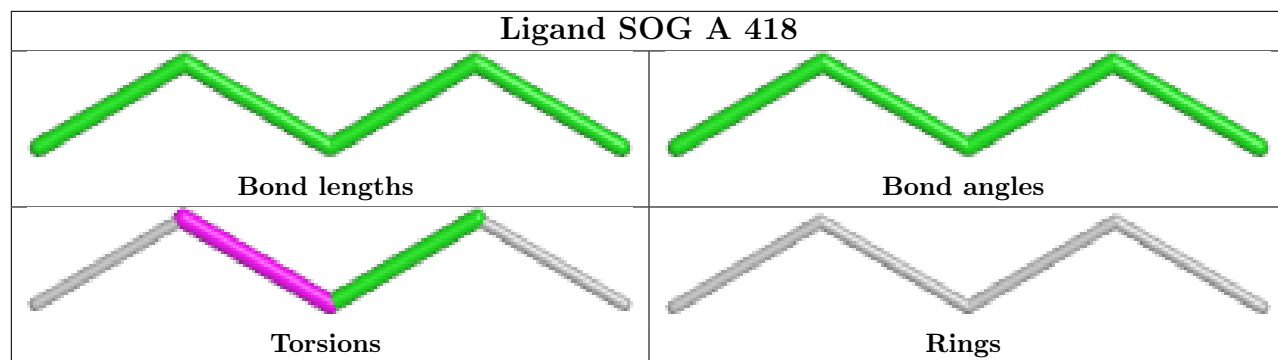


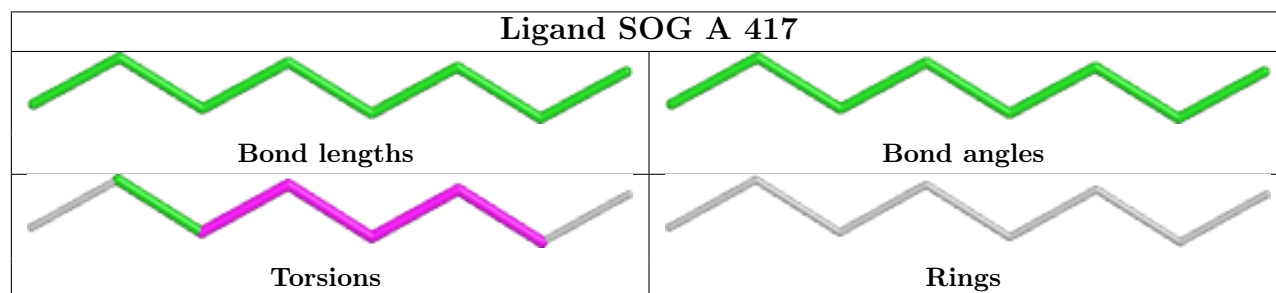
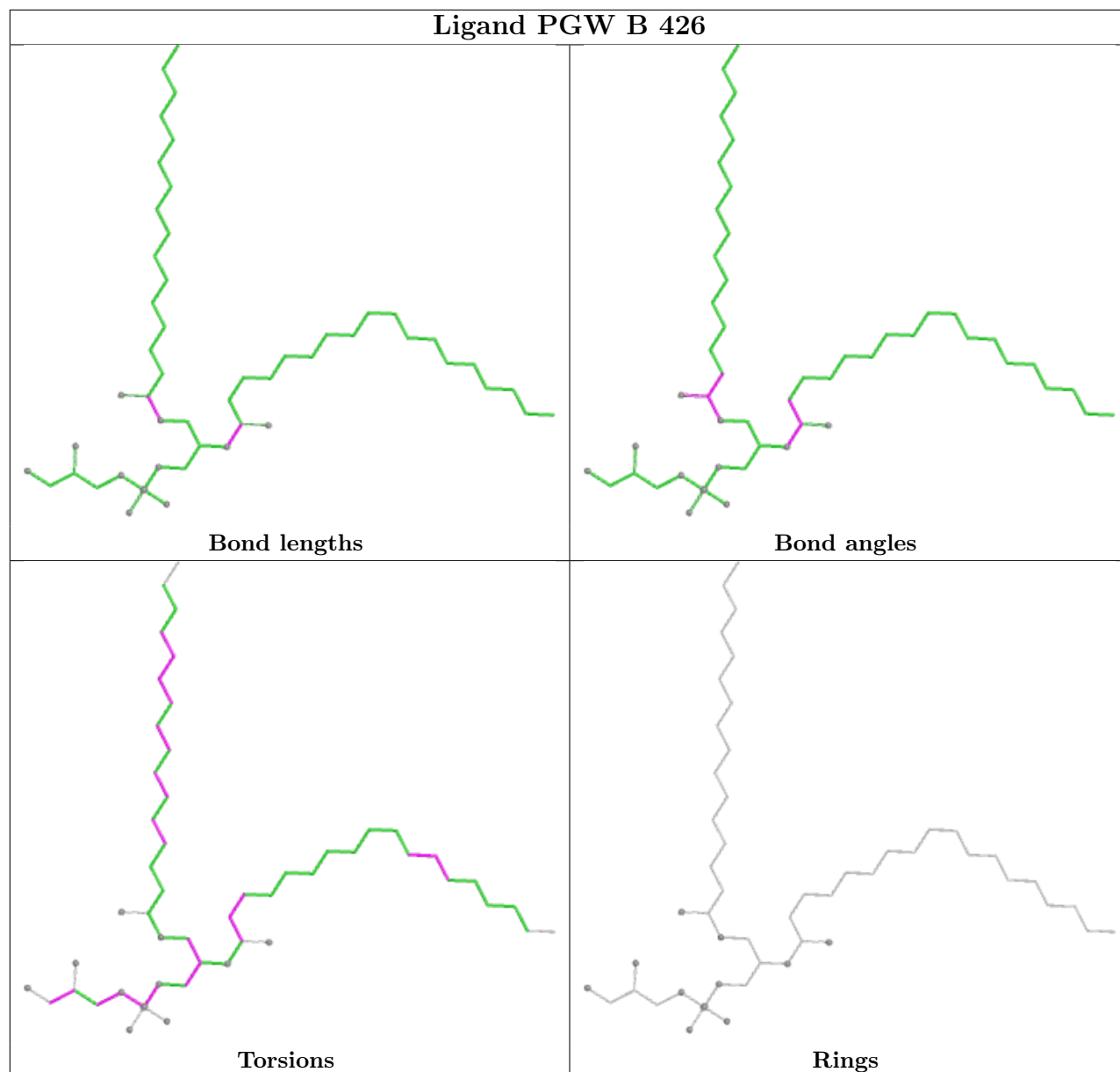


