Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2024 – 12:11 am GMT

PDB ID	:	6TOD
Title	:	Crystal structure of the Orexin-1 receptor in complex with EMPA
Authors	:	Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.
Deposited on	:	2019-12-11
Resolution	:	2.11 Å(reported)

This is a 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 (i) 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:

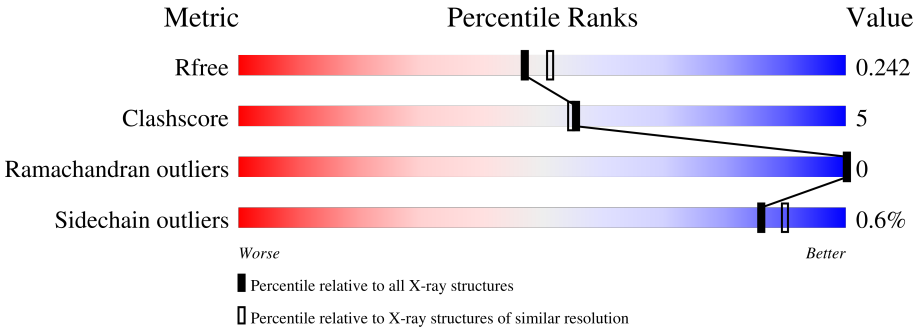
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

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

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6001 atoms, of which 52 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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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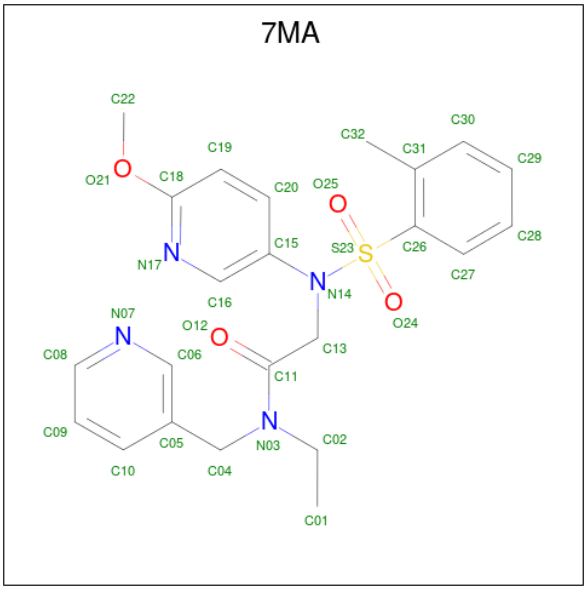
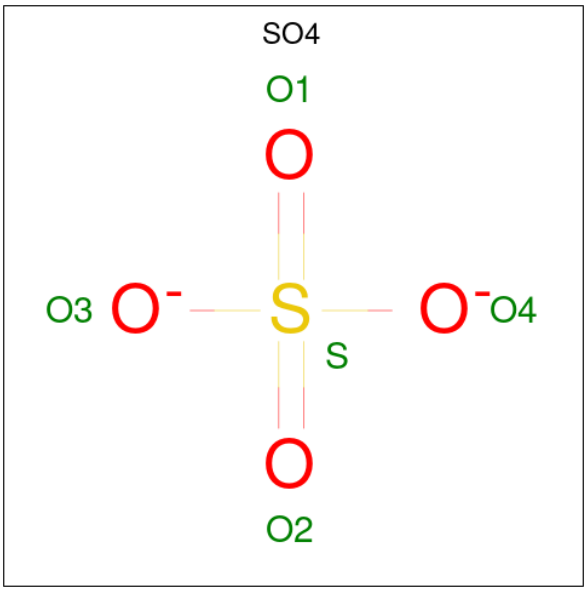
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	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 (three-letter code: 7MA) (formula: $C_{23}H_{26}N_4O_4S$) (labeled as "Ligand of Interest" by depositor).



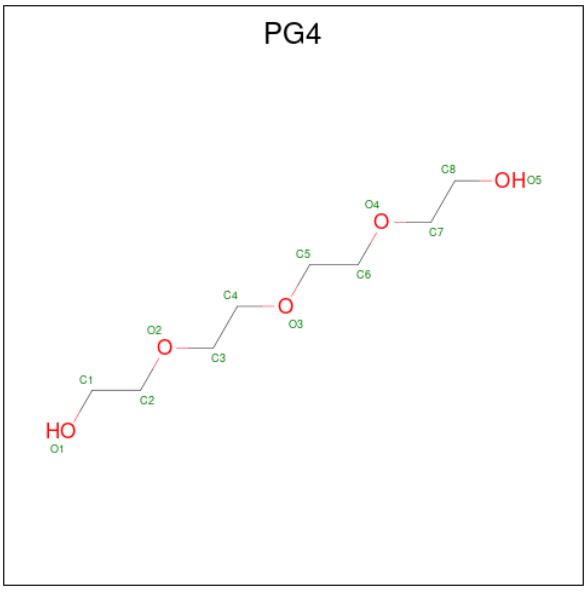
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			58	23	26	4	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			58	23	26	4	4	1		

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



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

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



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

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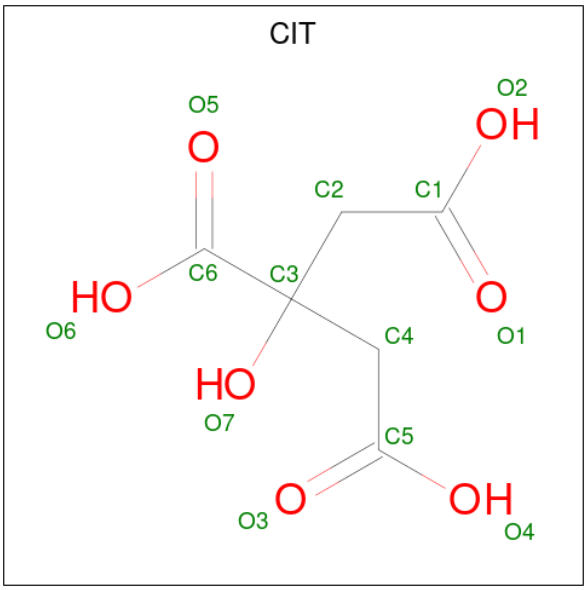
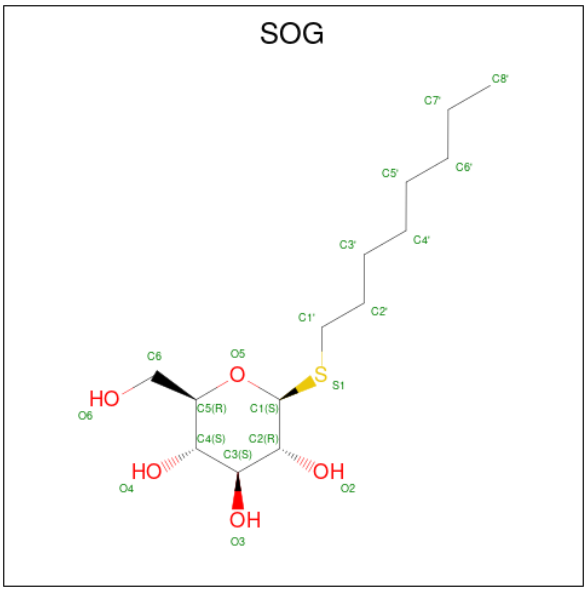
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0

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



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

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



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

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

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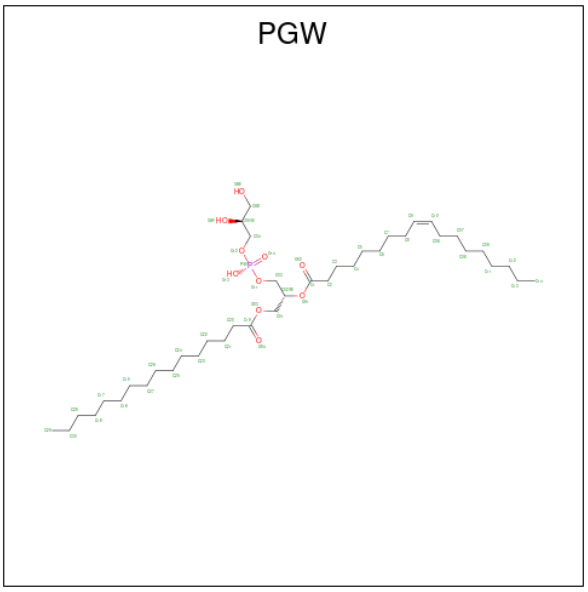
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C S 5 4 1	0	0
6	B	1	Total C O S 16 10 5 1	0	0
6	B	1	Total C S 8 7 1	0	0
6	B	1	Total C S 9 8 1	0	0
6	B	1	Total C S 6 5 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6 1	0	0
6	B	1	Total C S 7 6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

- Molecule 7 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



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

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

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

- Molecule 9 is water.

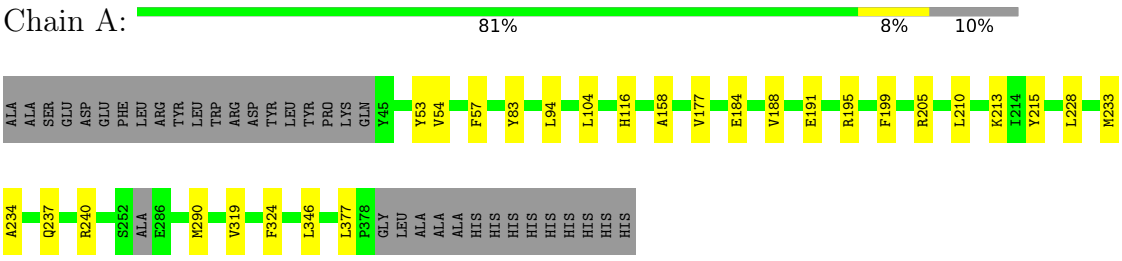
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	110	Total O 110 110	0	0
9	B	101	Total O 101 101	0	0

3 Residue-property plots (i)

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

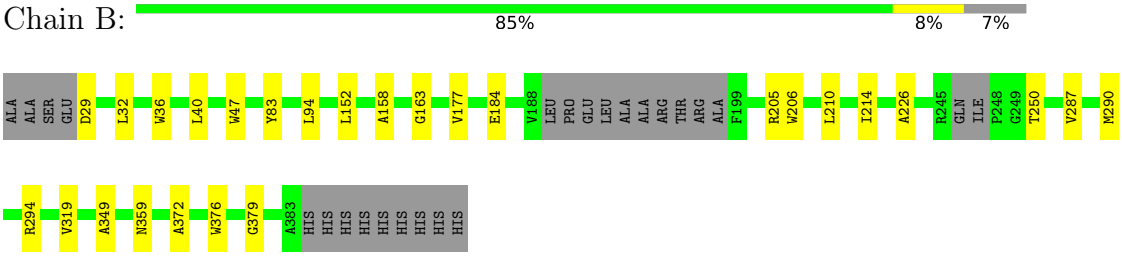
• Molecule 1: Orexin receptor type 1

Chain A:



• Molecule 1: Orexin receptor type 1

Chain B:



4 Data and refinement statistics (i)

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

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/2456	0.61	0/3350
1	B	0.51	0/2557	0.60	0/3485
All	All	0.50	0/5013	0.60	0/6835

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2390	0	2456	26	0
1	B	2486	0	2535	24	0
2	A	32	26	0	0	0
2	B	32	26	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	39	0	54	2	0
4	B	26	0	36	0	0
5	A	13	0	5	0	0
6	A	297	0	401	23	0
6	B	304	0	435	16	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:MET:HE3	1:B:294:ARG:NH2	1.68	1.08
1:B:290:MET:HE3	1:B:294:ARG:HH21	0.98	1.05
6:A:410:SOG:H5	6:A:411:SOG:S1	2.00	1.01
1:A:213:LYS:HD3	6:A:411:SOG:H1'1	1.46	0.93
1:B:290:MET:CE	1:B:294:ARG:HH21	1.88	0.84
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:LEU:HB3	4:A:404:PG4:H21	1.98	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
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:191:GLU:CD	1:A:191:GLU:H	2.25	0.40
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%)	249 (99%)	3 (1%)	71	77
1	B	260/280 (93%)	260 (100%)	0	100	100
All	All	512/560 (91%)	509 (99%)	3 (1%)	86	90