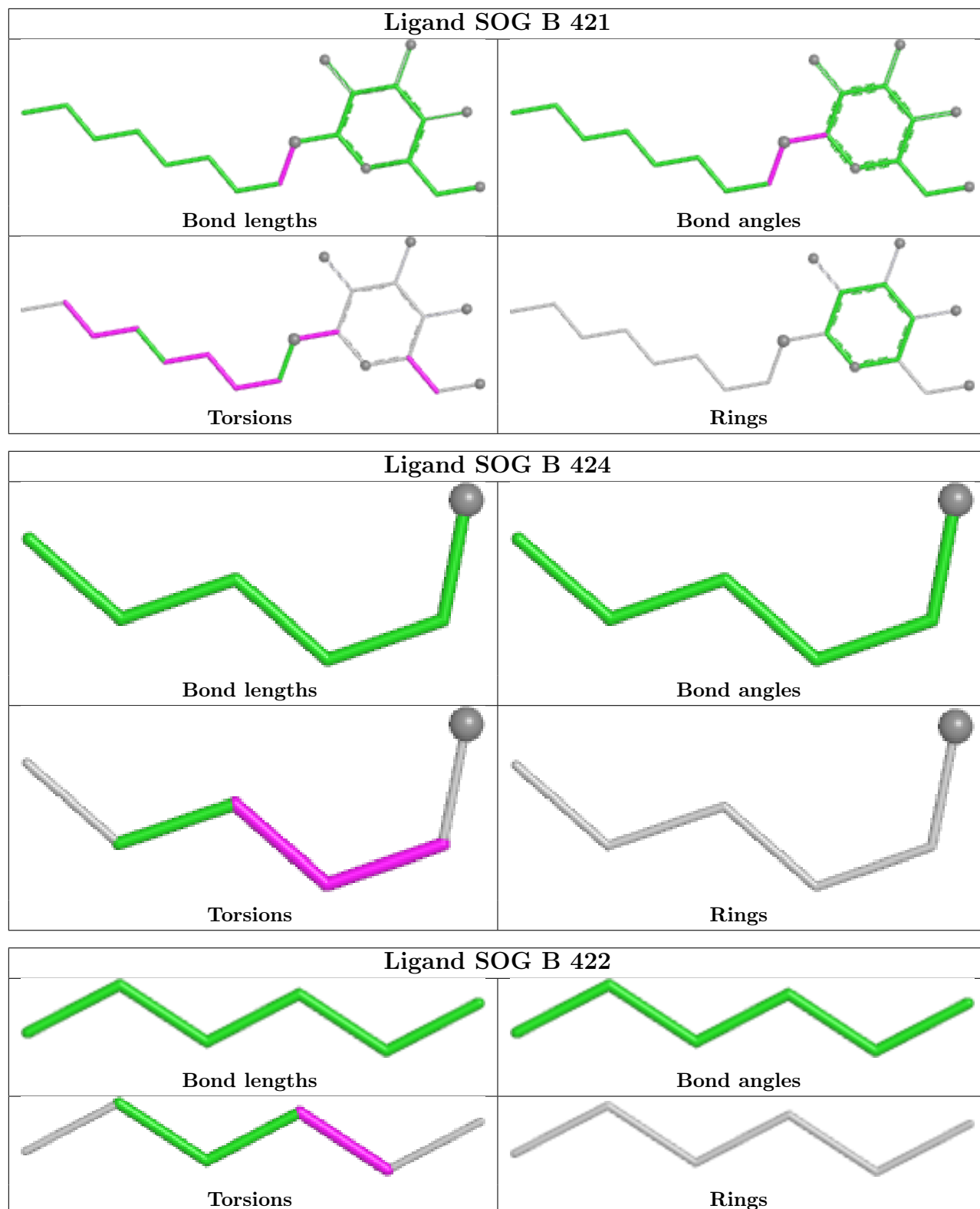




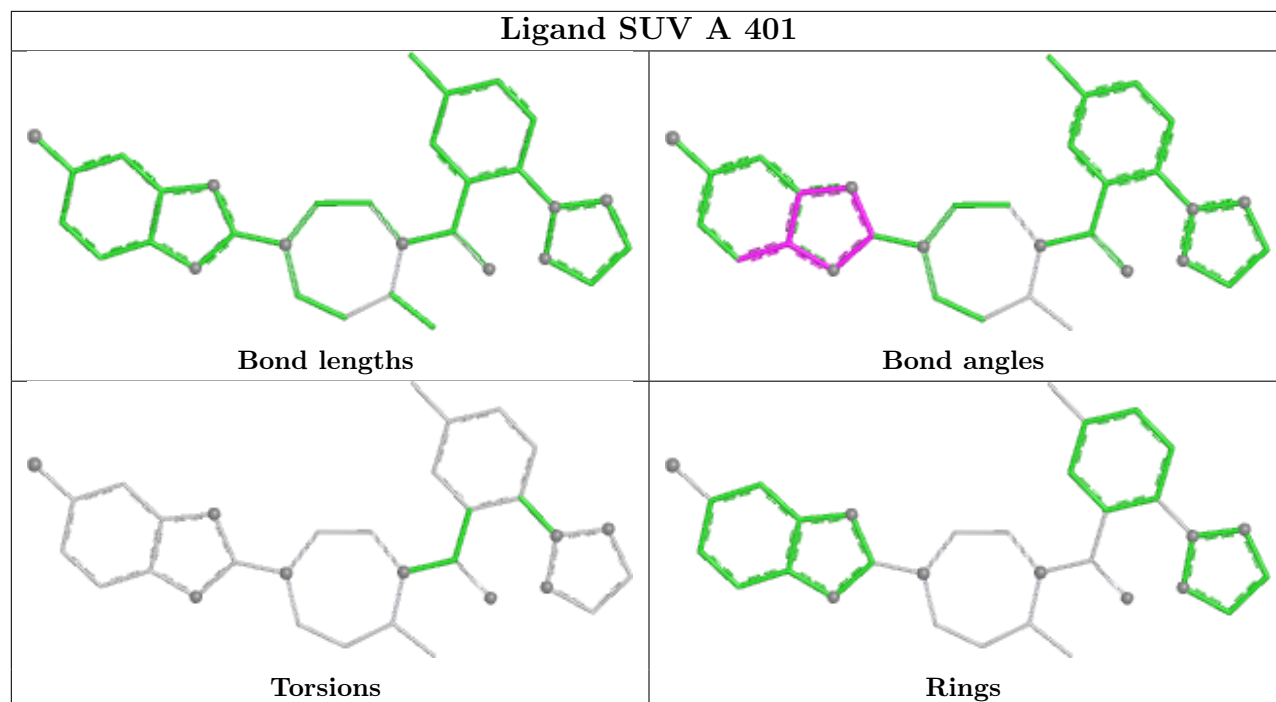




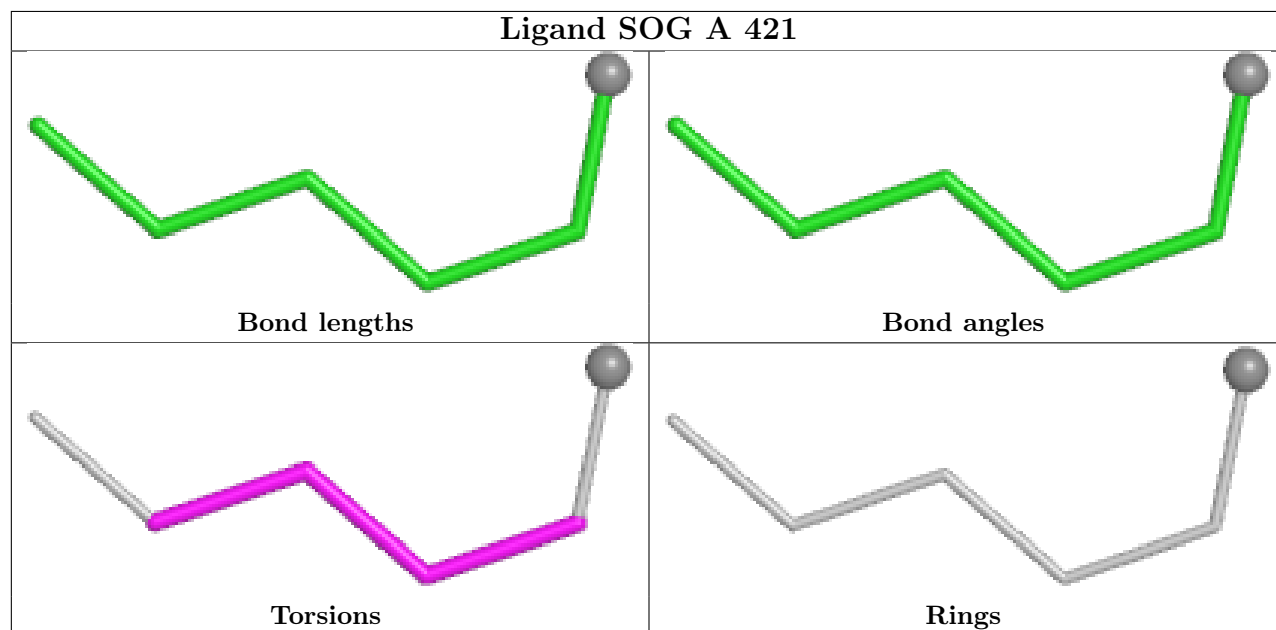


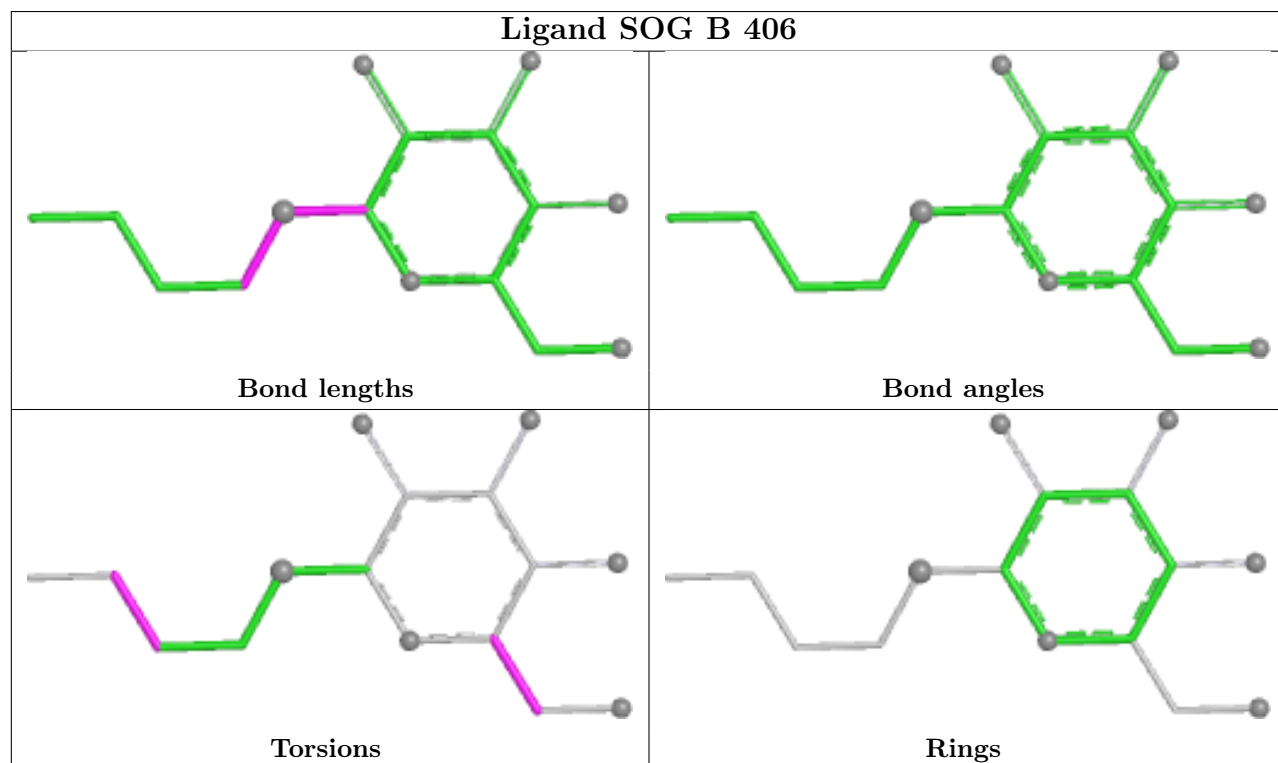
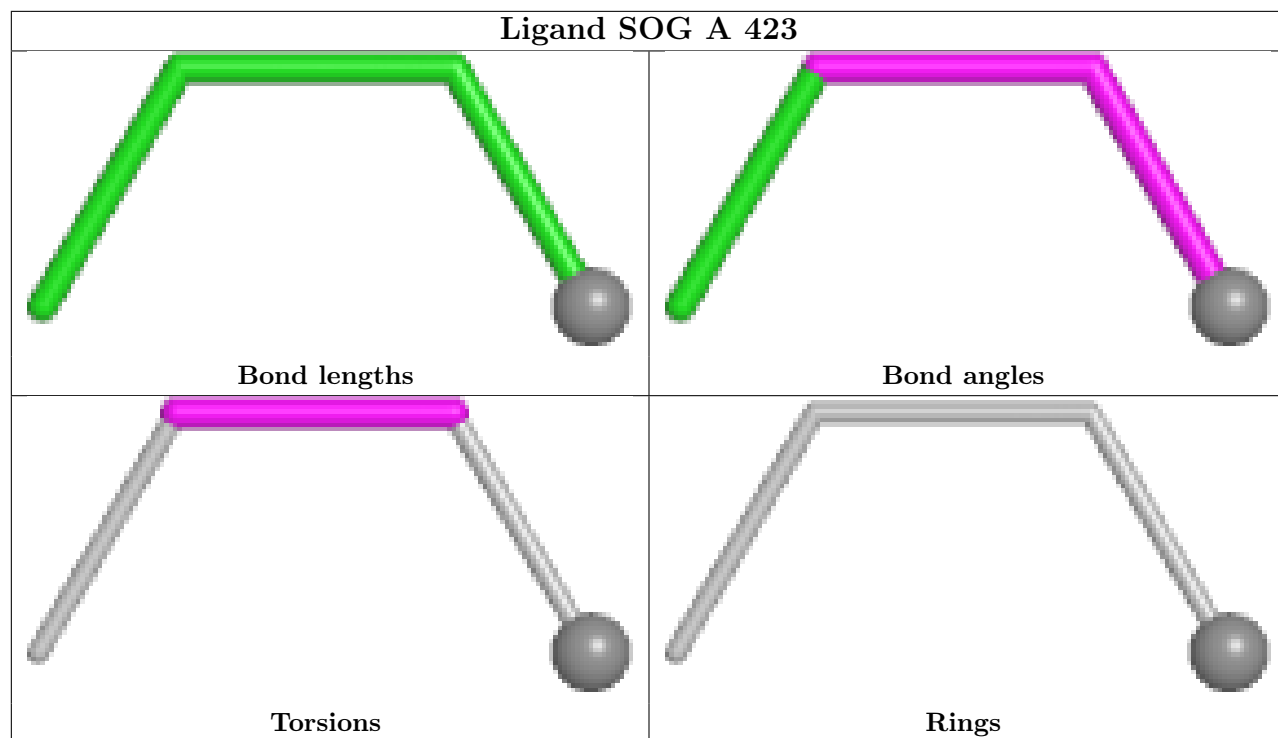