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 2 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PG4	A	404	-	12,12,12	0.58	0	11,11,11	0.18	0
6	SOG	A	412	-	20,20,20	1.10	2 (10%)	24,25,25	0.95	1 (4%)
6	SOG	A	425	-	6,6,20	0.53	0	5,5,25	0.71	0
6	SOG	B	421	-	16,16,20	1.12	1 (6%)	20,21,25	0.84	0
6	SOG	B	412	-	20,20,20	1.05	2 (10%)	24,25,25	0.74	0
6	SOG	A	413	-	20,20,20	0.95	1 (5%)	24,25,25	1.40	4 (16%)
6	SOG	B	411	-	20,20,20	0.98	2 (10%)	24,25,25	1.11	2 (8%)
6	SOG	B	429	-	6,6,20	0.52	0	5,5,25	0.80	0
2	7MA	A	401	-	34,34,34	5.53	11 (32%)	45,47,47	2.68	22 (48%)
6	SOG	A	418	-	20,20,20	0.99	1 (5%)	24,25,25	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SOG	A	415	-	14,14,20	0.91	1 (7%)	18,19,25	1.07	1 (5%)
6	SOG	B	418	-	7,7,20	0.51	0	6,6,25	0.91	0
6	SOG	A	414	-	20,20,20	1.10	2 (10%)	24,25,25	0.80	0
6	SOG	B	409	-	20,20,20	1.12	2 (10%)	24,25,25	1.60	5 (20%)
7	PGW	A	429	-	50,50,50	0.94	2 (4%)	53,56,56	1.15	3 (5%)
6	SOG	B	416	-	9,9,20	0.39	0	8,8,25	0.57	0
6	SOG	B	423	-	8,8,20	0.45	0	7,7,25	0.69	0
7	PGW	B	431	-	50,50,50	0.97	2 (4%)	53,56,56	0.94	2 (3%)
6	SOG	B	420	-	4,4,20	0.69	0	3,3,25	0.71	0
3	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.13	0
6	SOG	B	410	-	20,20,20	0.99	1 (5%)	24,25,25	0.82	0
6	SOG	B	424	-	5,5,20	0.52	0	4,4,25	0.45	0
4	PG4	A	405	-	12,12,12	0.15	0	11,11,11	0.14	0
6	SOG	B	430	-	6,6,20	0.49	0	5,5,25	0.82	0
6	SOG	A	422	-	6,6,20	0.48	0	5,5,25	0.54	0
4	PG4	B	404	-	12,12,12	0.41	0	11,11,11	0.59	0
6	SOG	A	419	-	6,6,20	0.52	0	5,5,25	0.63	0
6	SOG	A	427	-	6,6,20	0.51	0	5,5,25	0.55	0
6	SOG	A	407	-	17,17,20	1.05	2 (11%)	21,22,25	1.18	2 (9%)
6	SOG	A	410	-	20,20,20	0.85	1 (5%)	24,25,25	1.74	4 (16%)
6	SOG	B	414	-	20,20,20	0.99	1 (5%)	24,25,25	1.12	3 (12%)
6	SOG	B	419	-	8,8,20	0.49	0	7,7,25	0.64	0
6	SOG	A	411	-	20,20,20	0.76	1 (5%)	24,25,25	1.19	3 (12%)
6	SOG	A	408	-	16,16,20	1.15	2 (12%)	20,21,25	1.02	2 (10%)
6	SOG	B	408	-	20,20,20	1.01	2 (10%)	24,25,25	0.80	0
3	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.20	0
6	SOG	B	407	-	20,20,20	1.12	2 (10%)	24,25,25	0.74	1 (4%)
4	PG4	A	403	-	12,12,12	0.48	0	11,11,11	0.33	0
6	SOG	B	413	-	16,16,20	1.20	1 (6%)	20,21,25	0.94	2 (10%)
6	SOG	B	427	-	6,6,20	0.52	0	5,5,25	0.68	0
6	SOG	B	428	-	6,6,20	0.52	0	5,5,25	0.80	0
6	SOG	A	409	-	20,20,20	0.98	1 (5%)	24,25,25	0.92	1 (4%)
6	SOG	A	417	-	20,20,20	1.11	2 (10%)	24,25,25	1.29	4 (16%)
6	SOG	A	416	-	20,20,20	1.03	2 (10%)	24,25,25	0.87	1 (4%)
6	SOG	B	406	-	20,20,20	1.05	2 (10%)	24,25,25	1.17	1 (4%)
6	SOG	B	417	-	8,8,20	0.48	0	7,7,25	0.69	0
4	PG4	B	405	-	12,12,12	0.50	0	11,11,11	0.34	0
2	7MA	B	401	-	34,34,34	5.65	11 (32%)	45,47,47	2.58	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SOG	A	428	-	6,6,20	0.53	0	5,5,25	0.50	0
3	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.13	0
6	SOG	A	421	-	6,6,20	0.56	0	5,5,25	1.01	0
6	SOG	B	415	-	5,5,20	0.25	0	4,4,25	0.37	0
6	SOG	B	422	-	7,7,20	0.52	0	6,6,25	0.72	0
6	SOG	A	424	-	6,6,20	0.60	0	5,5,25	1.29	1 (20%)
6	SOG	B	425	-	6,6,20	0.54	0	5,5,25	0.88	0
6	SOG	A	423	-	6,6,20	0.52	0	5,5,25	0.80	0
6	SOG	A	420	-	6,6,20	0.50	0	5,5,25	0.75	0
6	SOG	A	426	-	6,6,20	0.52	0	5,5,25	0.63	0
5	CIT	A	406	-	12,12,12	0.99	0	17,17,17	1.67	3 (17%)
6	SOG	B	426	-	6,6,20	0.51	0	5,5,25	0.84	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
4	PG4	A	404	-	-	5/10/10/10	-
6	SOG	A	412	-	-	5/11/31/31	0/1/1/1
6	SOG	A	425	-	-	2/4/4/31	-
6	SOG	B	421	-	-	4/7/27/31	0/1/1/1
6	SOG	B	412	-	-	5/11/31/31	0/1/1/1
6	SOG	A	413	-	-	4/11/31/31	0/1/1/1
6	SOG	B	411	-	-	7/11/31/31	0/1/1/1
6	SOG	B	429	-	-	1/4/4/31	-
2	7MA	A	401	-	-	7/32/32/32	0/3/3/3
6	SOG	A	418	-	-	6/11/31/31	0/1/1/1
6	SOG	A	415	-	-	1/5/25/31	0/1/1/1
6	SOG	B	418	-	-	3/5/5/31	-
6	SOG	A	414	-	-	6/11/31/31	0/1/1/1
6	SOG	B	409	-	-	4/11/31/31	0/1/1/1
7	PGW	A	429	-	-	26/55/55/55	-
6	SOG	B	416	-	-	1/7/7/31	-
6	SOG	B	423	-	-	3/6/6/31	-
7	PGW	B	431	-	-	28/55/55/55	-
6	SOG	B	420	-	-	2/2/2/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	B	410	-	-	9/11/31/31	0/1/1/1
6	SOG	B	424	-	-	2/3/3/31	-
4	PG4	A	405	-	-	3/10/10/10	-
6	SOG	B	430	-	-	3/4/4/31	-
6	SOG	A	422	-	-	3/4/4/31	-
4	PG4	B	404	-	-	4/10/10/10	-
6	SOG	A	419	-	-	1/4/4/31	-
6	SOG	A	427	-	-	3/4/4/31	-
6	SOG	A	407	-	-	5/8/28/31	0/1/1/1
6	SOG	A	410	-	-	5/11/31/31	0/1/1/1
6	SOG	B	414	-	-	4/11/31/31	0/1/1/1
6	SOG	B	419	-	-	5/6/6/31	-
6	SOG	A	411	-	-	2/11/31/31	0/1/1/1
6	SOG	A	408	-	-	4/7/27/31	0/1/1/1
6	SOG	B	408	-	-	7/11/31/31	0/1/1/1
6	SOG	B	427	-	-	1/4/4/31	-
6	SOG	B	407	-	-	6/11/31/31	0/1/1/1
4	PG4	A	403	-	-	3/10/10/10	-
6	SOG	B	413	-	-	3/7/27/31	0/1/1/1
6	SOG	B	428	-	-	1/4/4/31	-
6	SOG	A	409	-	-	6/11/31/31	0/1/1/1
6	SOG	A	417	-	-	7/11/31/31	0/1/1/1
6	SOG	A	416	-	-	7/11/31/31	0/1/1/1
6	SOG	B	406	-	-	6/11/31/31	0/1/1/1
6	SOG	B	417	-	-	4/6/6/31	-
4	PG4	B	405	-	-	8/10/10/10	-
2	7MA	B	401	-	-	6/32/32/32	0/3/3/3
6	SOG	A	428	-	-	1/4/4/31	-
6	SOG	A	421	-	-	1/4/4/31	-
6	SOG	B	415	-	-	2/3/3/31	-
6	SOG	B	422	-	-	2/5/5/31	-
6	SOG	A	424	-	-	2/4/4/31	-
6	SOG	B	425	-	-	2/4/4/31	-
6	SOG	A	423	-	-	3/4/4/31	-
6	SOG	A	420	-	-	1/4/4/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOG	A	426	-	-	1/4/4/31	-
5	CIT	A	406	-	-	4/16/16/16	-
6	SOG	B	426	-	-	1/4/4/31	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7MA	O24-S23	20.06	1.65	1.43
2	A	401	7MA	O24-S23	19.73	1.65	1.43
2	B	401	7MA	O25-S23	17.26	1.62	1.43
2	A	401	7MA	O25-S23	17.07	1.62	1.43
2	B	401	7MA	S23-N14	13.63	1.84	1.65
2	A	401	7MA	S23-N14	13.47	1.84	1.65
2	B	401	7MA	C26-S23	8.94	1.89	1.78
2	A	401	7MA	C26-S23	8.04	1.88	1.78
2	A	401	7MA	C15-N14	5.50	1.52	1.44
2	B	401	7MA	C15-N14	5.47	1.52	1.44
2	B	401	7MA	C11-N03	4.90	1.45	1.35
7	B	431	PGW	O01-C1	4.64	1.47	1.34
2	A	401	7MA	C11-N03	4.58	1.44	1.35
7	A	429	PGW	O01-C1	4.30	1.46	1.34
6	B	409	SOG	C1'-S1	-4.21	1.76	1.81
7	A	429	PGW	O03-C19	4.18	1.45	1.33
7	B	431	PGW	O03-C19	4.05	1.45	1.33
6	A	417	SOG	C1'-S1	-3.81	1.76	1.81
6	B	413	SOG	C1'-S1	-3.74	1.76	1.81
6	A	412	SOG	C1'-S1	-3.73	1.76	1.81
6	A	414	SOG	C1'-S1	-3.69	1.76	1.81
6	B	407	SOG	C1'-S1	-3.69	1.76	1.81
6	B	406	SOG	C1'-S1	-3.65	1.76	1.81
6	A	416	SOG	C1'-S1	-3.53	1.76	1.81
6	A	408	SOG	C1'-S1	-3.53	1.76	1.81
6	B	412	SOG	C1'-S1	-3.49	1.77	1.81
6	B	421	SOG	C1'-S1	-3.38	1.77	1.81
6	B	408	SOG	C1'-S1	-3.35	1.77	1.81
6	A	418	SOG	C1'-S1	-3.34	1.77	1.81
6	A	409	SOG	C1'-S1	-3.30	1.77	1.81
6	B	414	SOG	C1'-S1	-3.29	1.77	1.81
6	B	410	SOG	C1'-S1	-3.27	1.77	1.81
6	A	413	SOG	C1'-S1	-3.21	1.77	1.81
6	B	411	SOG	C1'-S1	-3.19	1.77	1.81
6	A	407	SOG	C1'-S1	-3.08	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7MA	C20-C15	2.90	1.45	1.39
2	B	401	7MA	C13-C11	2.87	1.57	1.53
2	A	401	7MA	O21-C18	2.86	1.39	1.35
2	B	401	7MA	O21-C18	2.68	1.39	1.35
2	A	401	7MA	C19-C18	2.60	1.45	1.39
6	B	407	SOG	C1-S1	-2.54	1.76	1.80
6	A	410	SOG	C1'-S1	-2.54	1.78	1.81
2	B	401	7MA	C19-C18	2.52	1.45	1.39
2	A	401	7MA	C13-C11	2.50	1.56	1.53
2	A	401	7MA	C20-C15	2.49	1.44	1.39
6	A	417	SOG	C1-S1	-2.40	1.77	1.80
6	A	415	SOG	C1-S1	-2.39	1.77	1.80
6	B	406	SOG	C1-S1	-2.36	1.77	1.80
6	B	408	SOG	C1-S1	-2.35	1.77	1.80
6	A	412	SOG	C1-S1	-2.34	1.77	1.80
6	A	414	SOG	C1-S1	-2.26	1.77	1.80
2	B	401	7MA	C18-N17	2.22	1.36	1.32
6	A	408	SOG	C1-S1	-2.22	1.77	1.80
6	B	412	SOG	C1-S1	-2.16	1.77	1.80
6	B	409	SOG	C1-S1	-2.12	1.77	1.80
2	A	401	7MA	C18-N17	2.10	1.35	1.32
6	A	416	SOG	C1-S1	-2.10	1.77	1.80
6	A	407	SOG	C1-S1	-2.08	1.77	1.80
6	B	411	SOG	C1-S1	-2.01	1.77	1.80
6	A	411	SOG	C1'-S1	-2.00	1.78	1.81

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	7MA	C16-N17-C18	6.51	122.36	116.63
2	A	401	7MA	C16-N17-C18	6.01	121.92	116.63
2	A	401	7MA	O25-S23-O24	-5.79	110.13	119.52
6	A	410	SOG	C1-O5-C5	5.75	123.19	112.58
7	A	429	PGW	O01-C1-C2	5.61	123.59	111.50
2	B	401	7MA	C13-N14-C15	5.54	124.04	116.59
2	A	401	7MA	C13-C11-N03	5.15	123.57	117.08
2	B	401	7MA	C16-C15-N14	-5.13	112.43	120.14
2	B	401	7MA	O25-S23-O24	-5.03	111.38	119.52
2	A	401	7MA	O24-S23-N14	5.03	112.66	106.71
2	B	401	7MA	C13-C11-N03	4.84	123.18	117.08
2	A	401	7MA	C13-N14-C15	4.75	122.97	116.59
2	A	401	7MA	C16-C15-N14	-4.56	113.29	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	406	CIT	O6-C6-C3	4.42	120.73	113.05
2	A	401	7MA	O25-S23-N14	4.27	111.76	106.71
6	B	409	SOG	C3-C4-C5	4.02	117.42	110.24
6	B	406	SOG	C1'-S1-C1	3.96	107.49	100.09
6	A	407	SOG	C1-O5-C5	3.94	119.84	112.58
2	B	401	7MA	O25-S23-N14	3.68	111.07	106.71
7	B	431	PGW	O01-C1-C2	3.67	119.41	111.50
6	A	413	SOG	C3-C4-C5	3.56	116.60	110.24
2	B	401	7MA	C13-N14-S23	3.56	123.30	117.23
2	A	401	7MA	C13-N14-S23	3.49	123.18	117.23
2	B	401	7MA	C20-C15-N14	3.46	125.32	120.16
2	B	401	7MA	O24-S23-N14	3.44	110.78	106.71
6	A	410	SOG	C1'-S1-C1	3.38	106.42	100.09
2	A	401	7MA	C27-C26-S23	-3.28	112.89	117.42
6	A	411	SOG	C1-O5-C5	3.21	118.49	112.58
2	A	401	7MA	C20-C15-N14	3.20	124.93	120.16
2	A	401	7MA	C31-C26-S23	3.19	124.97	122.05
2	A	401	7MA	O12-C11-C13	-3.10	115.76	120.59
6	A	417	SOG	C4-C3-C2	3.08	116.20	110.82
6	A	412	SOG	C1-O5-C5	3.07	118.25	112.58
6	B	409	SOG	C4-C3-C2	3.03	116.12	110.82
6	A	411	SOG	C1'-S1-C1	3.03	105.76	100.09
6	B	409	SOG	O5-C5-C4	3.02	115.17	109.69
6	A	413	SOG	C4-C3-C2	3.01	116.08	110.82
6	A	407	SOG	O5-C1-C2	2.97	114.04	110.31
2	B	401	7MA	O12-C11-C13	-2.95	115.99	120.59
5	A	406	CIT	O5-C6-C3	-2.91	118.13	122.25
2	A	401	7MA	C08-N07-C06	2.84	121.76	116.85
2	A	401	7MA	C05-C04-N03	2.82	117.67	113.13
2	A	401	7MA	C04-N03-C02	2.82	119.83	116.54
6	A	415	SOG	C1-O5-C5	2.82	117.78	112.58
6	B	409	SOG	C1-O5-C5	2.81	117.77	112.58
6	B	411	SOG	C3-C4-C5	2.75	115.15	110.24
6	A	413	SOG	O5-C1-C2	-2.68	106.95	110.31
6	A	410	SOG	O5-C5-C4	2.65	114.50	109.69
2	B	401	7MA	C15-N14-S23	-2.63	112.46	117.73
2	B	401	7MA	C08-N07-C06	2.59	121.33	116.85
6	B	414	SOG	C4-C3-C2	2.58	115.33	110.82
2	B	401	7MA	C31-C26-S23	2.58	124.42	122.05
7	A	429	PGW	O03-C19-C20	2.57	119.98	111.91
2	A	401	7MA	O25-S23-C26	2.57	112.34	107.36
2	B	401	7MA	O21-C18-C19	2.57	121.18	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	7MA	C04-C05-C10	-2.56	115.96	120.77
2	B	401	7MA	C04-C05-C10	-2.55	115.97	120.77
6	B	411	SOG	C4-C3-C2	2.55	115.28	110.82
6	A	417	SOG	C3-C4-C5	2.55	114.79	110.24
2	A	401	7MA	C05-C06-N07	-2.54	118.77	123.72
6	B	409	SOG	C1'-S1-C1	2.50	104.78	100.09
2	A	401	7MA	O21-C18-C19	2.50	121.06	116.71
6	A	409	SOG	C4-C3-C2	2.48	115.15	110.82
6	B	414	SOG	C3-C4-C5	2.44	114.60	110.24
7	A	429	PGW	O01-C1-O02	-2.44	117.80	123.70
6	A	417	SOG	O5-C5-C4	2.44	114.12	109.69
2	B	401	7MA	C10-C05-C06	2.38	120.60	117.10
2	B	401	7MA	C30-C31-C26	2.36	118.89	116.27
2	B	401	7MA	C05-C06-N07	-2.35	119.14	123.72
7	B	431	PGW	O03-C19-C20	2.34	119.26	111.91
6	A	408	SOG	C1-O5-C5	2.28	116.79	112.58
2	A	401	7MA	C10-C05-C06	2.28	120.45	117.10
6	B	413	SOG	C4-C3-C2	2.28	114.80	110.82
2	B	401	7MA	C05-C04-N03	2.26	116.77	113.13
2	B	401	7MA	C27-C26-S23	-2.23	114.35	117.42
6	A	417	SOG	C1-O5-C5	2.22	116.67	112.58
2	A	401	7MA	C19-C18-N17	-2.21	121.57	124.87
6	A	410	SOG	O5-C1-C2	2.17	113.05	110.31
6	A	413	SOG	O5-C5-C4	2.16	113.61	109.69
6	A	408	SOG	O5-C5-C4	2.12	113.55	109.69
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
2	A	401	7MA	C19-C20-C15	-2.08	117.59	120.32
6	B	407	SOG	C1-O5-C5	2.06	116.39	112.58
5	A	406	CIT	O4-C5-C4	2.06	120.97	114.35
6	B	414	SOG	C1'-S1-C1	2.04	103.91	100.09
6	A	411	SOG	O5-C5-C4	2.03	113.39	109.69
6	A	416	SOG	C1-C2-C3	-2.01	106.63	110.59