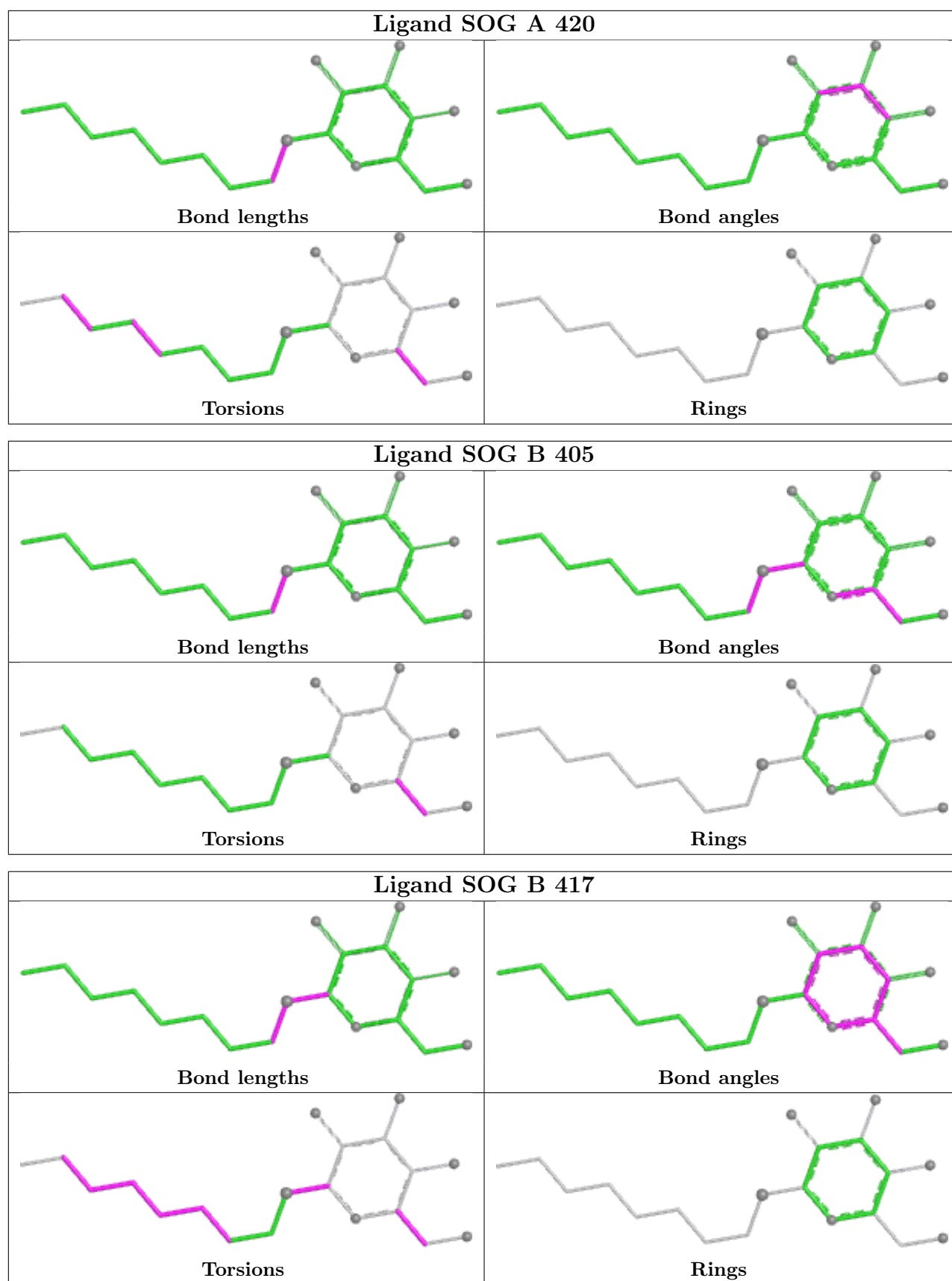
Ligand SUV A 401

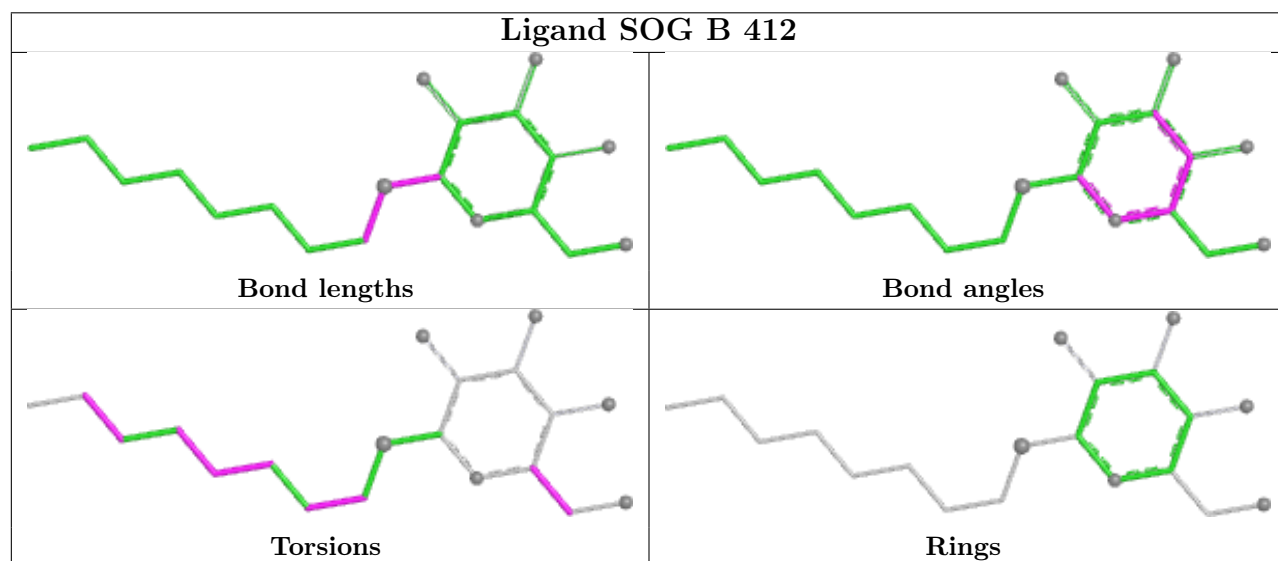
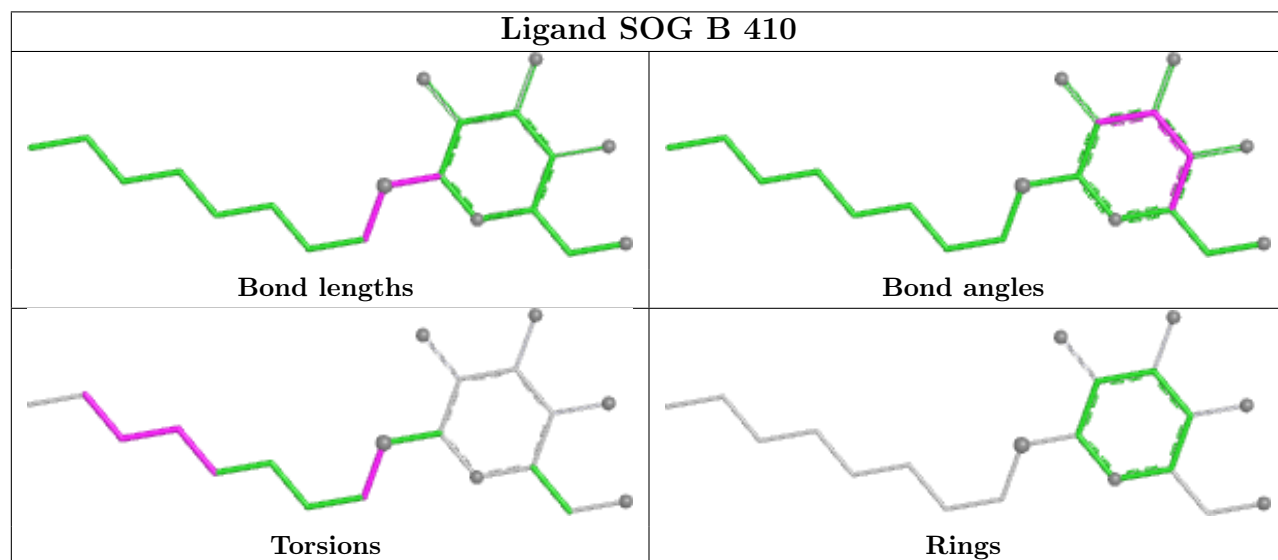
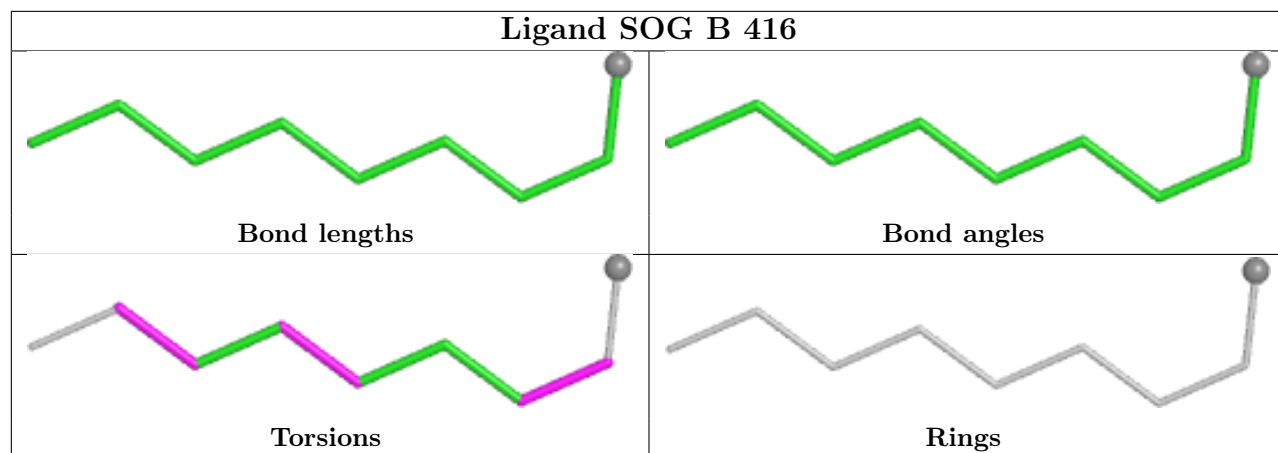


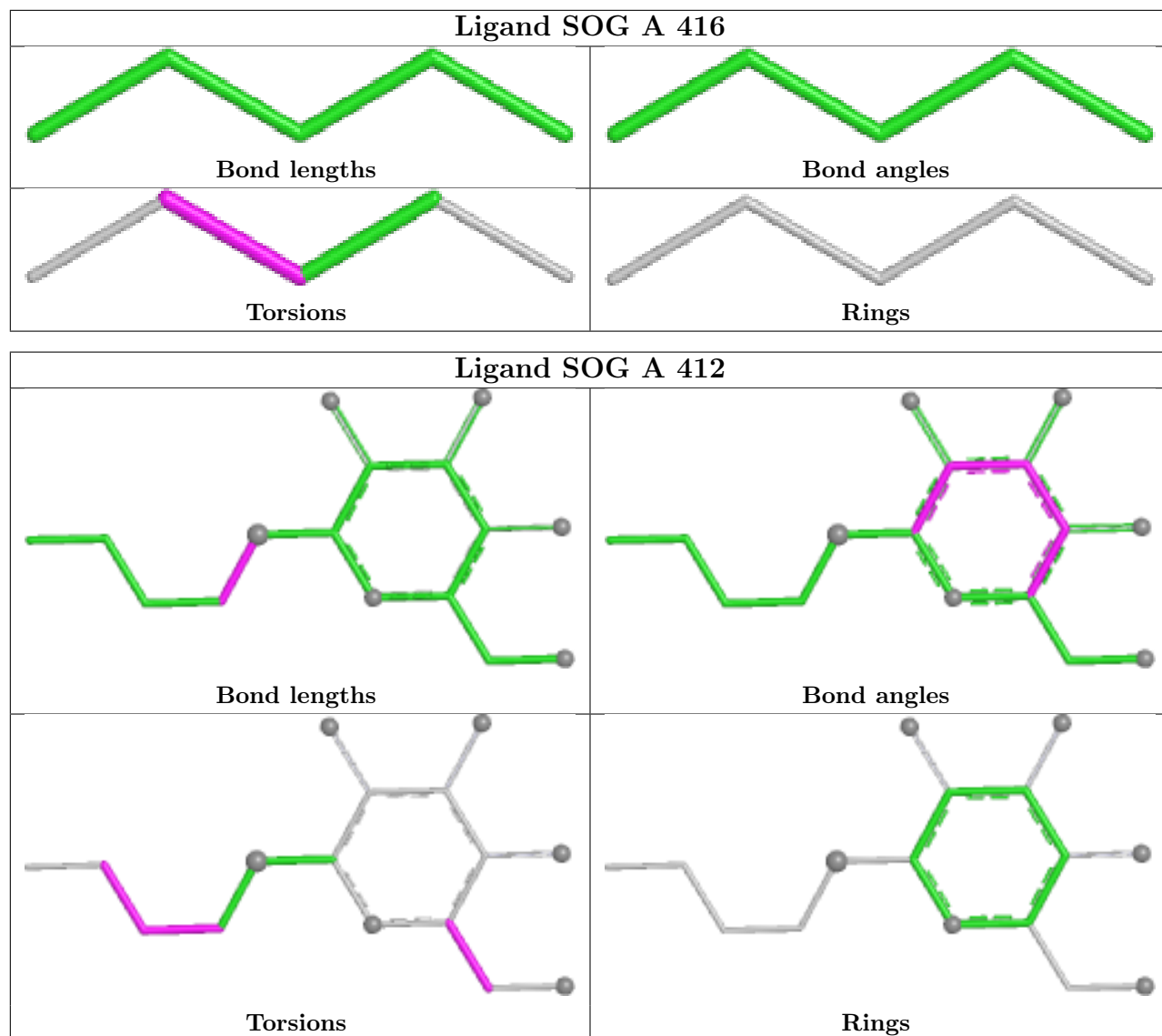
Ligand SOG A 421











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	300/336 (89%)	0.60	39 (13%) 7 6	18, 36, 83, 130	0
1	B	307/336 (91%)	0.60	41 (13%) 7 6	17, 33, 79, 130	0
All	All	607/672 (90%)	0.60	80 (13%) 7 6	17, 34, 82, 130	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	GLY	9.9
1	A	377	LEU	7.4
1	B	382	ALA	7.4
1	B	383	ALA	7.1
1	A	376	TRP	6.7
1	A	247	ILE	6.7
1	B	380	LEU	6.1
1	A	45	TYR	5.8
1	B	381	ALA	5.7
1	A	245	ARG	5.4
1	A	375	TRP	5.3
1	B	187	SER	5.2
1	B	199	PHE	5.1
1	A	189	LEU	4.7
1	B	376	TRP	4.7
1	B	375	TRP	4.6
1	B	250	THR	4.6
1	A	248	PRO	4.6
1	B	152	LEU	4.2
1	B	249	GLY	4.1
1	A	250	THR	4.1
1	A	249	GLY	4.0
1	A	47	TRP	4.0
1	A	188	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	377	LEU	3.9
1	A	332	ASP	3.9
1	B	244	GLY	3.8
1	B	329	GLN	3.8
1	A	373	PHE	3.7
1	A	191	GLU	3.6
1	B	159	ARG	3.6
1	B	72	TRP	3.6
1	A	192	LEU	3.6
1	B	251	THR	3.6
1	B	332	ASP	3.5
1	B	333	ARG	3.4
1	A	195	ARG	3.3
1	B	286	GLU	3.3
1	A	155	LYS	3.2
1	B	34	TYR	3.2
1	A	244	GLY	3.1
1	A	152	LEU	3.1
1	B	31	PHE	3.1
1	A	72	TRP	3.0
1	A	166	LEU	3.0
1	A	333	ARG	2.9
1	B	186	SER	2.8
1	B	378	PRO	2.8
1	B	155	LYS	2.8
1	A	75	HIS	2.8
1	A	160	ARG	2.7
1	B	291	ARG	2.7
1	A	193	ALA	2.6
1	A	337	TYR	2.6
1	A	108	ILE	2.6
1	B	32	LEU	2.6
1	B	47	TRP	2.6
1	B	73	ARG	2.5
1	A	286	GLU	2.5
1	B	33	ARG	2.5
1	B	201	VAL	2.4
1	A	46	ALA	2.4
1	A	330	ALA	2.4
1	A	374	SER	2.4
1	B	166	LEU	2.4
1	B	330	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	154	PHE	2.3
1	A	162	LEU	2.3
1	B	160	ARG	2.3
1	A	83	TYR	2.2
1	B	373	PHE	2.2
1	B	331	SER	2.2
1	A	329	GLN	2.2
1	B	205	ARG	2.2
1	B	30	GLU	2.2
1	B	328	ARG	2.1
1	A	290	MET	2.1
1	B	75	HIS	2.1
1	A	291	ARG	2.1
1	A	209	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	SOG	A	420	20/20	0.43	0.35	115,120,121,121	0
5	SOG	B	417	20/20	0.54	0.46	102,106,108,108	0
5	SOG	B	421	20/20	0.63	0.37	79,93,95,96	0
5	SOG	A	418	5/20	0.65	0.36	51,53,53,54	0
5	SOG	A	423	4/20	0.65	0.42	75,76,78,80	0
5	SOG	A	422	6/20	0.71	0.32	67,72,77,78	0
5	SOG	A	416	5/20	0.71	0.35	54,56,59,59	0
5	SOG	B	424	6/20	0.72	0.35	75,76,77,79	0
5	SOG	A	406	16/20	0.73	0.27	94,97,100,100	0