There are no chirality outliers.

All (258) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	410	SOG	O5-C1-S1-C1'
6	A	413	SOG	C2'-C1'-S1-C1
6	A	417	SOG	C2-C1-S1-C1'
6	A	417	SOG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
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	411	SOG	C2'-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	411	SOG	O5-C5-C6-O6
6	A	412	SOG	S1-C1'-C2'-C3'
6	A	417	SOG	S1-C1'-C2'-C3'
6	A	418	SOG	S1-C1'-C2'-C3'
6	B	416	SOG	S1-C1'-C2'-C3'
6	B	410	SOG	O5-C5-C6-O6
6	B	412	SOG	O5-C5-C6-O6
6	B	413	SOG	O5-C5-C6-O6
7	A	429	PGW	O04-C19-O03-C01
6	B	421	SOG	O5-C5-C6-O6
6	A	416	SOG	O5-C5-C6-O6
6	A	418	SOG	O5-C5-C6-O6
6	B	406	SOG	O5-C5-C6-O6
6	A	416	SOG	S1-C1'-C2'-C3'
6	B	406	SOG	S1-C1'-C2'-C3'
6	B	410	SOG	C4-C5-C6-O6
4	B	405	PG4	O3-C5-C6-O4
6	B	413	SOG	C4-C5-C6-O6
7	A	429	PGW	C16-C15-C27-C26

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Mol	Chain	Res	Type	Atoms
6	A	407	SOG	O5-C5-C6-O6
7	A	429	PGW	O12-C04-C05-CAD
6	B	408	SOG	C1'-C2'-C3'-C4'
6	B	412	SOG	C4-C5-C6-O6
4	A	404	PG4	O3-C5-C6-O4
6	B	414	SOG	O5-C5-C6-O6
6	B	414	SOG	C4-C5-C6-O6
6	A	414	SOG	O5-C5-C6-O6
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	406	SOG	C4-C5-C6-O6
4	A	403	PG4	O1-C1-C2-O2
4	B	405	PG4	O1-C1-C2-O2
6	A	421	SOG	C1'-C2'-C3'-C4'
2	B	401	7MA	N03-C11-C13-N14
4	A	405	PG4	C3-C4-O3-C5
7	B	431	PGW	C04-O12-P-O11
6	A	407	SOG	C1'-C2'-C3'-C4'
6	A	424	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'
4	B	404	PG4	O1-C1-C2-O2
6	A	416	SOG	C2'-C3'-C4'-C5'
6	B	419	SOG	C1'-C2'-C3'-C4'
6	B	422	SOG	C1'-C2'-C3'-C4'
6	B	430	SOG	C1'-C2'-C3'-C4'
6	A	426	SOG	C2'-C3'-C4'-C5'
6	B	409	SOG	C4'-C5'-C6'-C7'
6	B	407	SOG	S1-C1'-C2'-C3'
6	B	418	SOG	C3'-C4'-C5'-C6'
6	B	423	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C16-C17-C18-C28
6	A	410	SOG	C2'-C3'-C4'-C5'
6	B	412	SOG	C4'-C5'-C6'-C7'
2	A	401	7MA	C13-N14-S23-O25
2	B	401	7MA	C13-N14-S23-O25
7	B	431	PGW	C08-C09-C11-C12
7	B	431	PGW	C09-C11-C12-C13
7	A	429	PGW	C09-C11-C12-C13
4	A	404	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	A	417	SOG	C4'-C5'-C6'-C7'
6	B	408	SOG	C3'-C4'-C5'-C6'
6	A	408	SOG	C4-C5-C6-O6
6	B	411	SOG	C3'-C4'-C5'-C6'
6	A	410	SOG	S1-C1'-C2'-C3'
6	A	414	SOG	C2'-C3'-C4'-C5'
6	A	416	SOG	C4'-C5'-C6'-C7'
6	A	417	SOG	C2'-C3'-C4'-C5'
6	A	414	SOG	C4'-C5'-C6'-C7'
6	A	416	SOG	C3'-C4'-C5'-C6'
6	A	428	SOG	C2'-C3'-C4'-C5'
6	B	410	SOG	C3'-C4'-C5'-C6'
7	A	429	PGW	C25-C26-C27-C15
7	A	429	PGW	C22-C23-C24-C25
6	A	427	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C06-C07-C08-C09
6	A	423	SOG	C2'-C3'-C4'-C5'
7	A	429	PGW	C23-C24-C25-C26
6	B	408	SOG	O5-C5-C6-O6
6	A	413	SOG	C2'-C3'-C4'-C5'
6	A	414	SOG	C3'-C4'-C5'-C6'
6	A	407	SOG	S1-C1'-C2'-C3'
6	A	409	SOG	C2'-C3'-C4'-C5'
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	413	SOG	C4'-C5'-C6'-C7'
4	A	404	PG4	O4-C7-C8-O5
7	B	431	PGW	C1-C2-C3-C4
6	B	407	SOG	C1'-C2'-C3'-C4'
6	A	415	SOG	O5-C5-C6-O6
6	A	418	SOG	C4-C5-C6-O6
6	B	421	SOG	C4-C5-C6-O6
6	A	411	SOG	C3'-C4'-C5'-C6'
2	A	401	7MA	N03-C11-C13-N14
6	A	417	SOG	C1'-C2'-C3'-C4'
6	B	417	SOG	C3'-C4'-C5'-C6'
7	B	431	PGW	C21-C22-C23-C24
6	A	412	SOG	C4'-C5'-C6'-C7'
6	A	407	SOG	C4-C5-C6-O6
7	A	429	PGW	C21-C22-C23-C24
4	B	405	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
7	A	429	PGW	O03-C01-C02-C03
7	B	431	PGW	O03-C01-C02-C03
6	A	422	SOG	C3'-C4'-C5'-C6'
6	A	409	SOG	O5-C5-C6-O6
6	A	424	SOG	C3'-C4'-C5'-C6'
6	A	413	SOG	C3'-C4'-C5'-C6'
6	B	415	SOG	C3'-C4'-C5'-C6'
2	A	401	7MA	C13-N14-S23-C26
6	A	422	SOG	C1'-C2'-C3'-C4'
6	B	420	SOG	C1'-C2'-C3'-C4'
6	B	408	SOG	S1-C1'-C2'-C3'
6	A	409	SOG	C4'-C5'-C6'-C7'
6	B	424	SOG	C2'-C3'-C4'-C5'
6	A	412	SOG	C2'-C3'-C4'-C5'
6	B	414	SOG	C5'-C6'-C7'-C8'
6	B	408	SOG	C5'-C6'-C7'-C8'
6	B	428	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C11-C12-C13-C14
6	B	408	SOG	C4'-C5'-C6'-C7'
6	A	414	SOG	C4-C5-C6-O6
7	A	429	PGW	C4-C5-C6-C7
7	A	429	PGW	C19-C20-C21-C22
7	B	431	PGW	C25-C26-C27-C15
6	A	408	SOG	O5-C5-C6-O6
6	A	427	SOG	C3'-C4'-C5'-C6'
6	A	417	SOG	C5'-C6'-C7'-C8'
6	B	419	SOG	C5'-C6'-C7'-C8'
6	B	409	SOG	C5'-C6'-C7'-C8'
2	A	401	7MA	C13-N14-S23-O24
2	B	401	7MA	C13-N14-S23-O24
2	B	401	7MA	O12-C11-C13-N14
6	B	417	SOG	C5'-C6'-C7'-C8'
6	B	413	SOG	S1-C1'-C2'-C3'
2	A	401	7MA	O12-C11-C13-N14
6	B	427	SOG	C2'-C3'-C4'-C5'
6	B	407	SOG	C3'-C4'-C5'-C6'
6	B	409	SOG	C2'-C1'-S1-C1
6	B	410	SOG	C2'-C1'-S1-C1
6	B	421	SOG	C2'-C1'-S1-C1
7	B	431	PGW	C20-C19-O03-C01
6	B	411	SOG	C2'-C3'-C4'-C5'
6	B	422	SOG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
4	B	405	PG4	C1-C2-O2-C3
7	B	431	PGW	C15-C16-C17-C18
2	B	401	7MA	C13-N14-S23-C26
4	B	404	PG4	O4-C7-C8-O5
7	B	431	PGW	O04-C19-O03-C01
6	A	416	SOG	C4-C5-C6-O6
4	B	405	PG4	C3-C4-O3-C5
6	A	425	SOG	S1-C1'-C2'-C3'
6	B	424	SOG	S1-C1'-C2'-C3'
6	A	407	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	C04-O12-P-O13
7	B	431	PGW	C04-O12-P-O14
6	A	423	SOG	C1'-C2'-C3'-C4'
6	A	409	SOG	C3'-C4'-C5'-C6'
6	A	409	SOG	C2-C1-S1-C1'
4	B	405	PG4	C5-C6-O4-C7
6	B	415	SOG	C4'-C5'-C6'-C7'
6	B	410	SOG	C5'-C6'-C7'-C8'
4	A	404	PG4	C6-C5-O3-C4
7	B	431	PGW	O03-C01-C02-O01
4	B	405	PG4	C6-C5-O3-C4
6	B	412	SOG	C3'-C4'-C5'-C6'
6	B	430	SOG	C3'-C4'-C5'-C6'
6	A	408	SOG	C1'-C2'-C3'-C4'
6	B	419	SOG	C3'-C4'-C5'-C6'
6	B	407	SOG	C4-C5-C6-O6
4	A	403	PG4	C8-C7-O4-C6
6	A	412	SOG	C3'-C4'-C5'-C6'
6	A	418	SOG	C1'-C2'-C3'-C4'
5	A	406	CIT	O7-C3-C4-C5
6	B	410	SOG	C4'-C5'-C6'-C7'
7	B	431	PGW	C07-C08-C09-C11
6	A	410	SOG	C1'-C2'-C3'-C4'
7	A	429	PGW	O03-C01-C02-O01
7	A	429	PGW	C03-O11-P-O12
7	A	429	PGW	C04-O12-P-O11
7	A	429	PGW	C17-C18-C28-C30
6	A	408	SOG	S1-C1'-C2'-C3'
6	B	410	SOG	S1-C1'-C2'-C3'
4	B	405	PG4	O2-C3-C4-O3
7	B	431	PGW	C05-C04-O12-P
7	A	429	PGW	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
7	A	429	PGW	C10-C06-C07-C08
7	B	431	PGW	C7-C8-C9-C10
6	B	407	SOG	C2'-C3'-C4'-C5'
5	A	406	CIT	C3-C4-C5-O4
6	B	411	SOG	S1-C1'-C2'-C3'
5	A	406	CIT	C3-C4-C5-O3
6	B	409	SOG	S1-C1'-C2'-C3'
6	B	417	SOG	C2'-C3'-C4'-C5'
4	A	403	PG4	C1-C2-O2-C3
4	B	404	PG4	C5-C6-O4-C7
6	B	419	SOG	C4'-C5'-C6'-C7'
6	B	423	SOG	C5'-C6'-C7'-C8'
6	B	406	SOG	C1'-C2'-C3'-C4'
6	A	409	SOG	O5-C1-S1-C1'
6	A	410	SOG	C2'-C1'-S1-C1
6	B	408	SOG	C2'-C1'-S1-C1
6	B	410	SOG	O5-C1-S1-C1'
6	A	416	SOG	C5'-C6'-C7'-C8'
4	A	404	PG4	C5-C6-O4-C7
4	B	404	PG4	C3-C4-O3-C5
7	A	429	PGW	C15-C16-C17-C18
7	B	431	PGW	C23-C24-C25-C26
2	A	401	7MA	C15-N14-S23-O25
6	A	418	SOG	C2'-C3'-C4'-C5'
7	A	429	PGW	C06-C07-C08-C09
6	B	419	SOG	C2'-C3'-C4'-C5'
7	B	431	PGW	O01-C1-C2-C3
6	B	430	SOG	C2'-C3'-C4'-C5'
6	B	412	SOG	S1-C1'-C2'-C3'
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	407	SOG	C5'-C6'-C7'-C8'
4	A	405	PG4	O2-C3-C4-O3
5	A	406	CIT	C6-C3-C4-C5
2	A	401	7MA	C11-C13-N14-C15
2	B	401	7MA	C11-C13-N14-C15
7	A	429	PGW	C03-O11-P-O14
7	B	431	PGW	O02-C1-C2-C3
7	A	429	PGW	O03-C19-C20-C21
4	A	405	PG4	O3-C5-C6-O4
6	A	414	SOG	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
6	A	418	SOG	C2-C1-S1-C1'
6	A	412	SOG	C1'-C2'-C3'-C4'

There are no ring outliers.

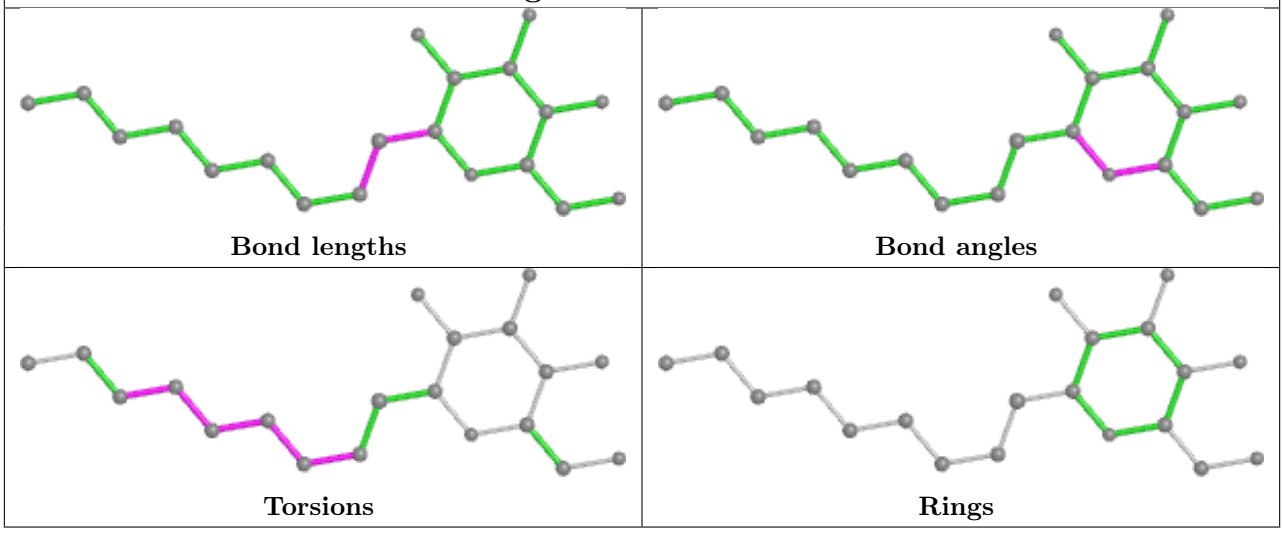
25 monomers are involved in 45 short contacts:

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

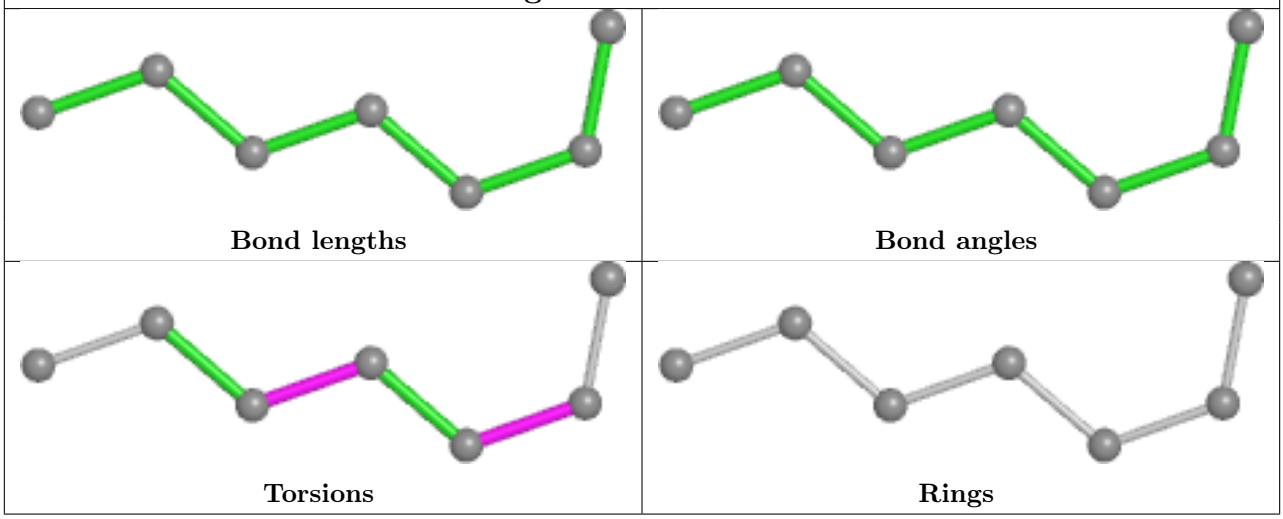
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