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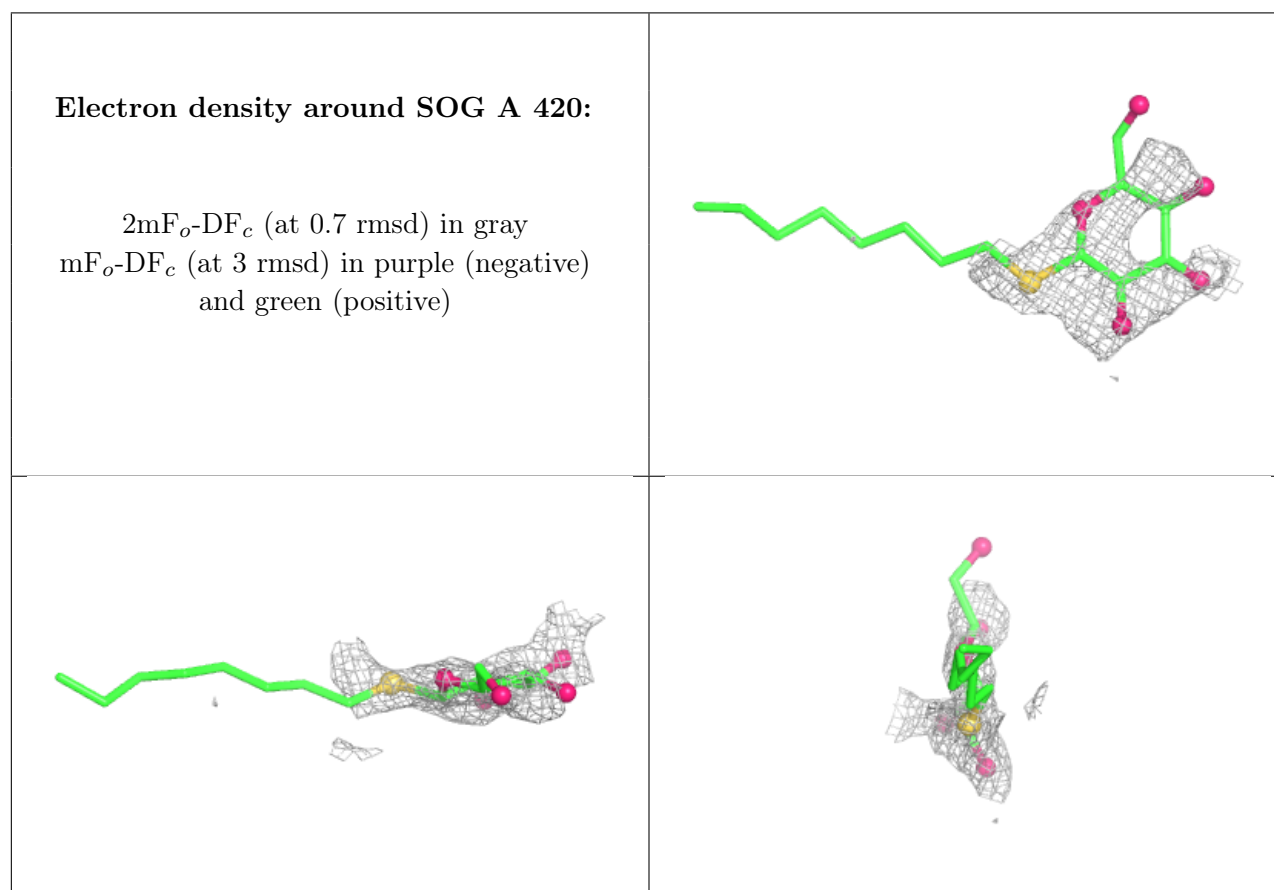
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SOG	A	413	10/20	0.75	0.34	55,71,92,92	0
3	PG4	B	404	11/13	0.75	0.26	73,73,76,76	0
5	SOG	B	412	20/20	0.75	0.28	100,102,105,105	0
5	SOG	B	423	5/20	0.76	0.32	62,62,63,63	0
5	SOG	A	417	8/20	0.76	0.28	41,51,55,56	0
5	SOG	A	412	16/20	0.77	0.26	72,91,96,96	0
5	SOG	A	424	4/20	0.77	0.41	77,78,79,79	0
5	SOG	B	418	6/20	0.77	0.36	88,91,95,95	0
5	SOG	A	419	9/20	0.78	0.27	74,75,81,82	0
5	SOG	B	414	20/20	0.78	0.24	61,95,101,102	0
5	SOG	B	419	4/20	0.78	0.35	92,92,93,93	0
5	SOG	B	411	20/20	0.79	0.22	66,89,93,94	0
5	SOG	A	409	20/20	0.80	0.18	33,74,79,79	0
5	SOG	B	416	9/20	0.80	0.33	33,44,60,65	9
5	SOG	A	415	8/20	0.80	0.26	57,61,72,77	0
5	SOG	A	407	14/20	0.80	0.20	92,98,101,102	0
5	SOG	B	408	20/20	0.81	0.21	44,93,100,100	0
5	SOG	B	409	20/20	0.81	0.25	70,88,91,93	0
5	SOG	A	425	4/20	0.81	0.35	62,63,63,63	0
5	SOG	A	405	20/20	0.82	0.23	60,101,108,109	0
5	SOG	A	408	20/20	0.82	0.24	60,95,99,101	0
5	SOG	A	404	20/20	0.82	0.23	81,89,93,93	0
5	SOG	A	421	6/20	0.84	0.27	66,70,74,77	0
3	PG4	B	403	13/13	0.85	0.20	54,60,63,64	0
5	SOG	B	422	6/20	0.85	0.30	61,64,66,66	0
5	SOG	B	425	6/20	0.85	0.25	53,55,56,58	0
7	NA	A	427	1/1	0.85	0.15	50,50,50,50	0
4	CIT	A	403	13/13	0.86	0.15	55,60,67,69	0
5	SOG	A	414	9/20	0.86	0.38	69,70,79,83	9
5	SOG	B	413	20/20	0.86	0.20	63,77,83,83	0
3	PG4	A	402	13/13	0.86	0.19	56,58,70,71	0
5	SOG	B	415	20/20	0.86	0.21	45,79,86,87	20
5	SOG	A	411	6/20	0.87	0.36	75,77,83,87	6
5	SOG	A	410	20/20	0.87	0.14	35,59,71,74	0
5	SOG	B	420	6/20	0.87	0.26	71,72,72,73	0
6	PGW	A	426	51/51	0.88	0.16	17,43,94,97	0
5	SOG	B	407	20/20	0.88	0.21	60,81,88,90	0
5	SOG	B	410	20/20	0.89	0.13	36,61,70,71	0
6	PGW	B	426	51/51	0.89	0.16	21,40,95,97	0
5	SOG	B	405	20/20	0.89	0.15	32,48,55,58	0
7	NA	B	427	1/1	0.91	0.10	44,44,44,44	0
3	PG4	B	402	13/13	0.92	0.12	44,46,50,51	0

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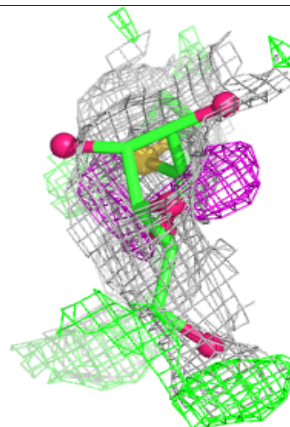
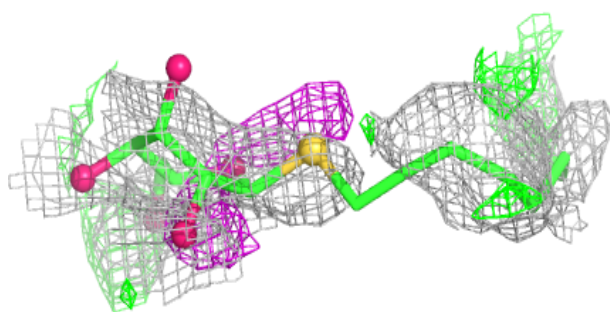
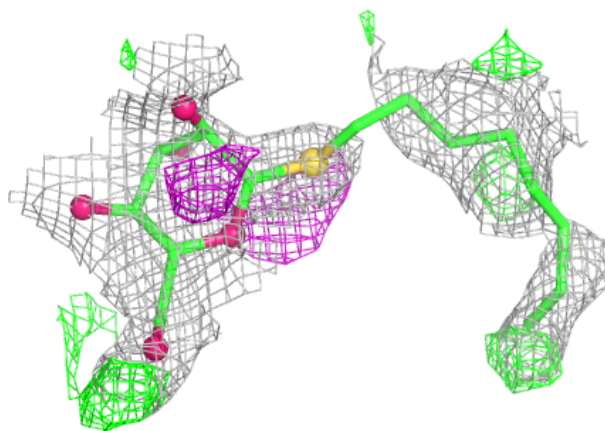
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SOG	B	406	16/20	0.94	0.11	39,45,48,48	0
2	SUV	B	401	32/32	0.94	0.08	20,31,44,46	0
2	SUV	A	401	32/32	0.95	0.08	18,27,34,46	0

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

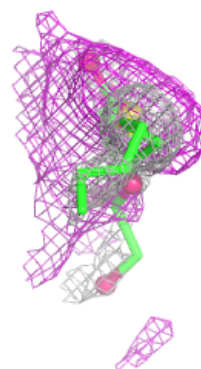
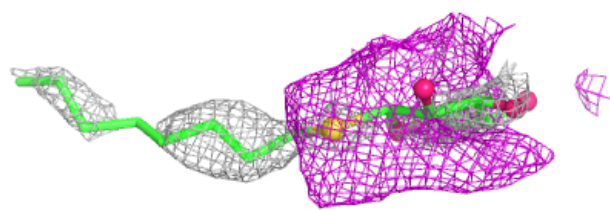
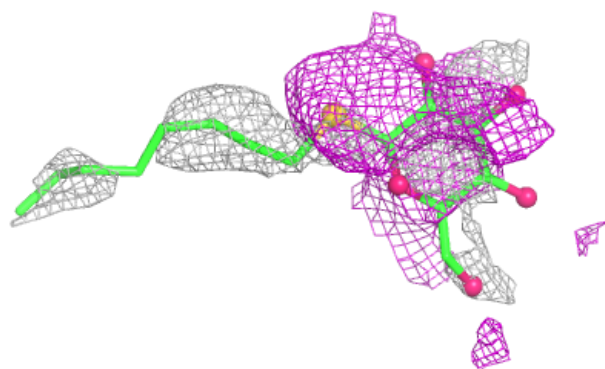


Electron density around SOG B 417:

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

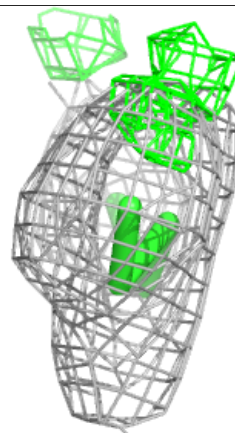
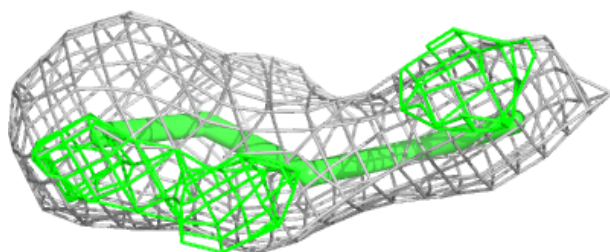
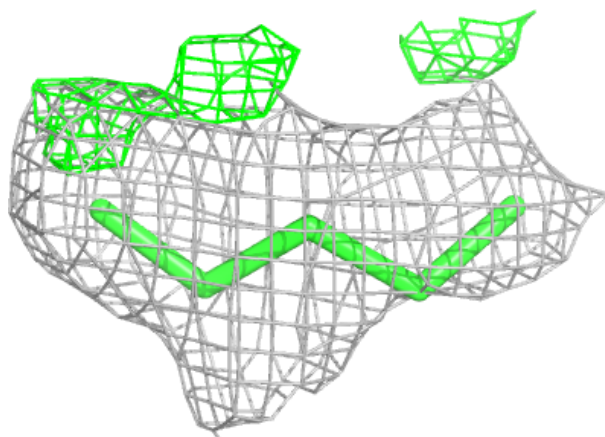
**Electron density around SOG B 421:**