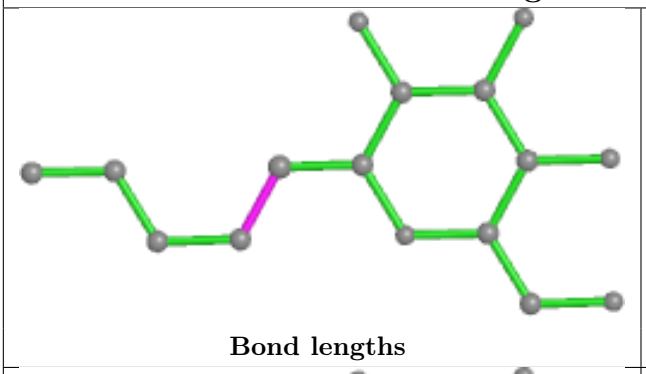
Ligand SOG A 412



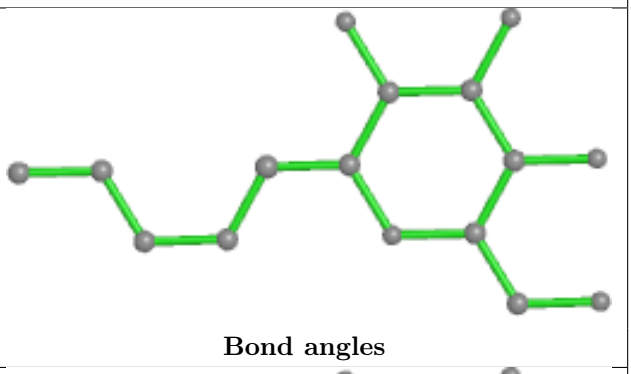
Ligand SOG A 425



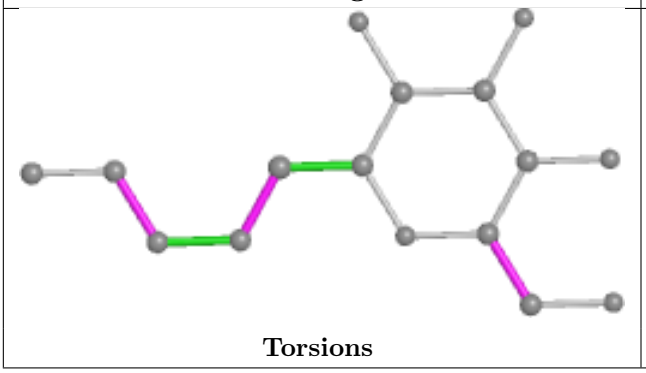
Ligand SOG B 421



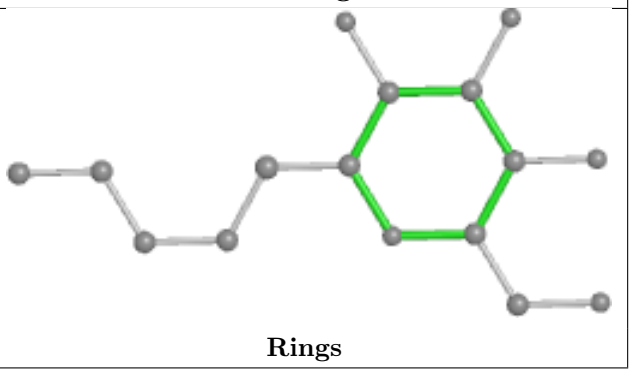
Bond lengths



Bond angles

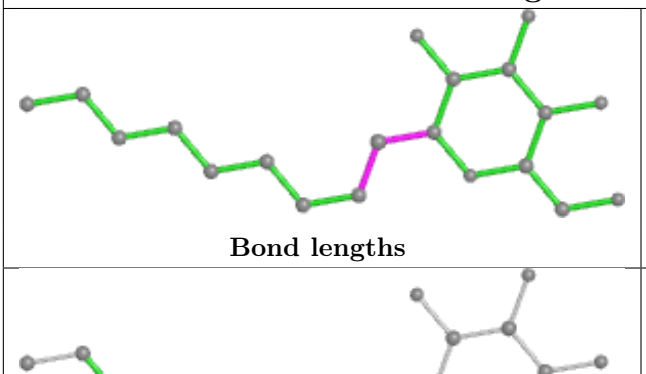


Torsions

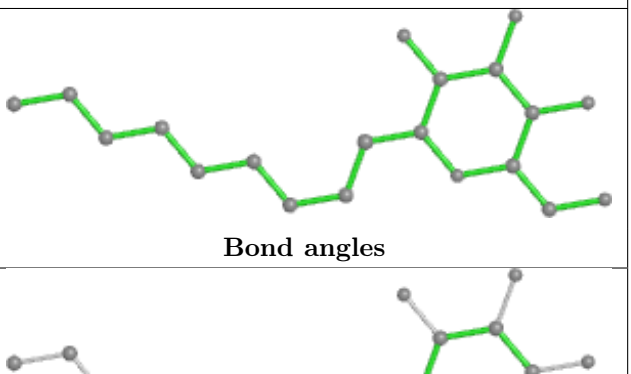


Rings

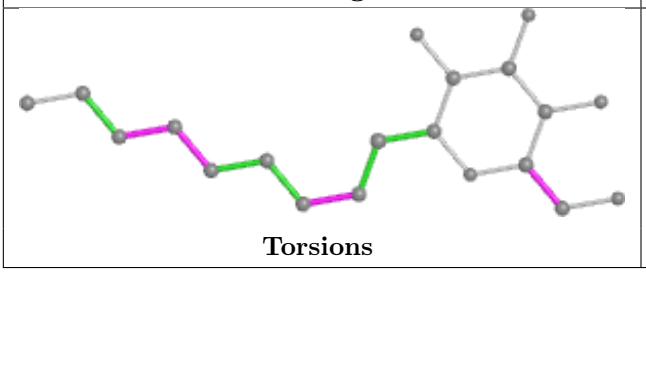
Ligand SOG B 412



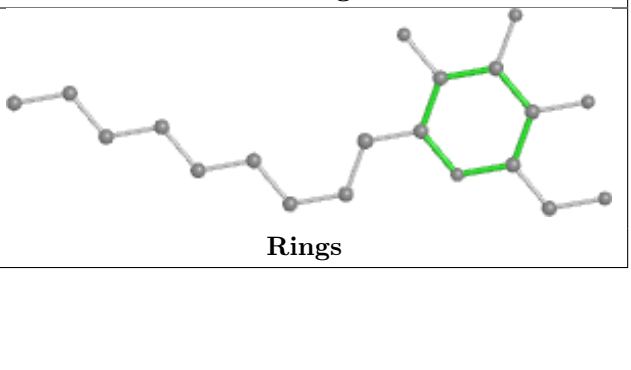
Bond lengths



Bond angles

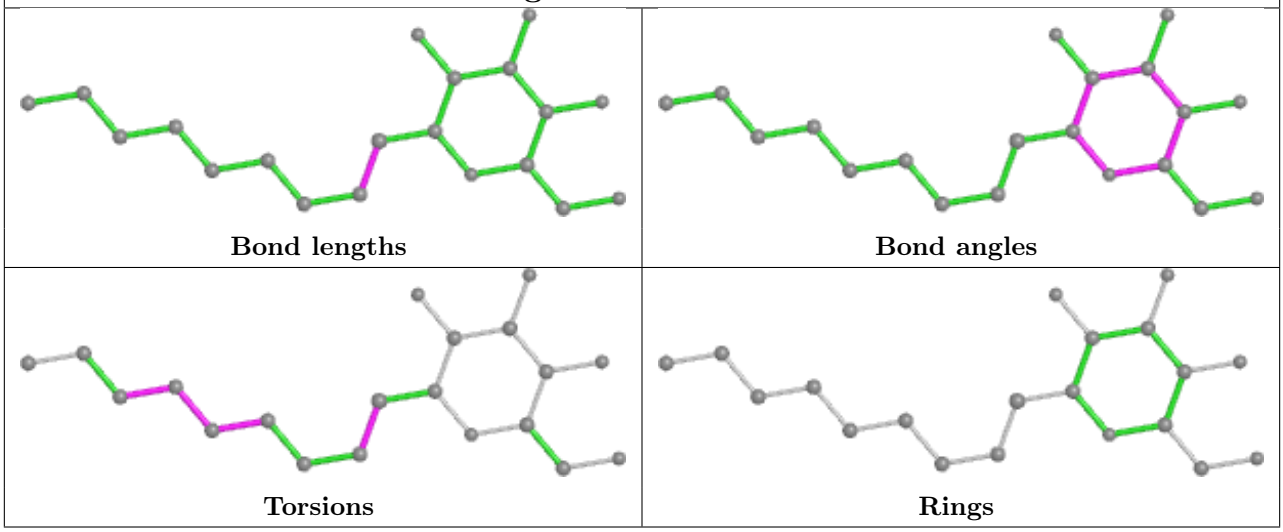


Torsions

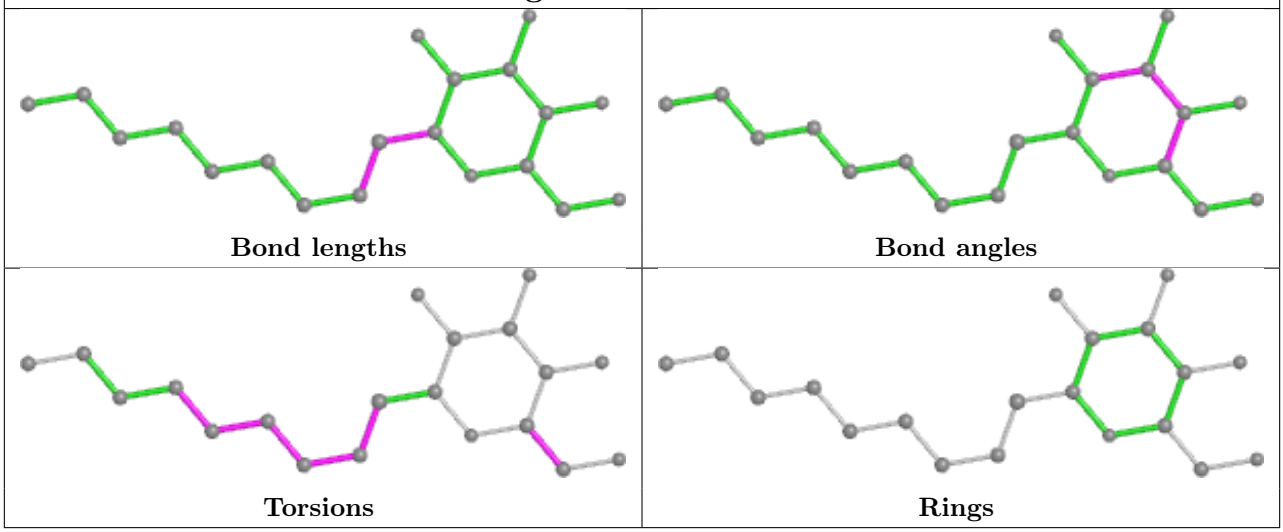


Rings

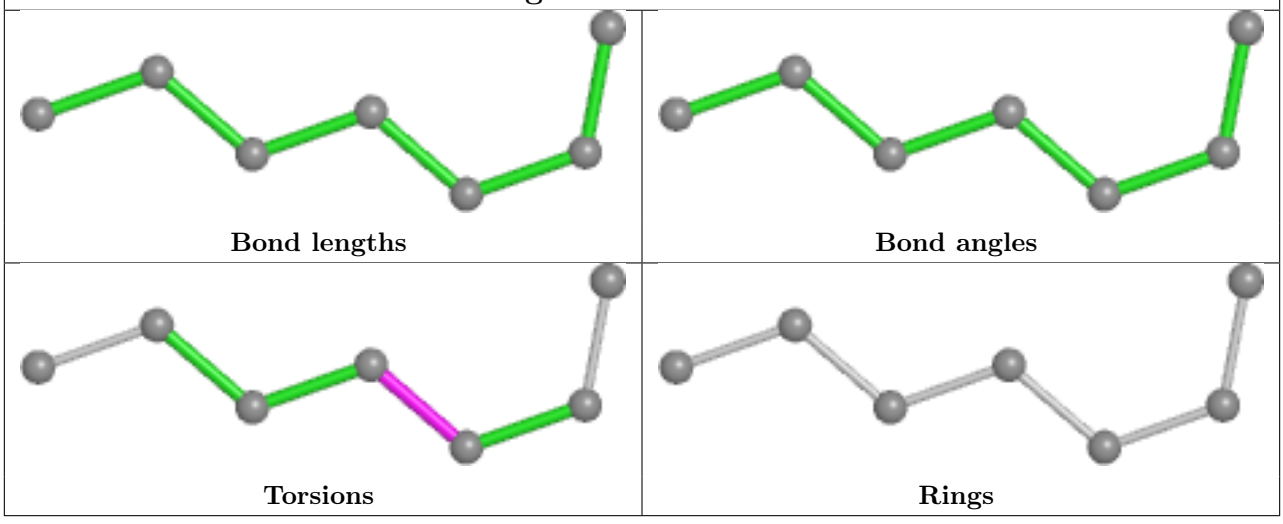
Ligand SOG A 413



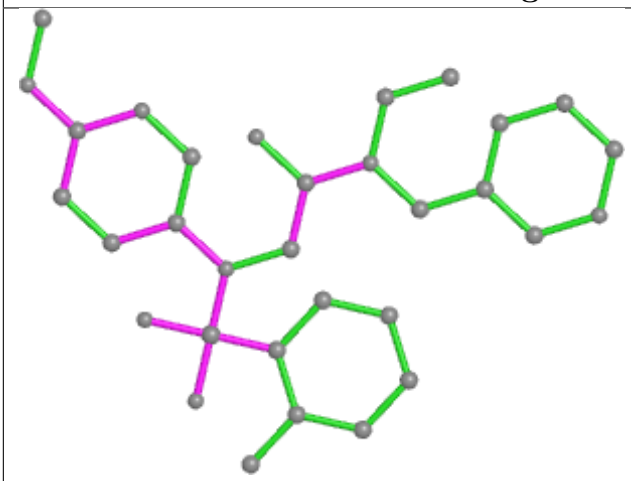
Ligand SOG B 411



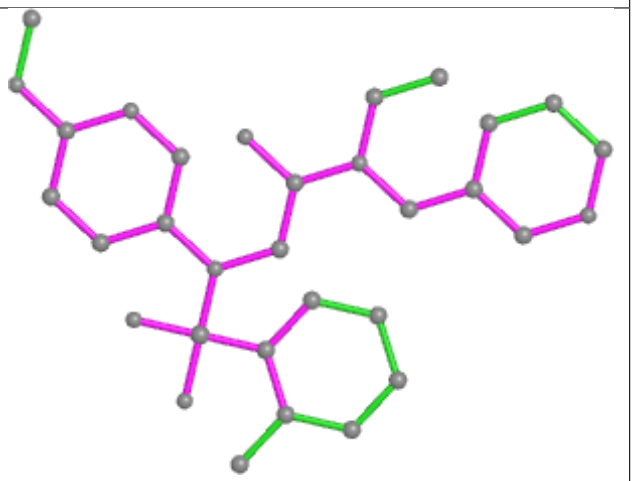
Ligand SOG B 429



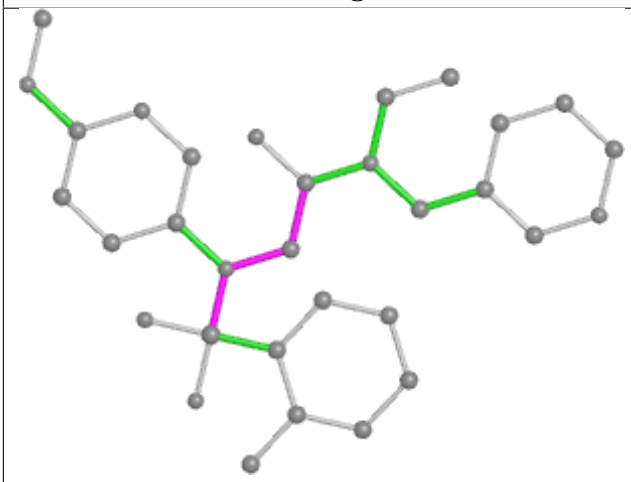
Ligand 7MA A 401



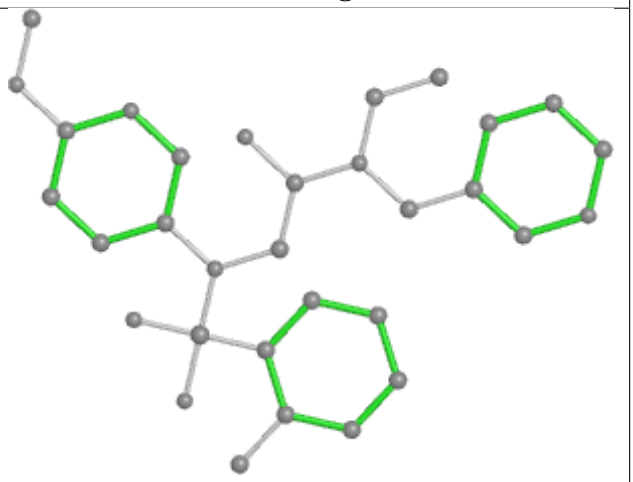
Bond lengths



Bond angles

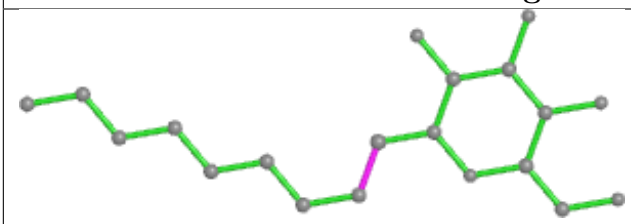


Torsions



Rings

Ligand SOG A 418



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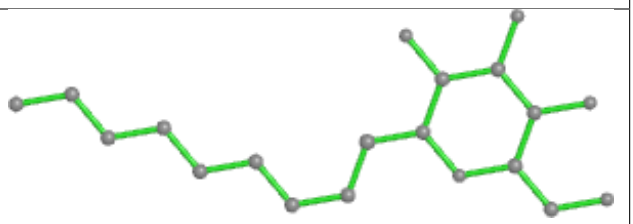
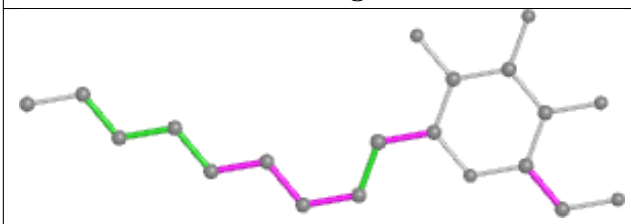


Bond angles



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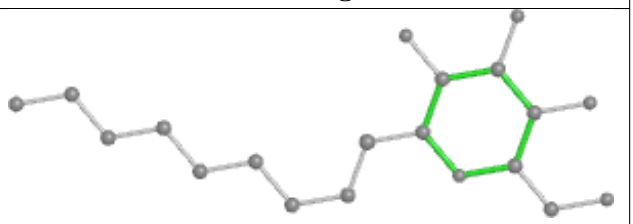
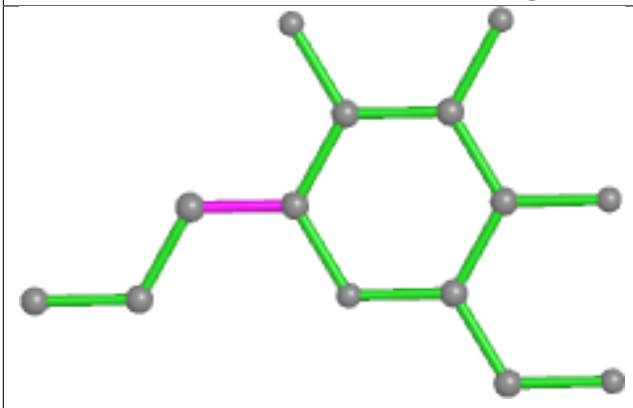


Rings

Ligand SOG A 415



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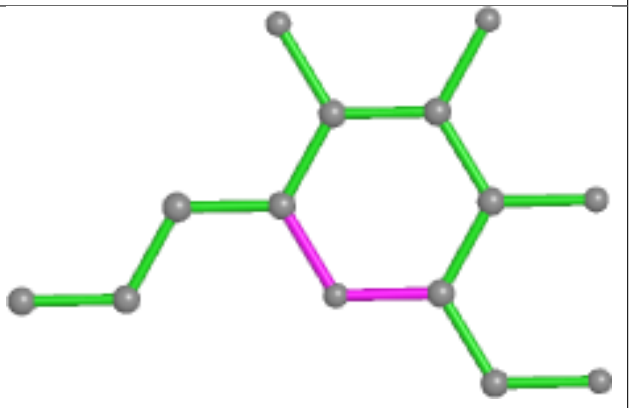
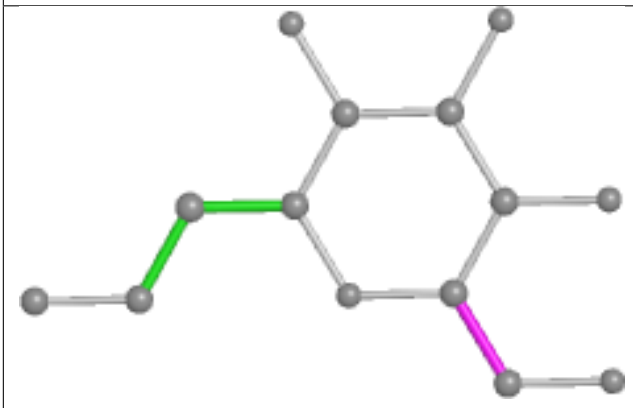


Bond angles



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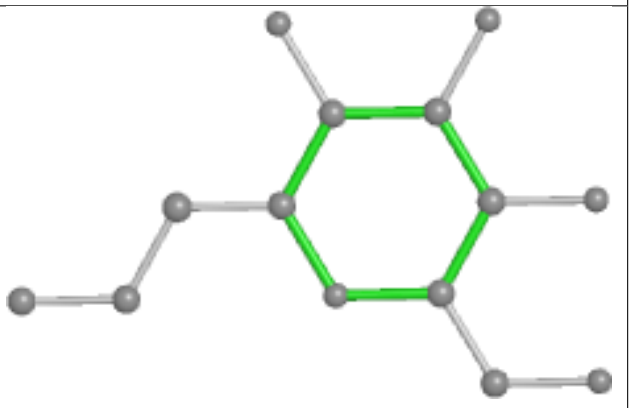
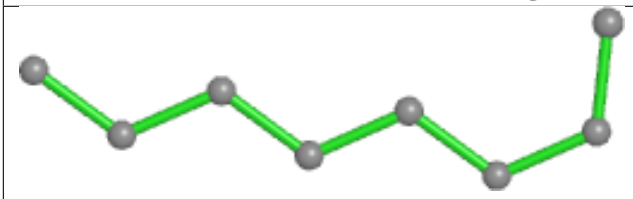
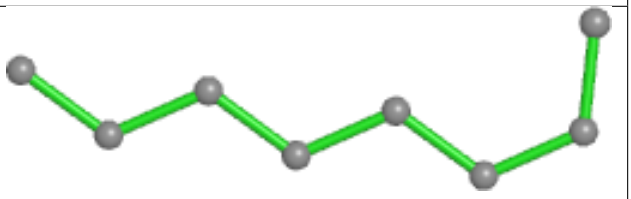