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

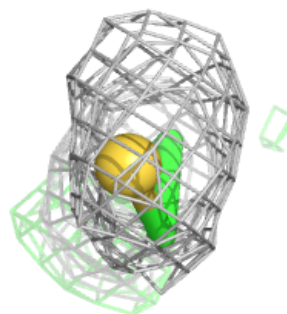
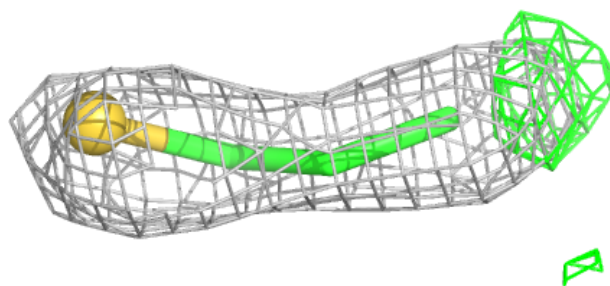
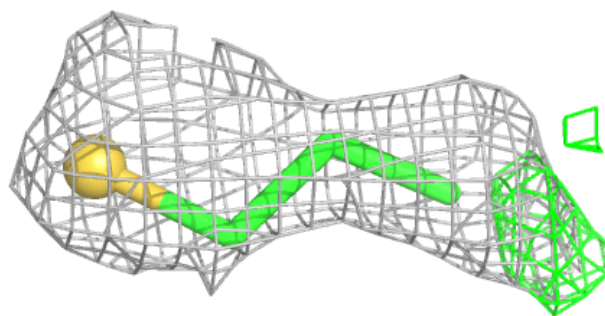


Electron density around SOG A 418:

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

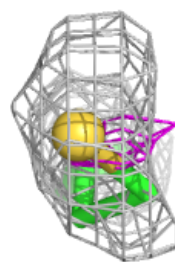
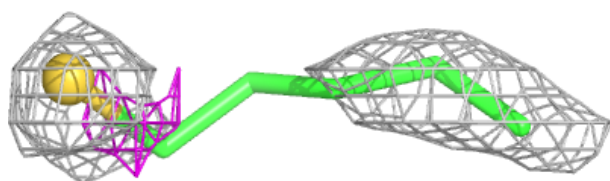
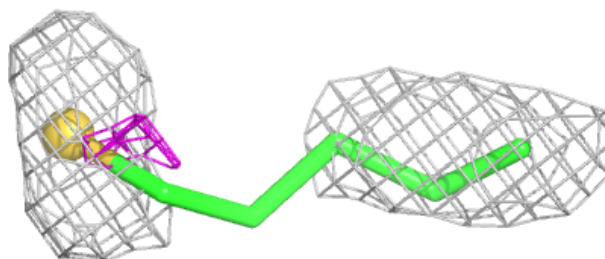
**Electron density around SOG A 423:**

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

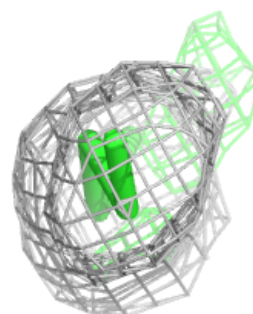
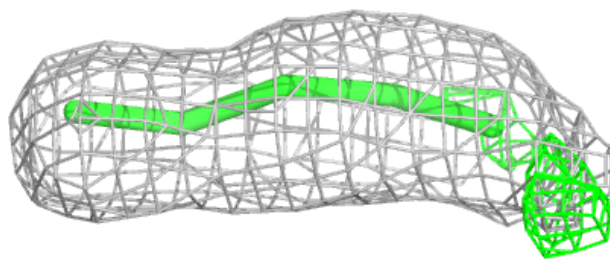
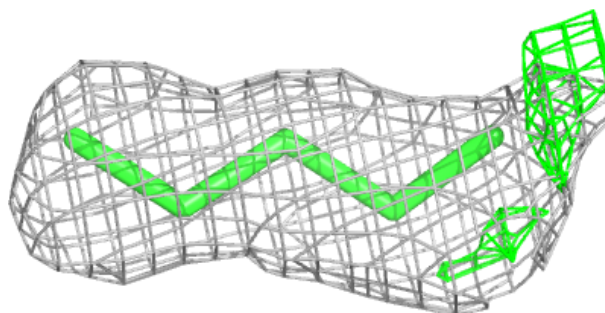


Electron density around SOG A 422:

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

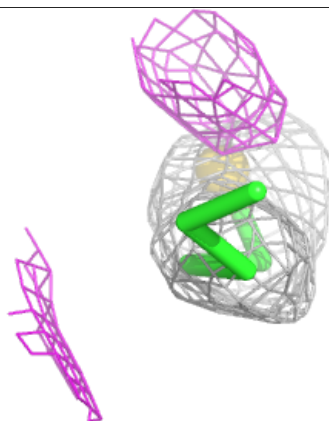
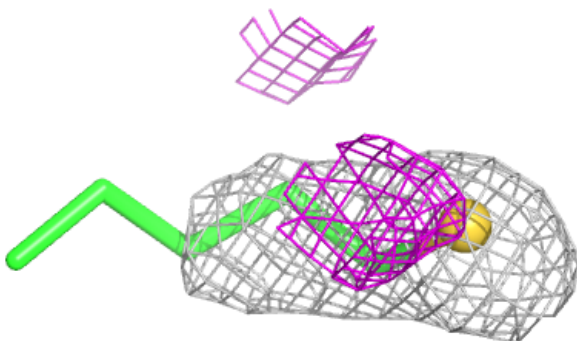
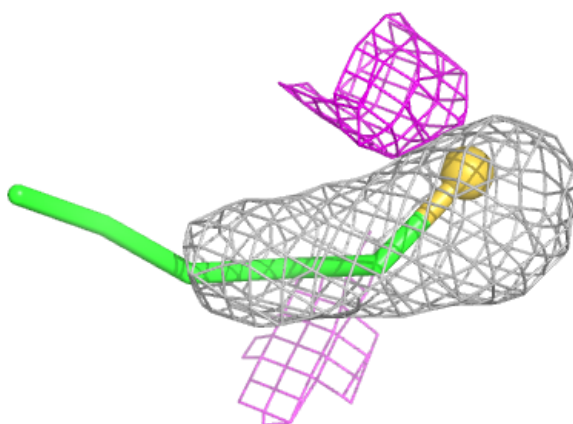
**Electron density around SOG A 416:**

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

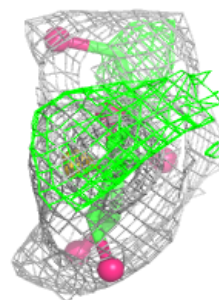
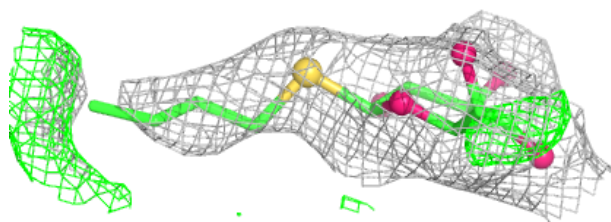
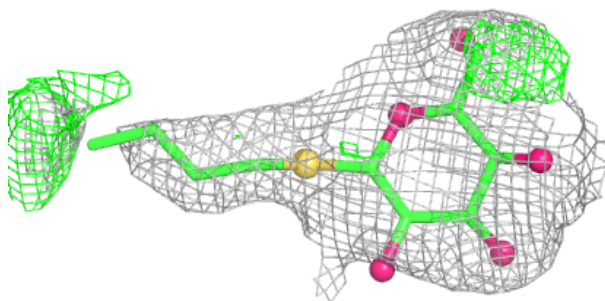


Electron density around SOG B 424:

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

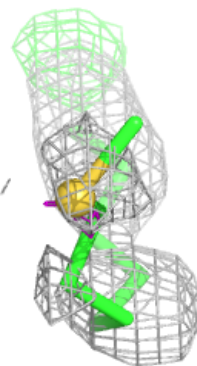
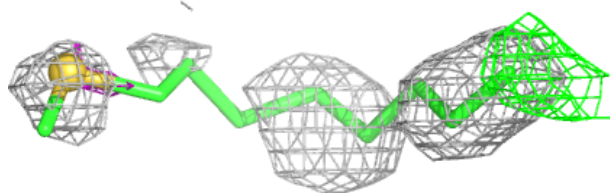
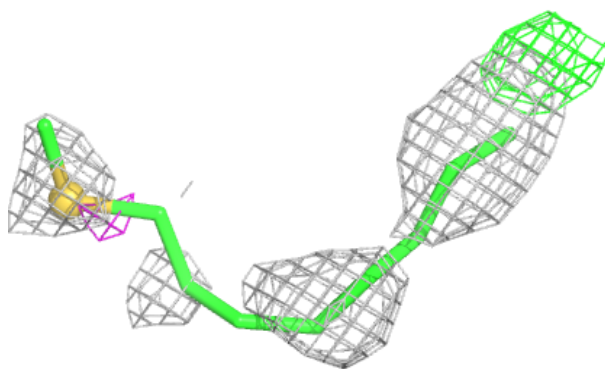
**Electron density around SOG A 406:**

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

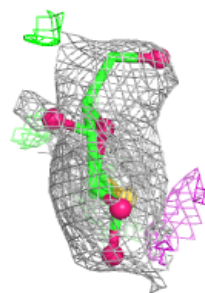
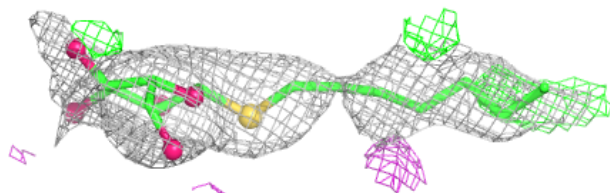
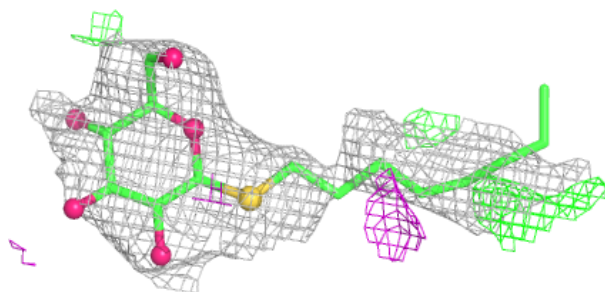


Electron density around SOG A 413:

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

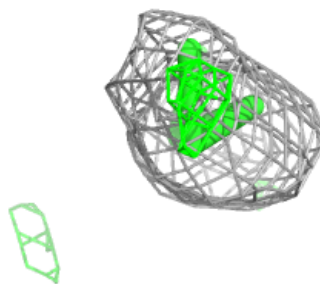
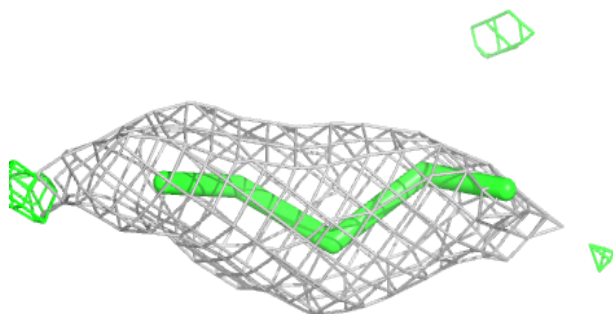
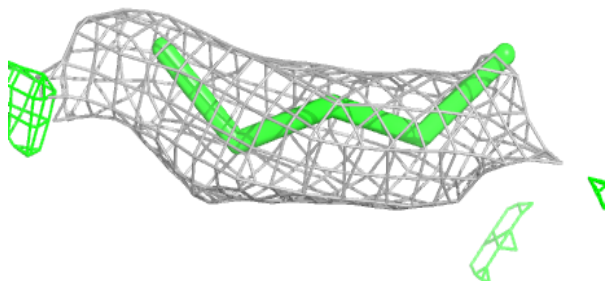
**Electron density around SOG B 412:**

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

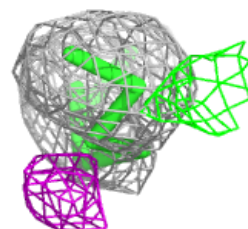
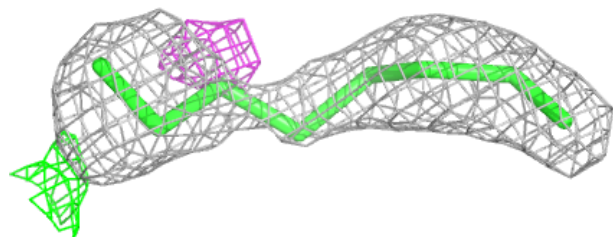
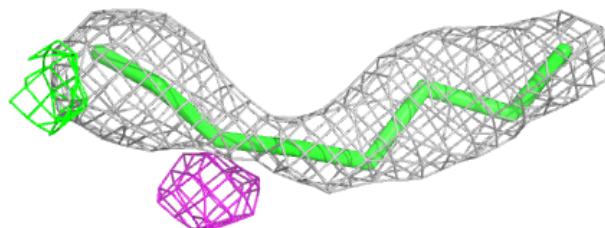


Electron density around SOG B 423:

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

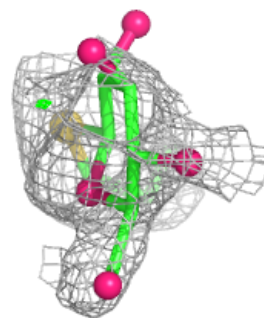
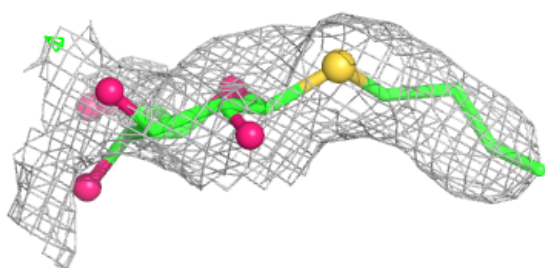
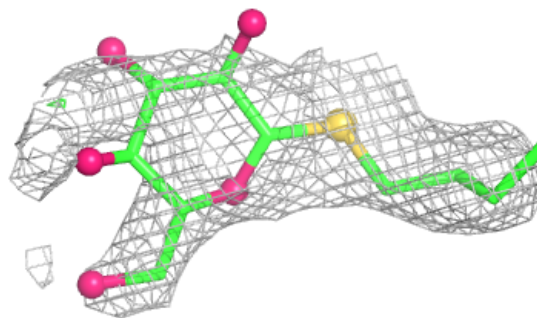
**Electron density around SOG A 417:**

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

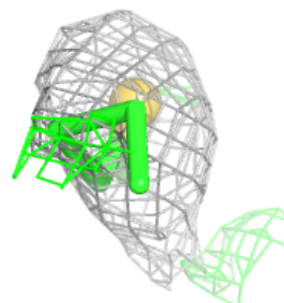
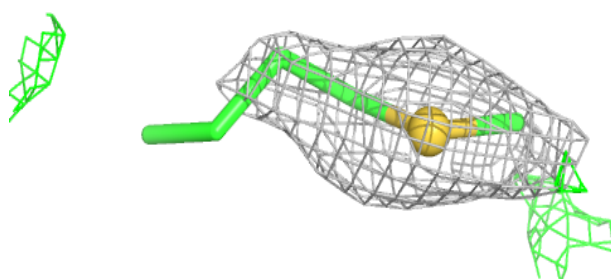
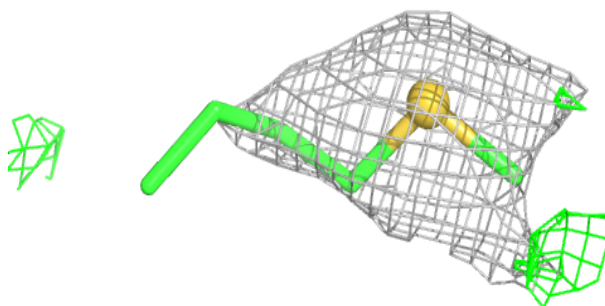


Electron density around SOG A 412:

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

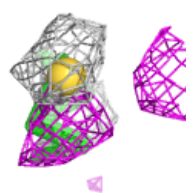
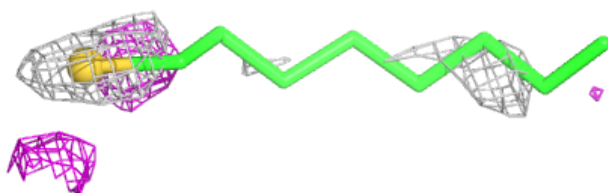
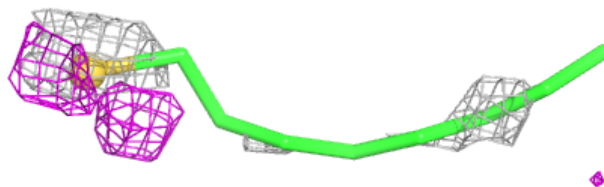
**Electron density around SOG B 418:**

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

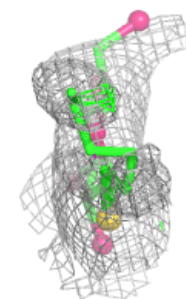
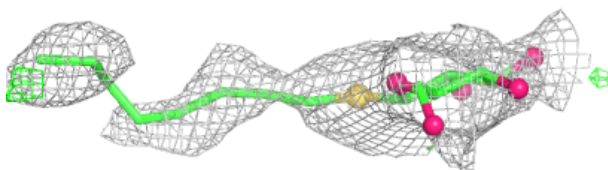
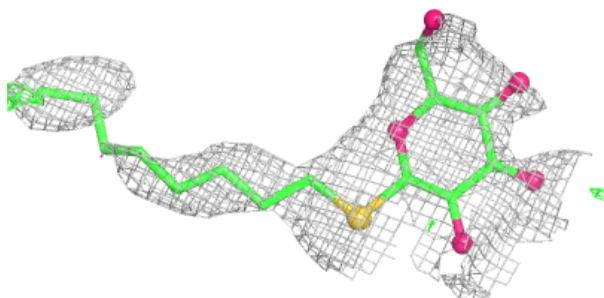


Electron density around SOG A 419:

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

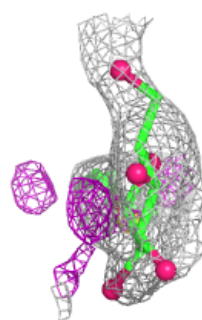
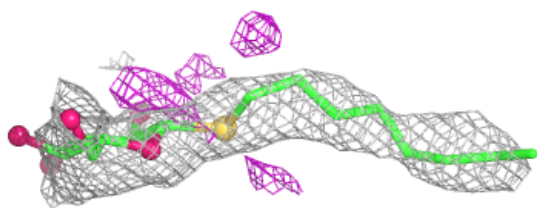
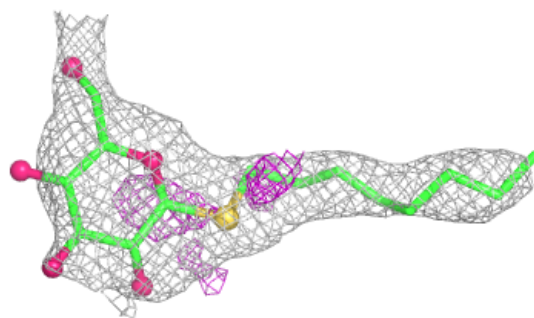
**Electron density around SOG B 414:**

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

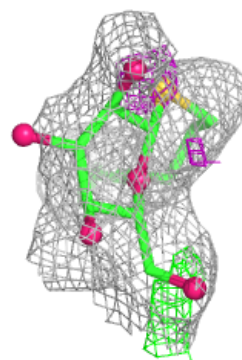
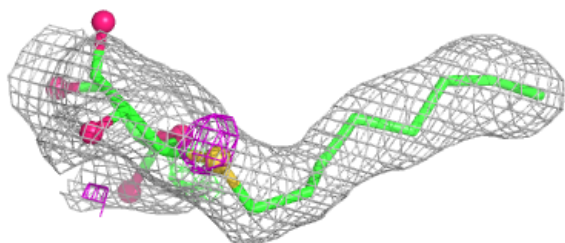
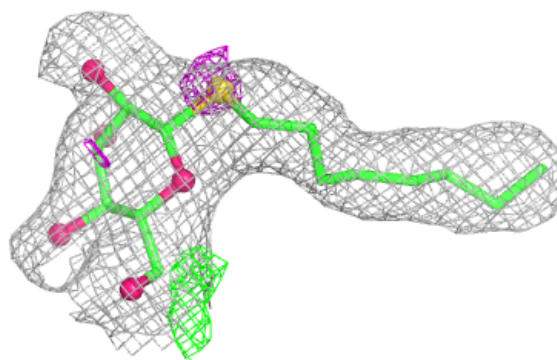


Electron density around SOG B 411:

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

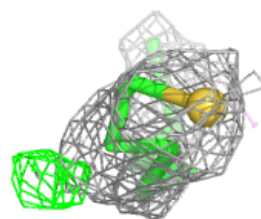
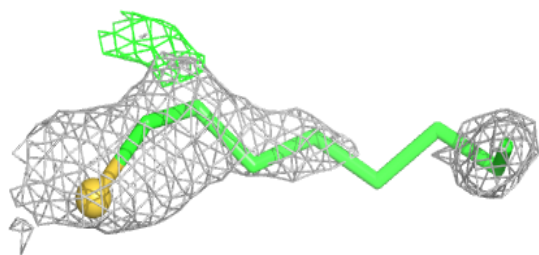
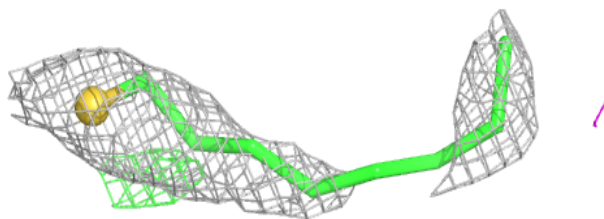
**Electron density around SOG A 409:**

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

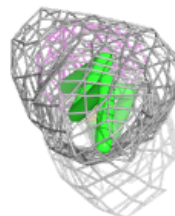
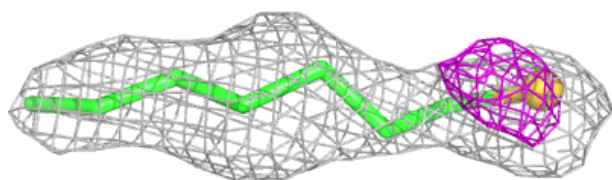
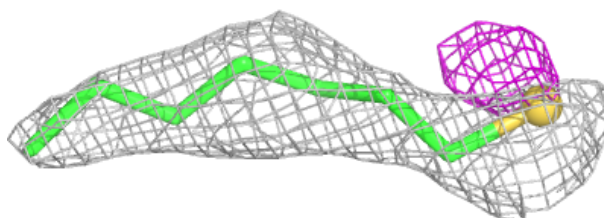


Electron density around SOG B 416:

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

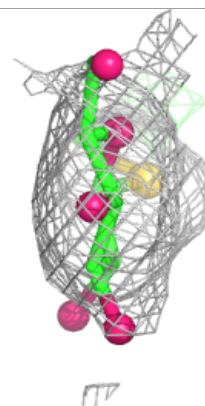
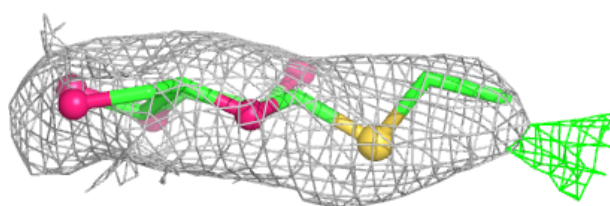
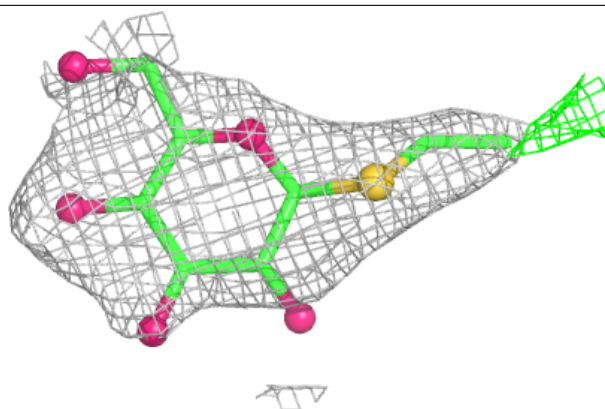
**Electron density around SOG A 415:**

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

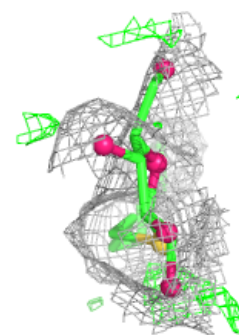
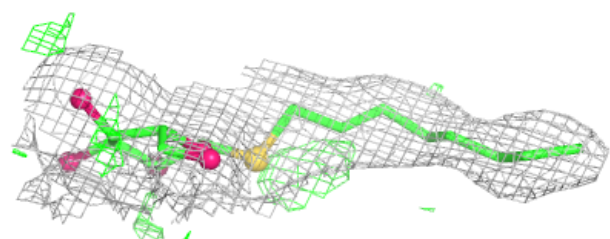
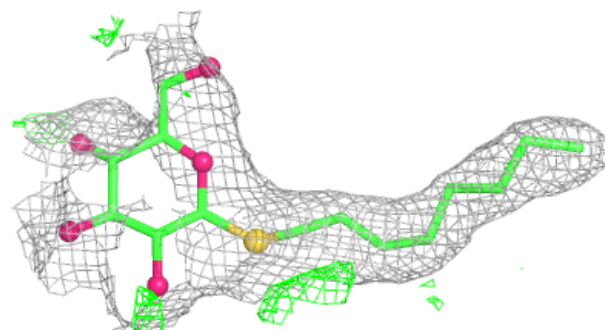


Electron density around SOG A 407:

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

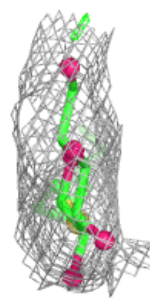
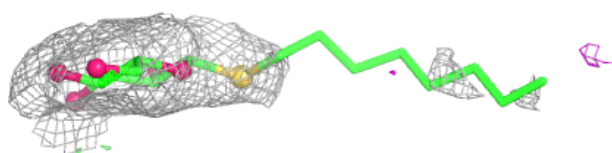
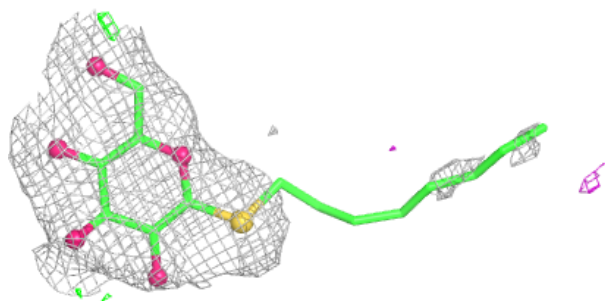
**Electron density around SOG B 408:**