Rings

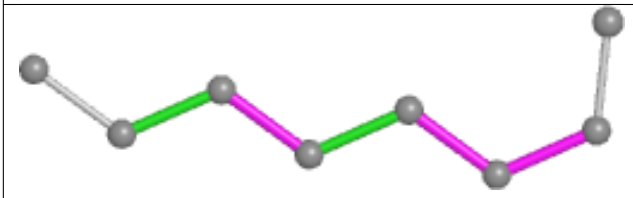
Ligand SOG B 418



Bond lengths



Bond angles



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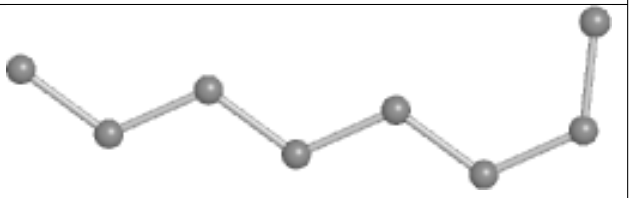
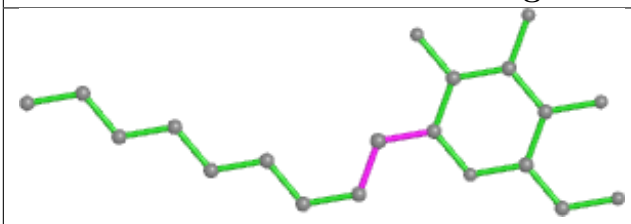
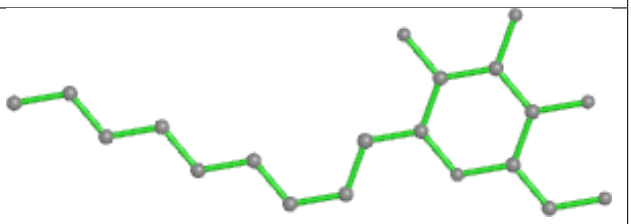
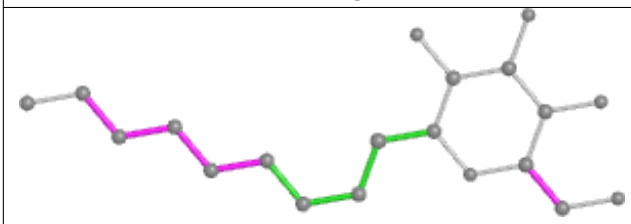
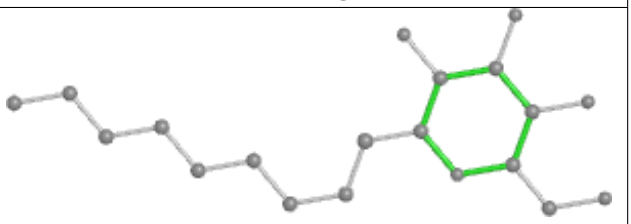
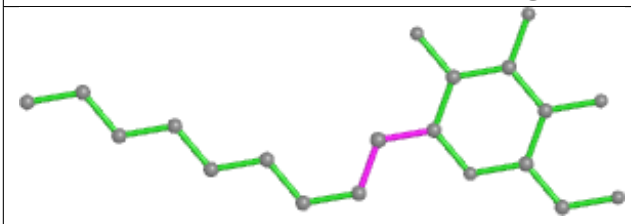
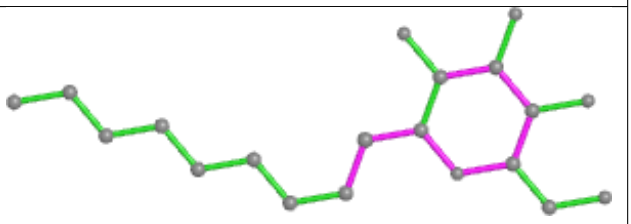
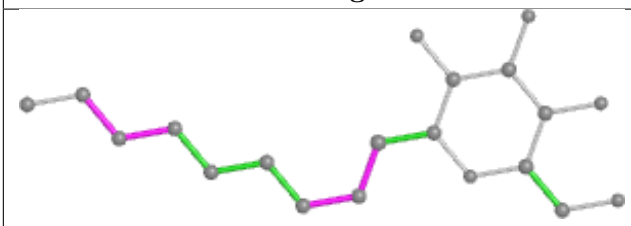
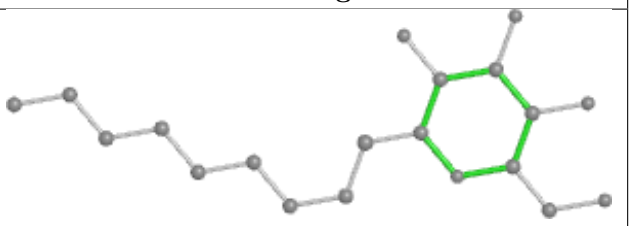
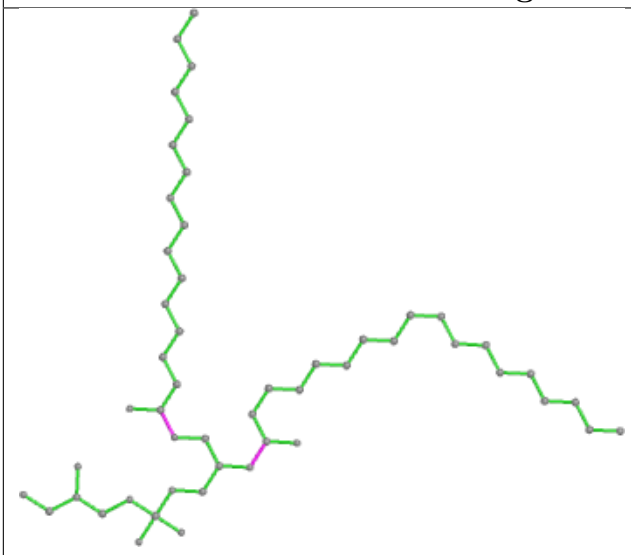


Rings

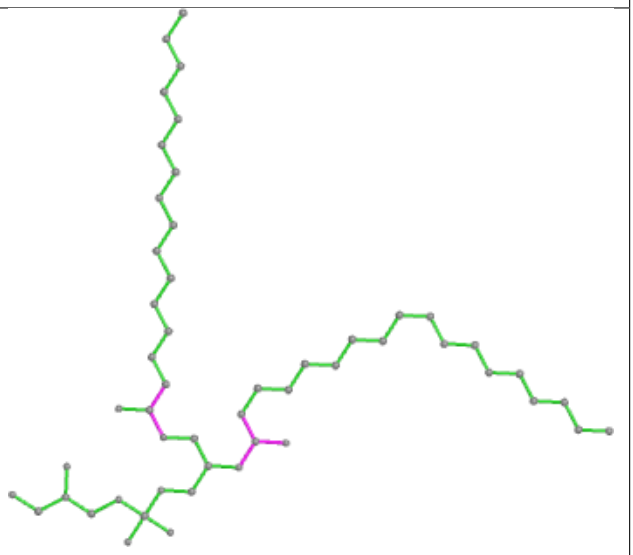
Ligand SOG A 414	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SOG B 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

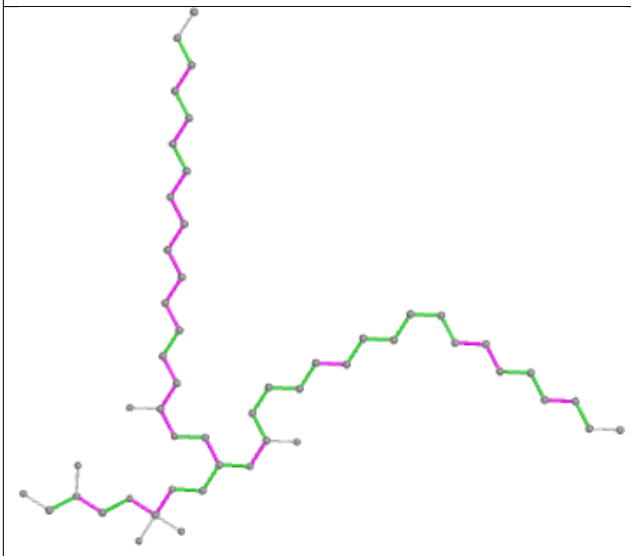
Ligand PGW A 429



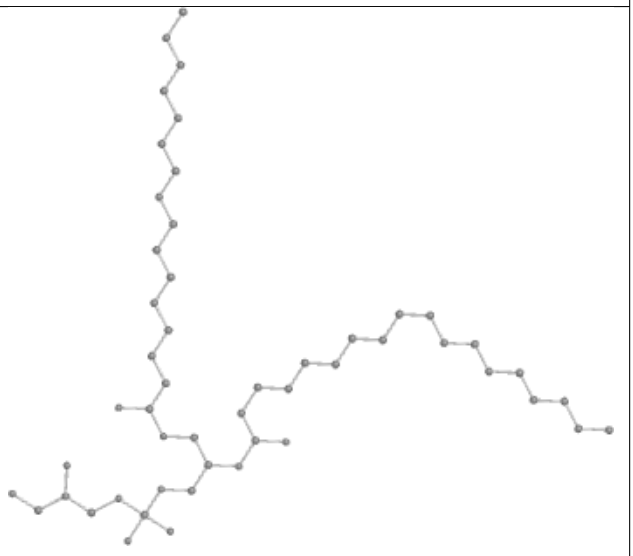
Bond lengths



Bond angles

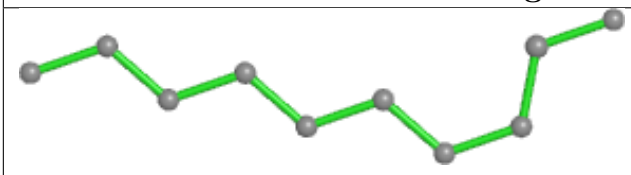


Torsions

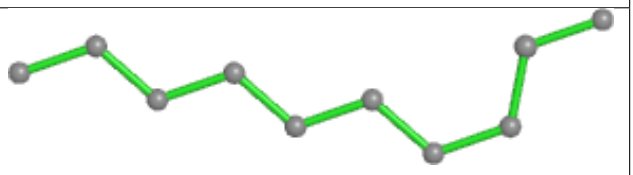


Rings

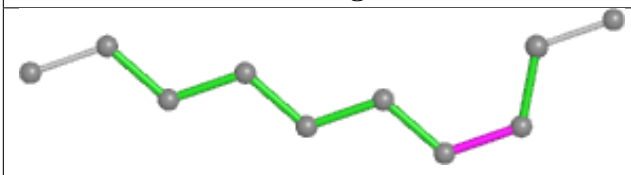
Ligand SOG B 416



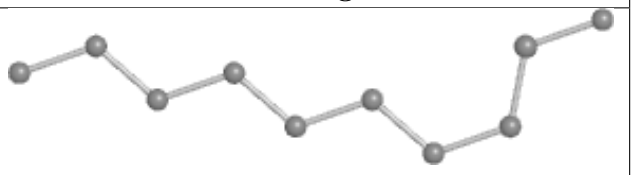
Bond lengths



Bond angles

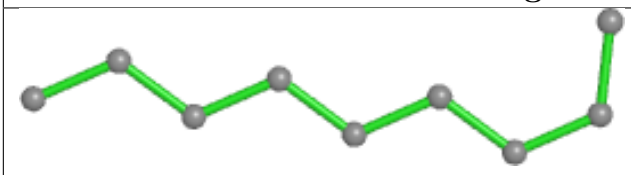


Torsions

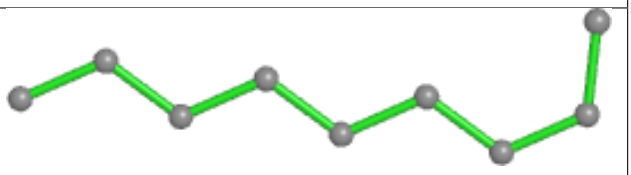


Rings

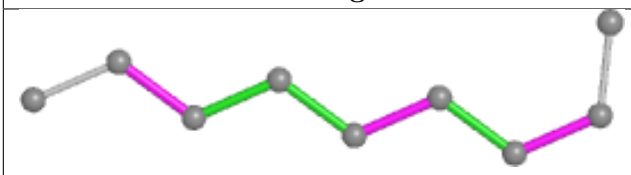
Ligand SOG B 423



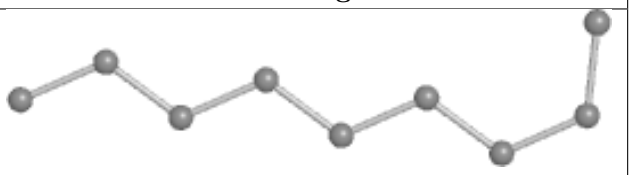
Bond lengths



Bond angles

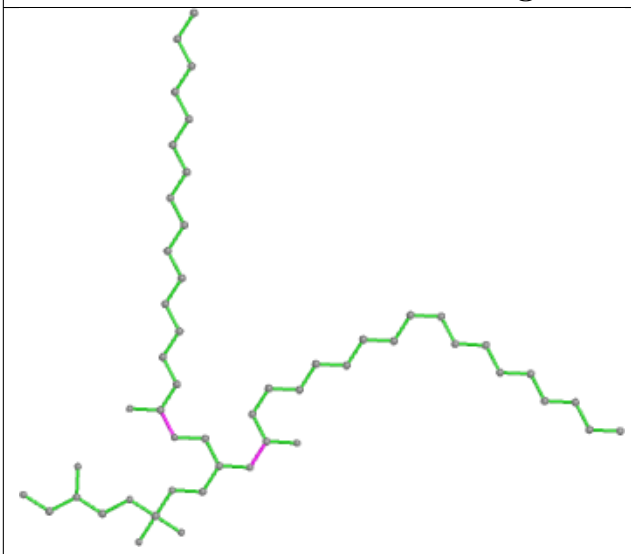


Torsions

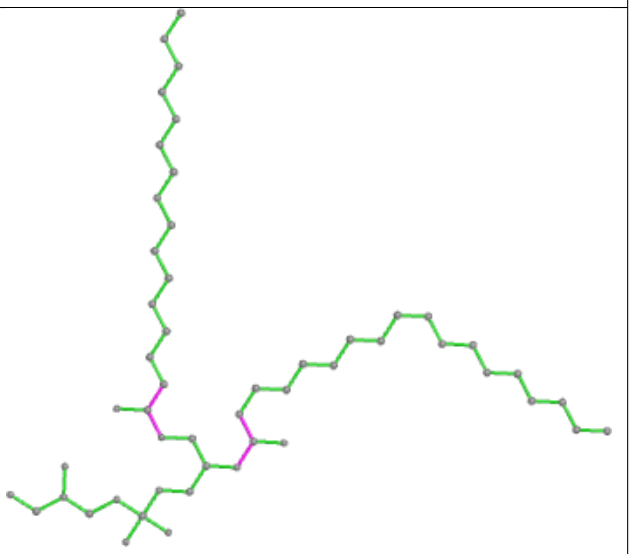


Rings

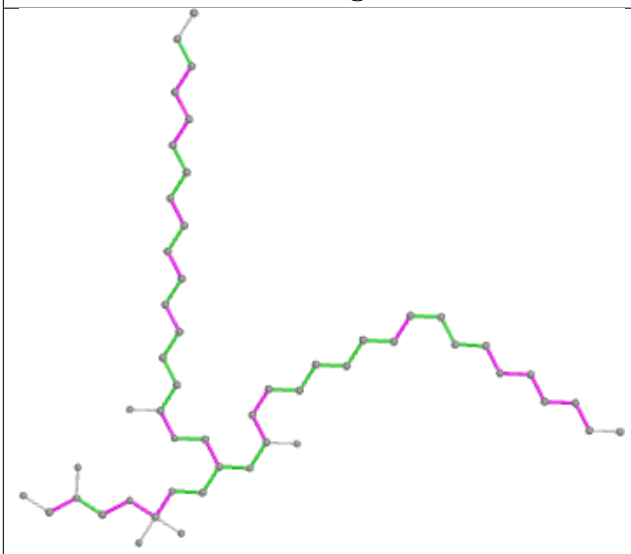
Ligand PGW B 431



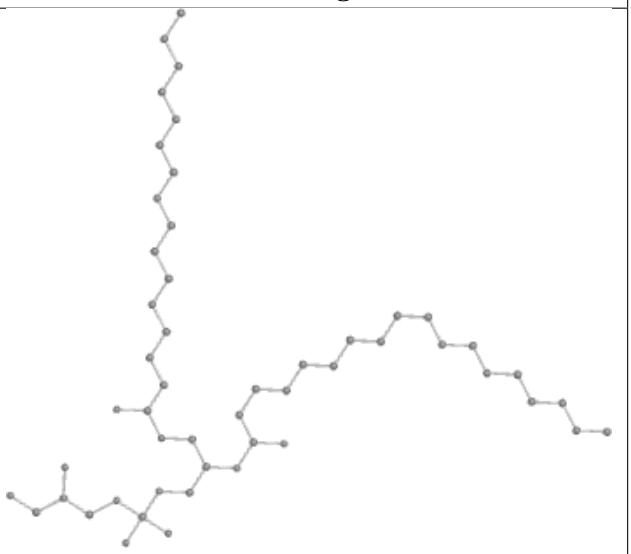
Bond lengths



Bond angles

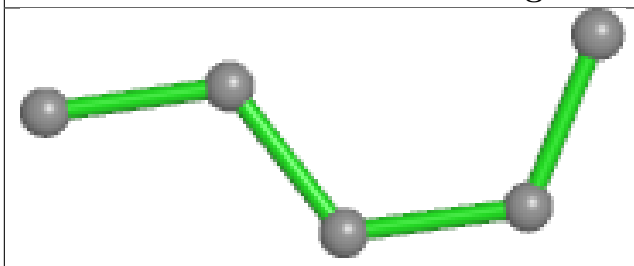


Torsions

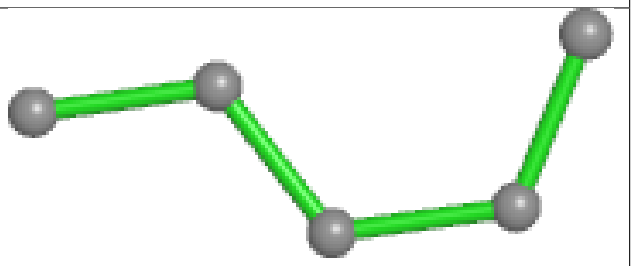


Rings

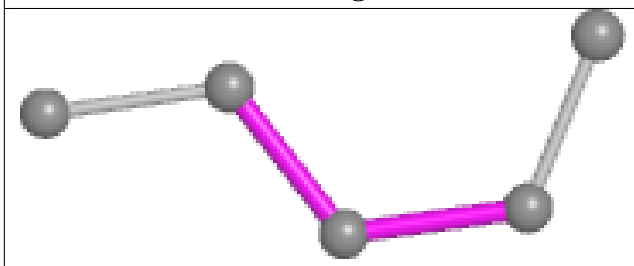
Ligand SOG B 420



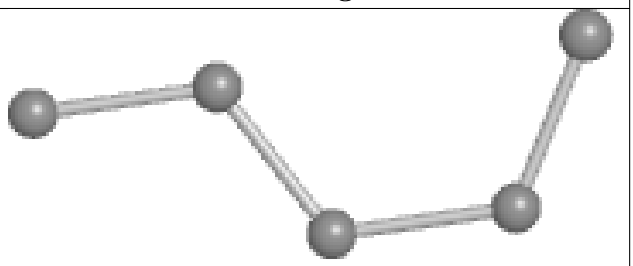
Bond lengths



Bond angles

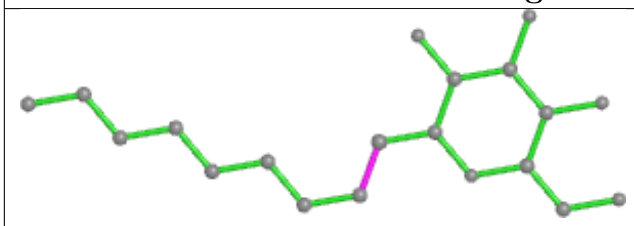


Torsions

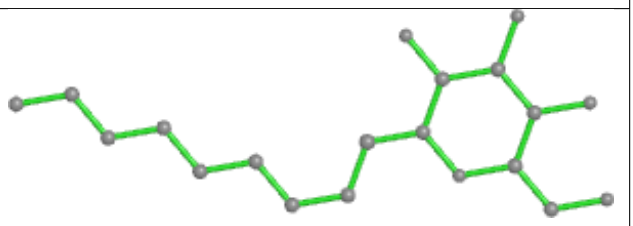


Rings

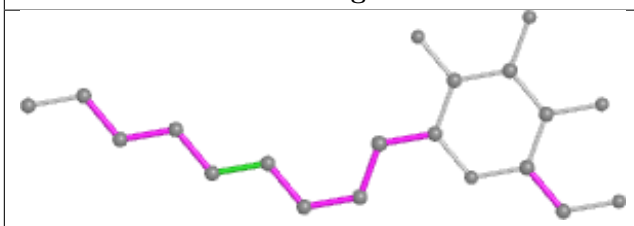
Ligand SOG B 410



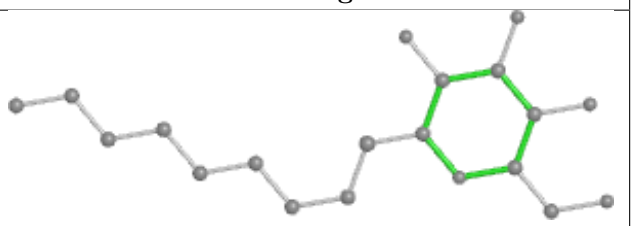
Bond lengths



Bond angles

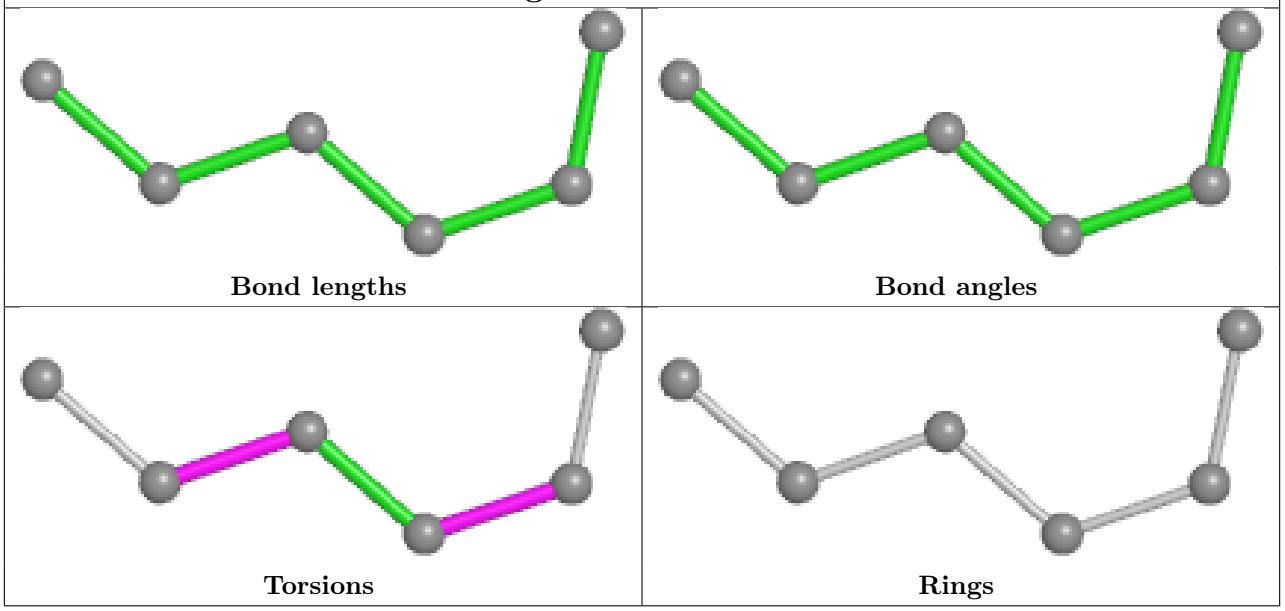


Torsions

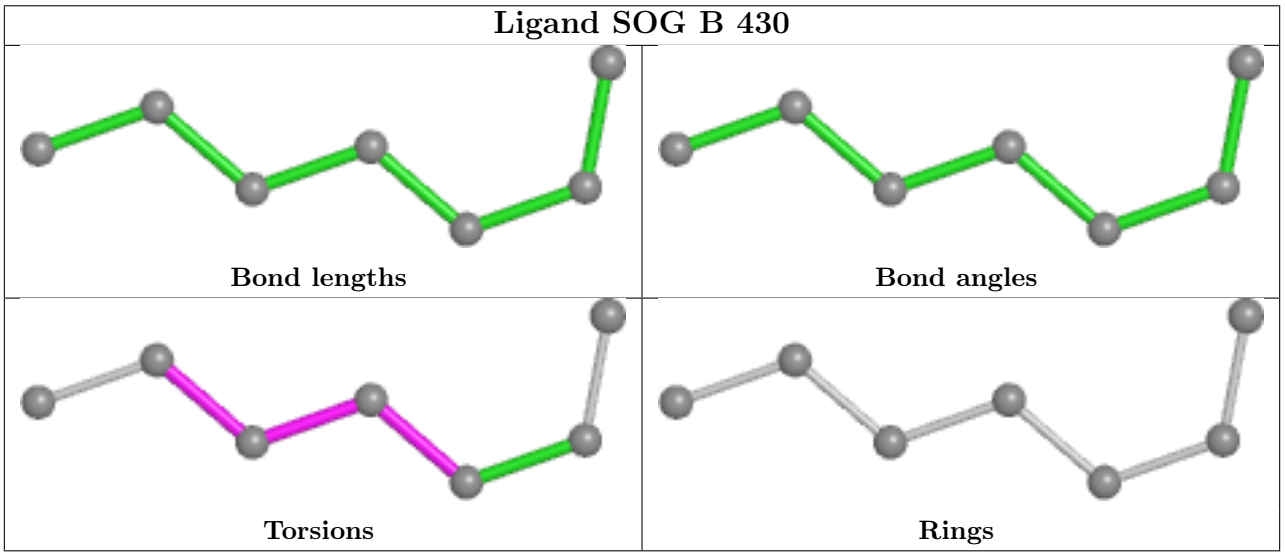


Rings

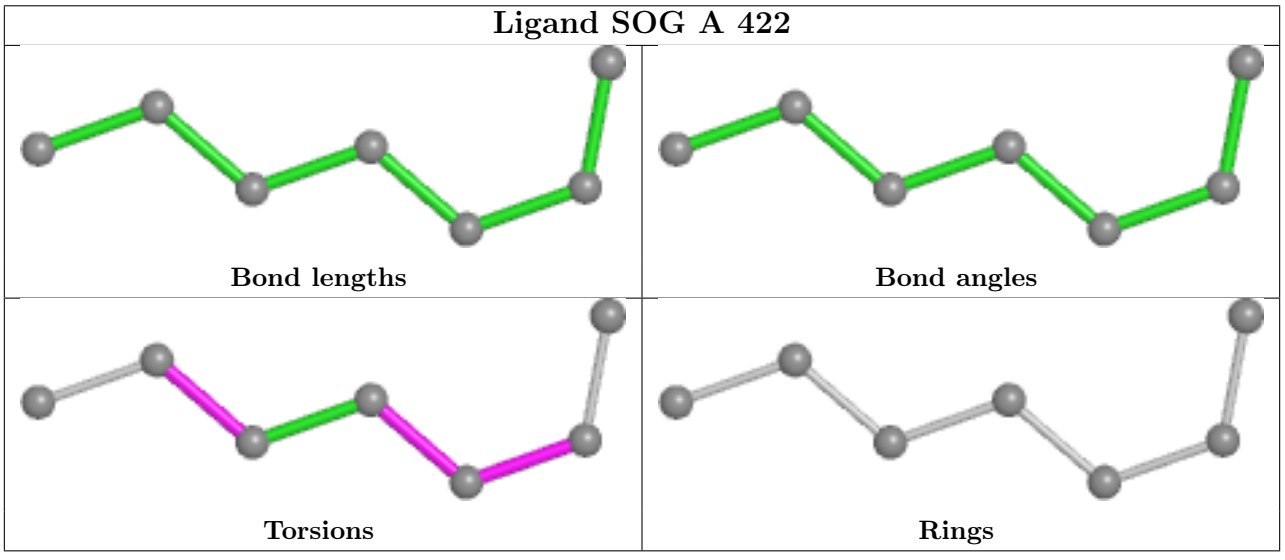
Ligand SOG B 424

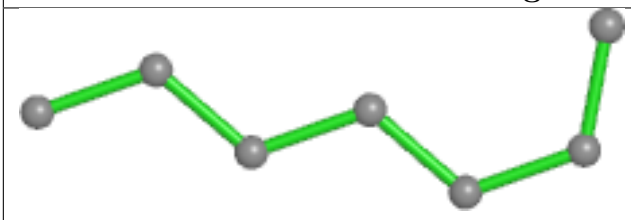
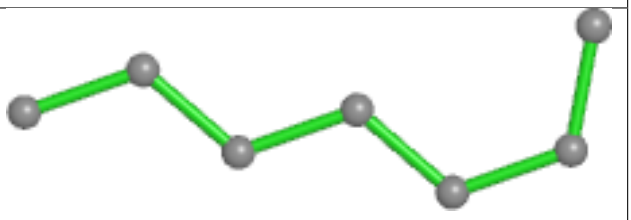
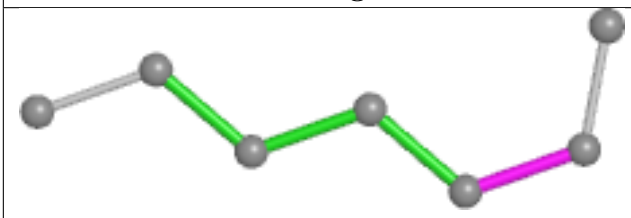
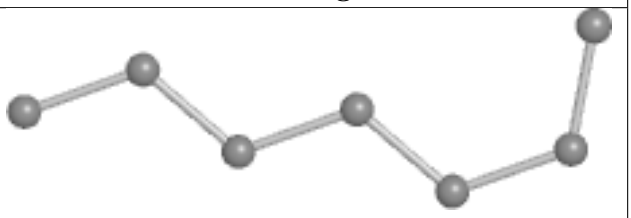