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

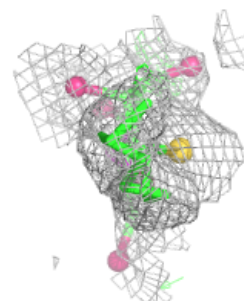
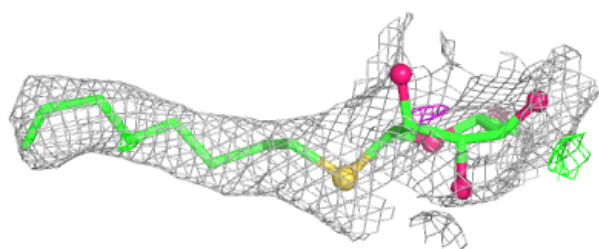
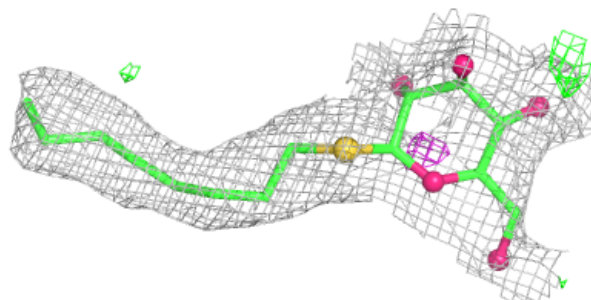


Electron density around SOG B 409:

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

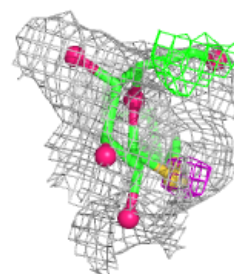
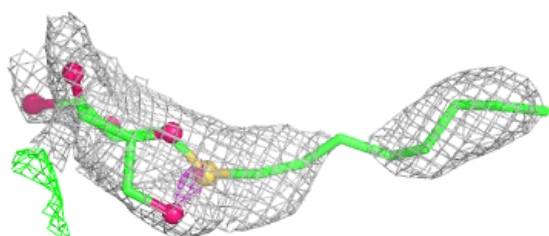
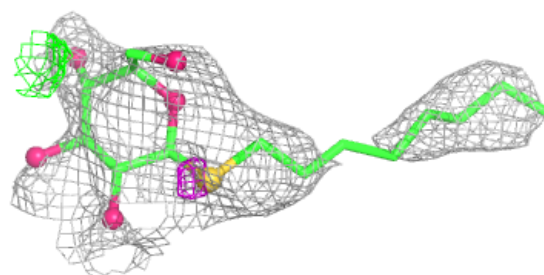
**Electron density around SOG A 405:**

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

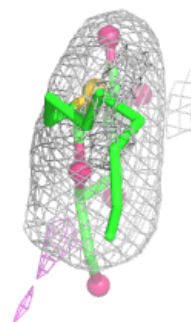
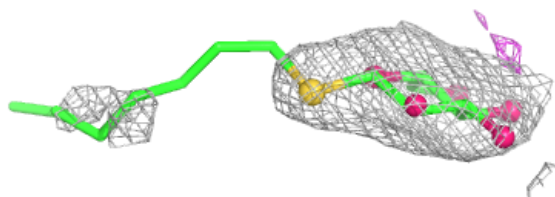
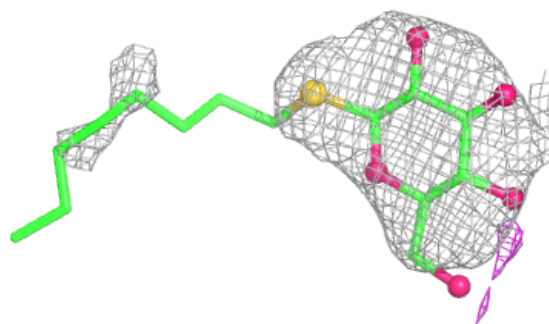


Electron density around SOG A 408:

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

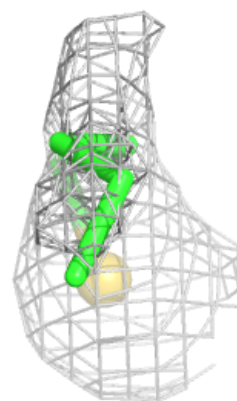
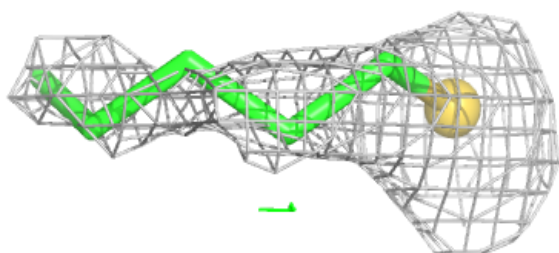
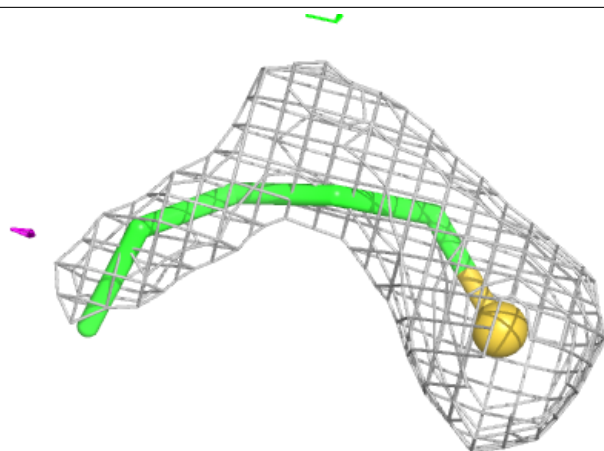
**Electron density around SOG A 404:**

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



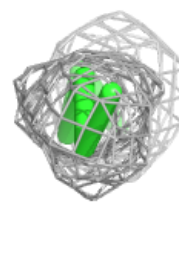
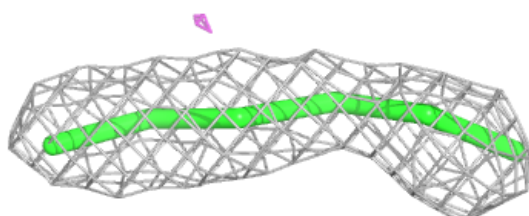
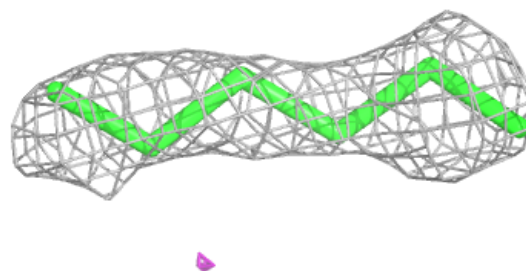
Electron density around SOG A 421:

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

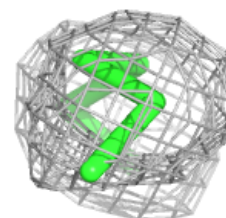
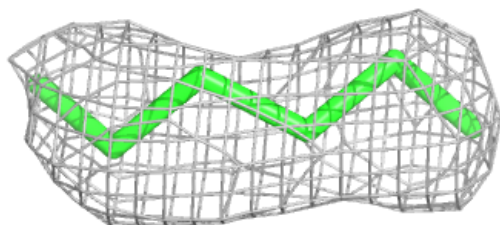
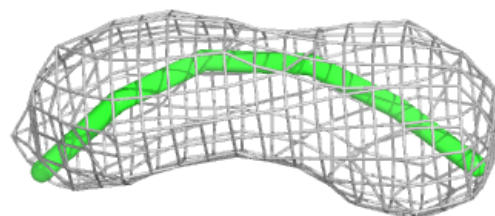


Electron density around SOG B 422:

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

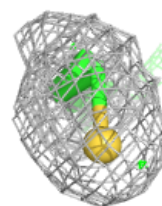
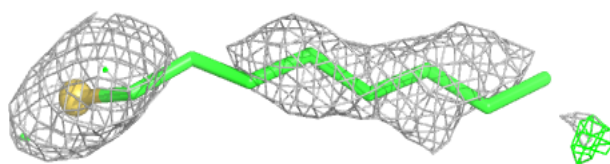
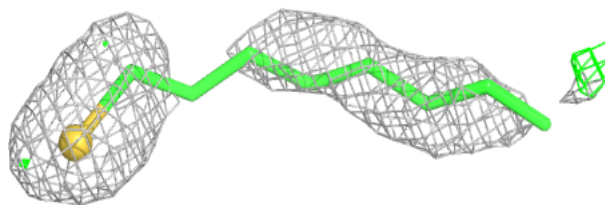
**Electron density around SOG B 425:**

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

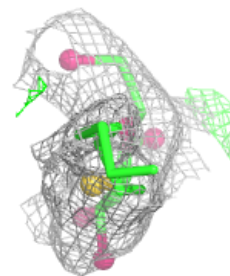
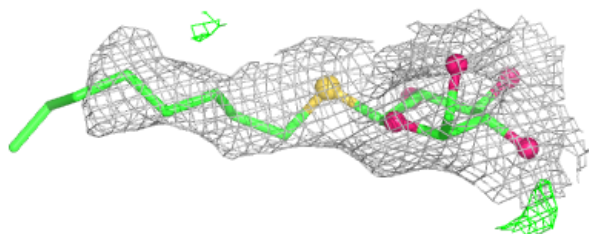


Electron density around SOG A 414:

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

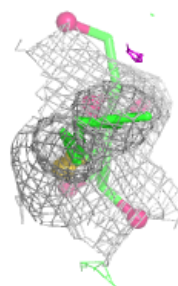
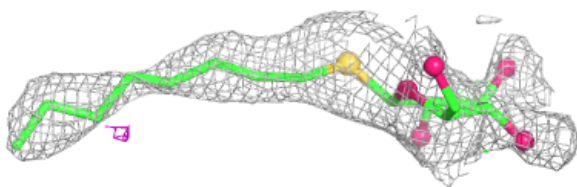
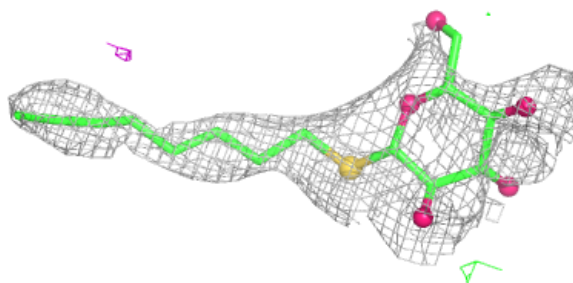
**Electron density around SOG B 413:**

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

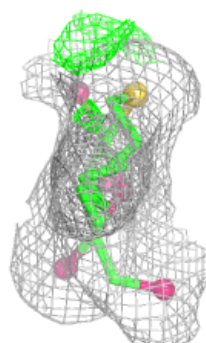
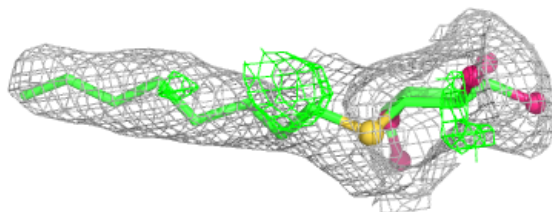
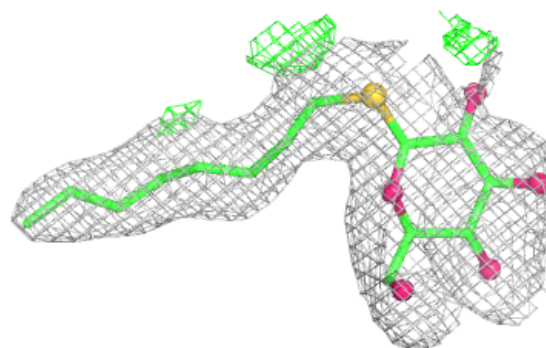


Electron density around SOG B 415:

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

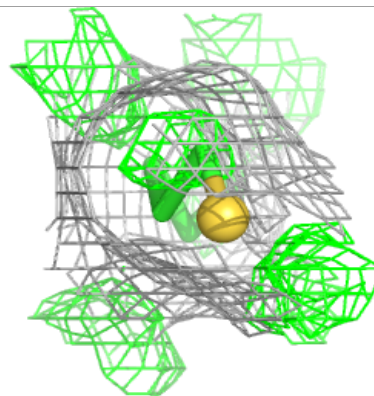
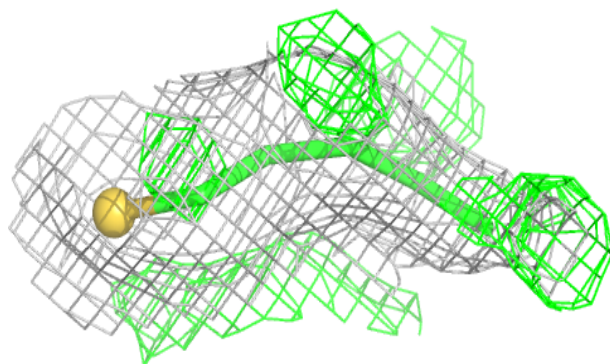
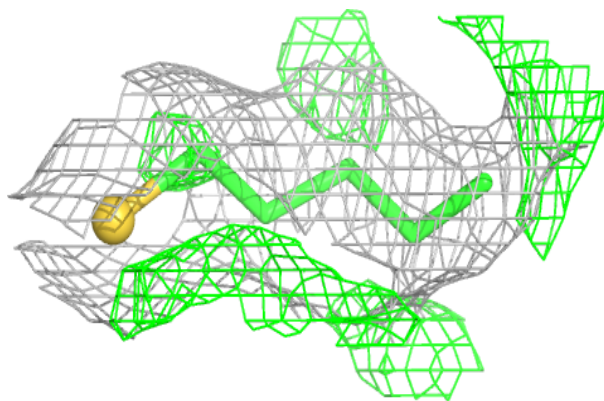
**Electron density around SOG A 410:**

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

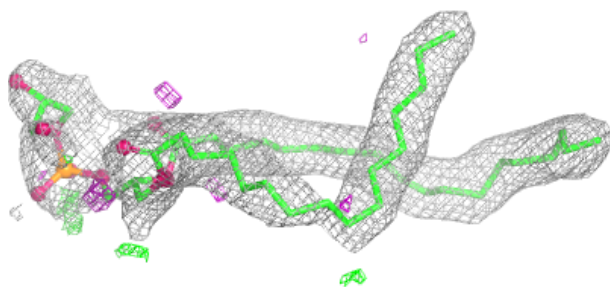
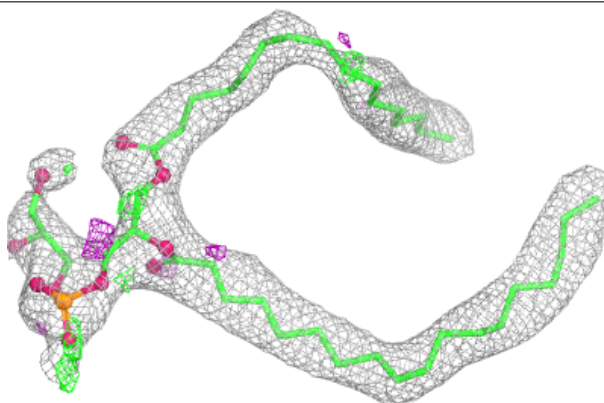


Electron density around SOG B 420:

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

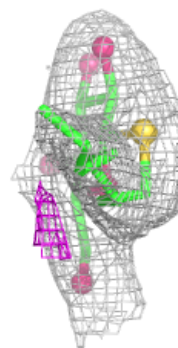
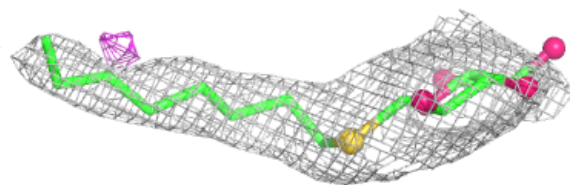
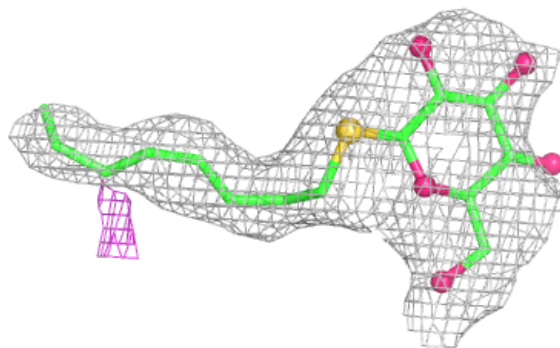
**Electron density around PGW A 426:**

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

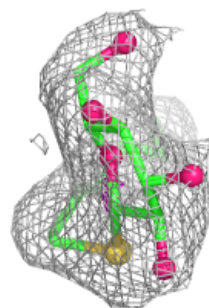
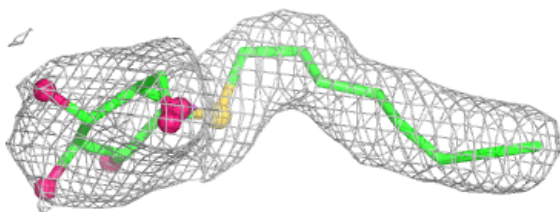
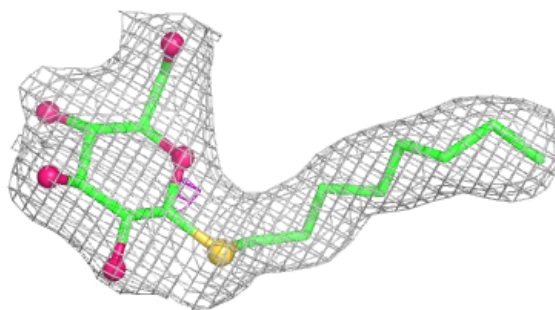


Electron density around SOG B 407:

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

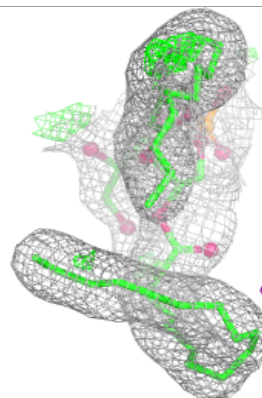
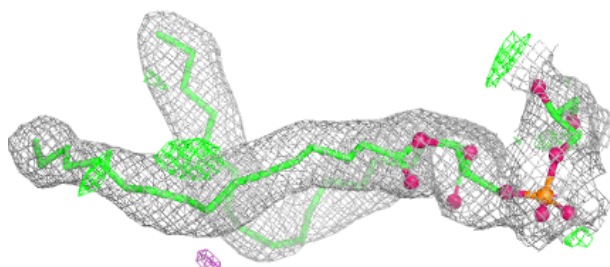
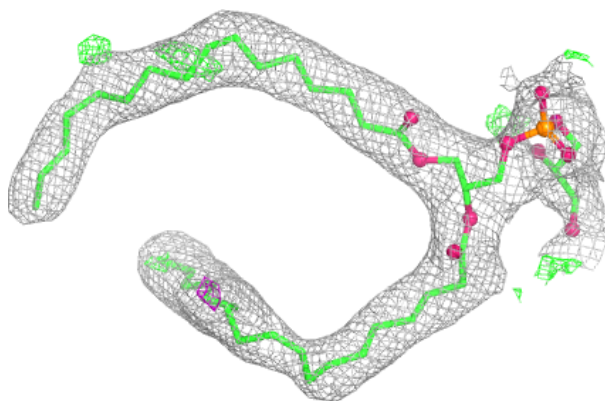
**Electron density around SOG B 410:**

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

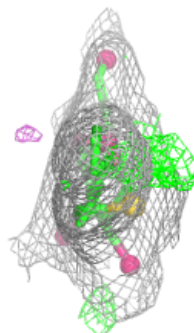
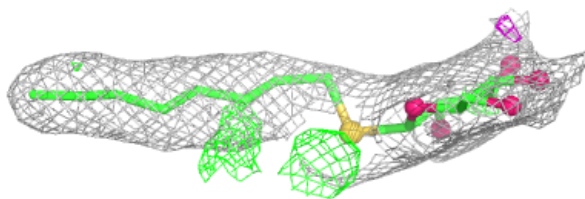
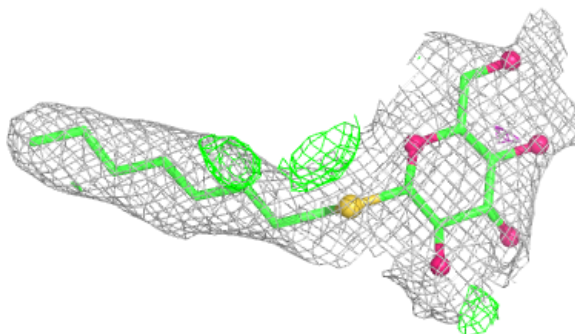


Electron density around PGW B 426:

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

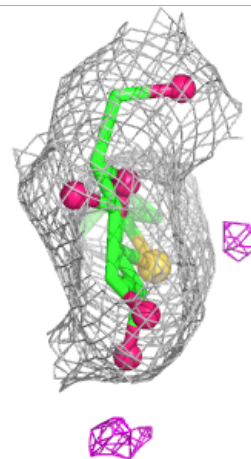
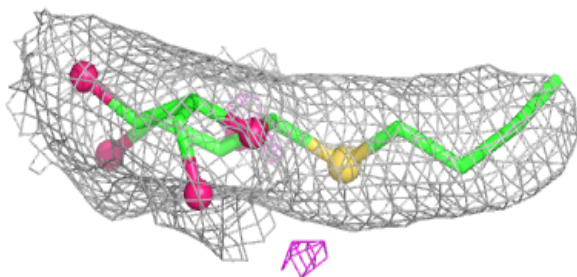
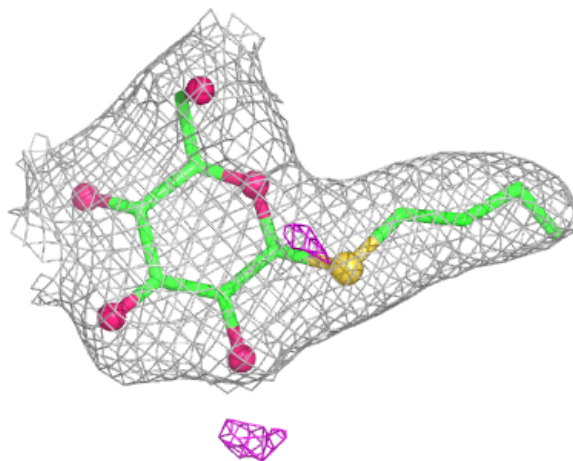
**Electron density around SOG B 405:**

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



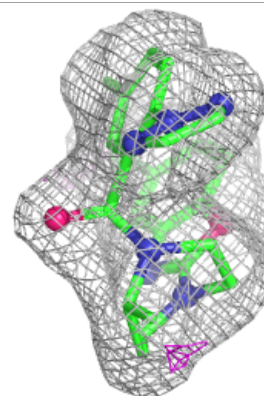
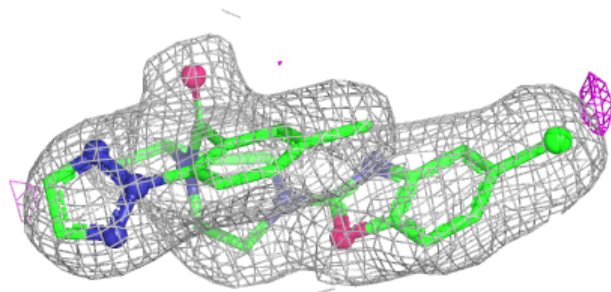
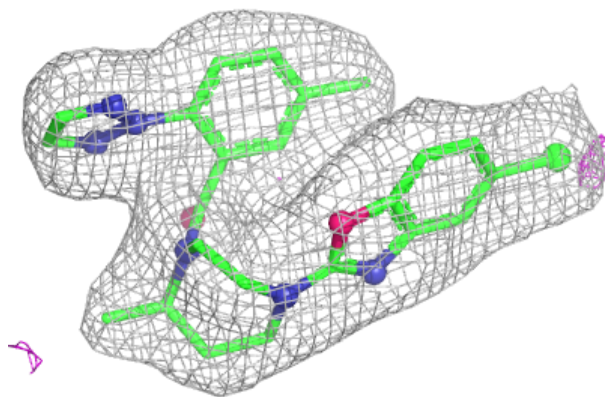
Electron density around SOG B 406:

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

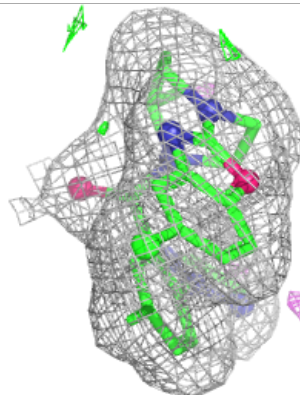
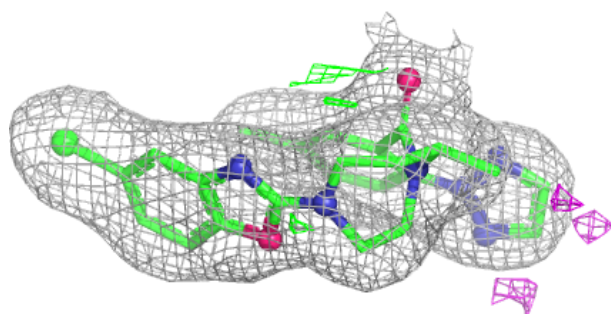
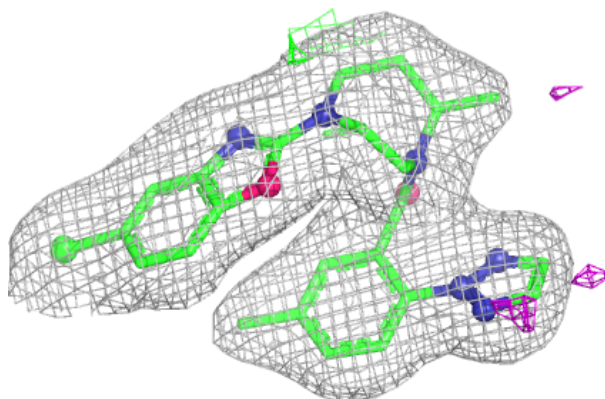


Electron density around SUV B 401:

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

**Electron density around SUV 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.