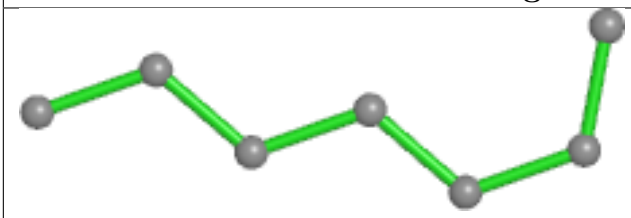
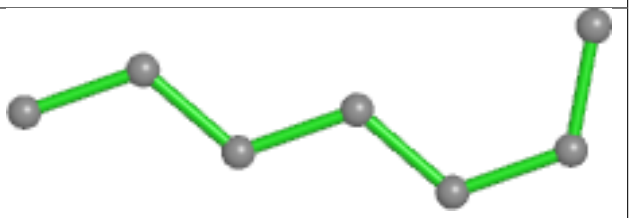
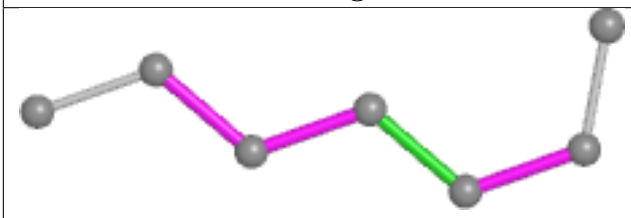
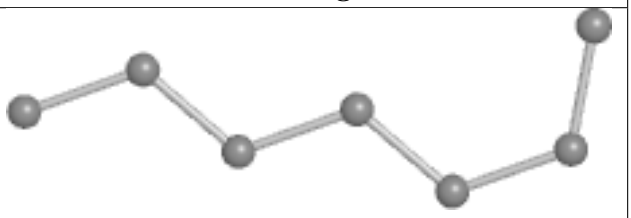
Ligand SOG B 430



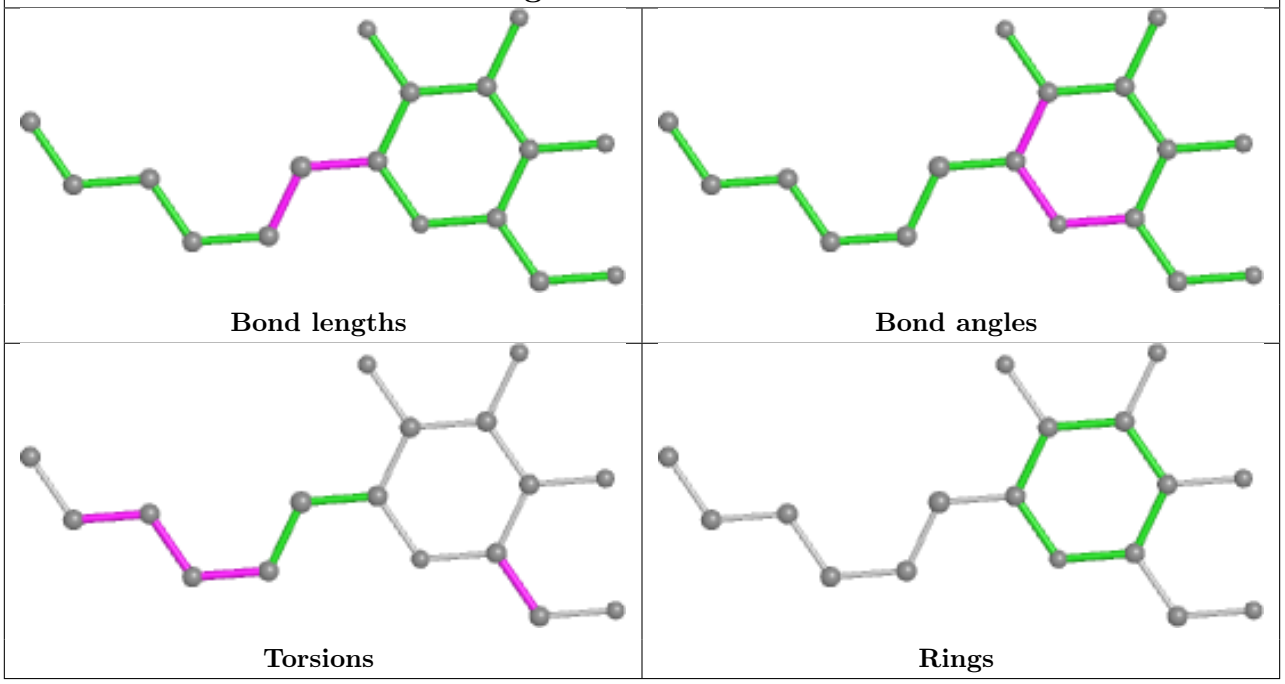
Ligand SOG A 422



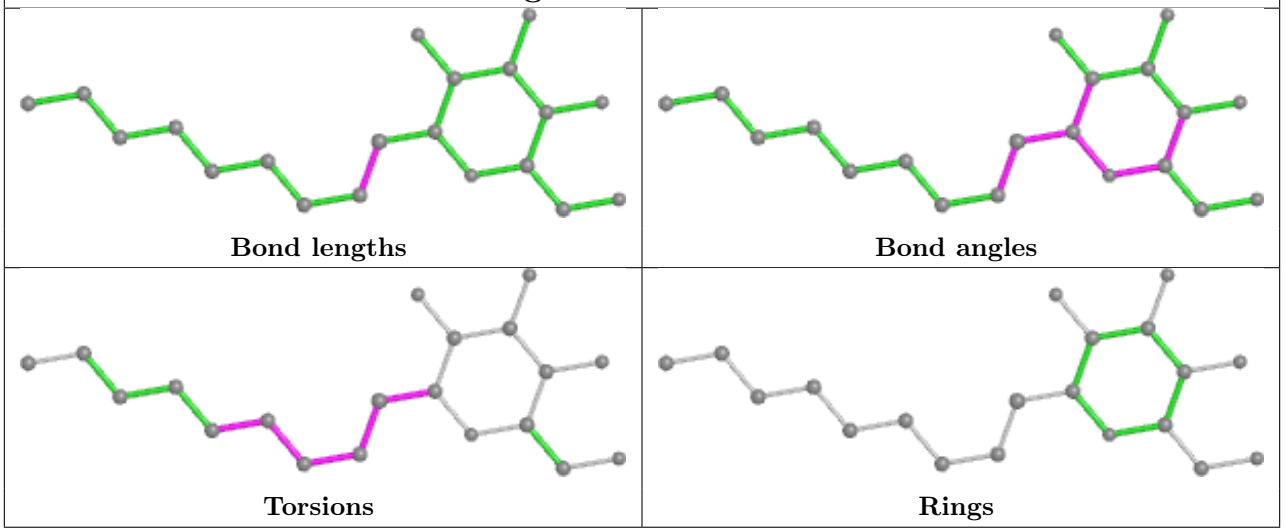
Ligand SOG A 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SOG A 427	
 Bond lengths	 Bond angles
 Torsions	 Rings

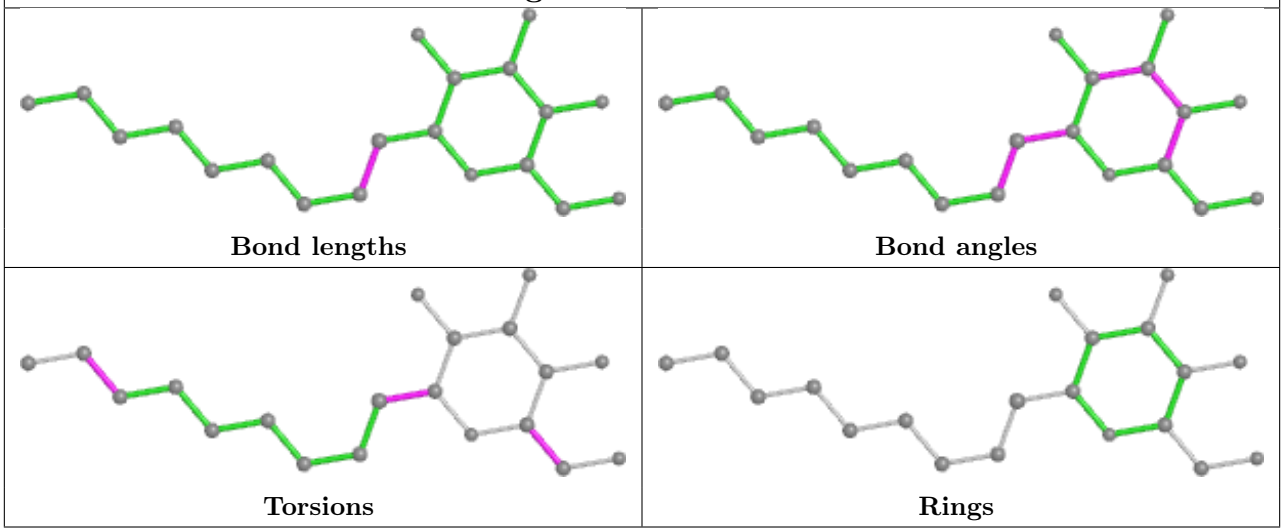
Ligand SOG A 407



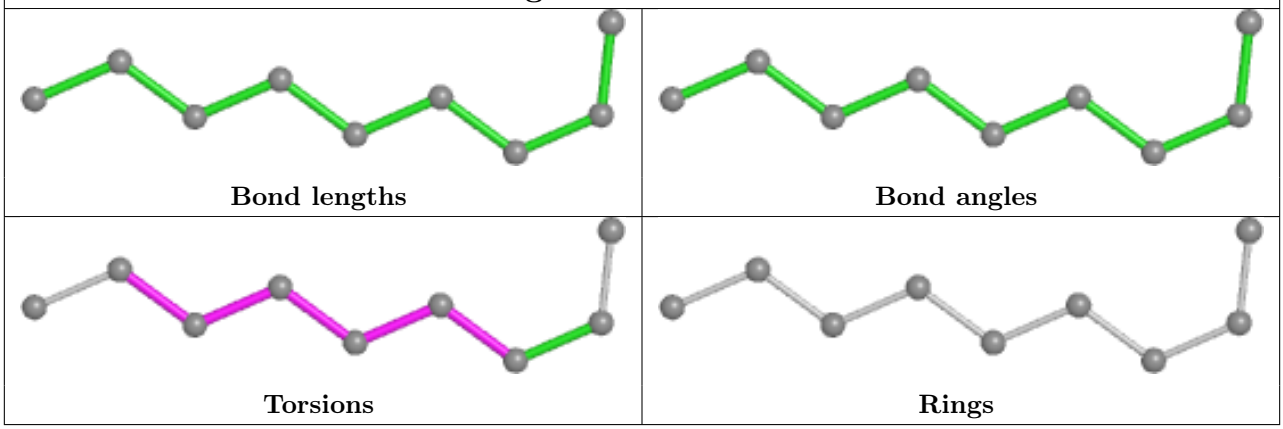
Ligand SOG A 410



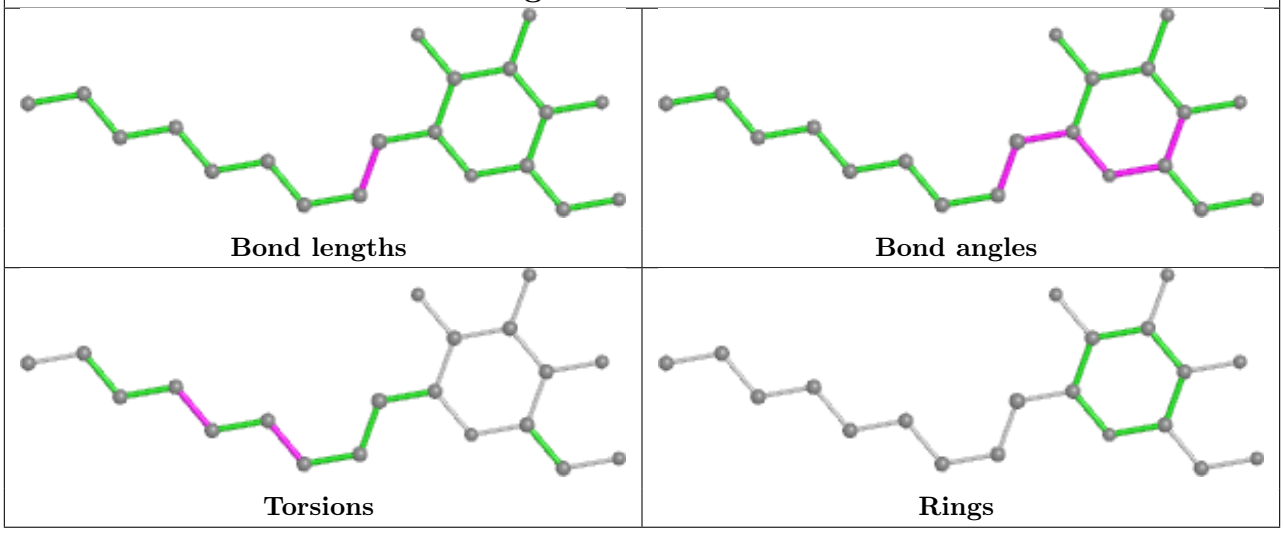
Ligand SOG B 414



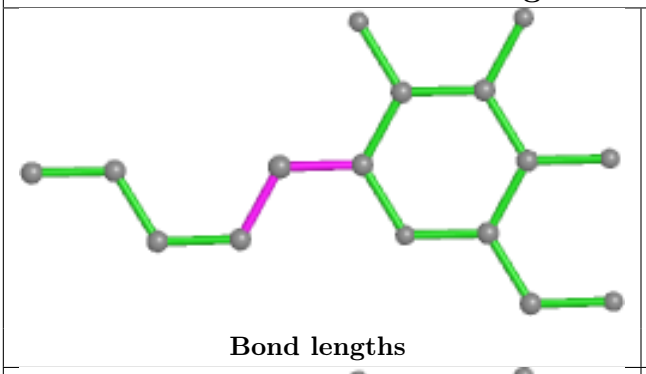
Ligand SOG B 419



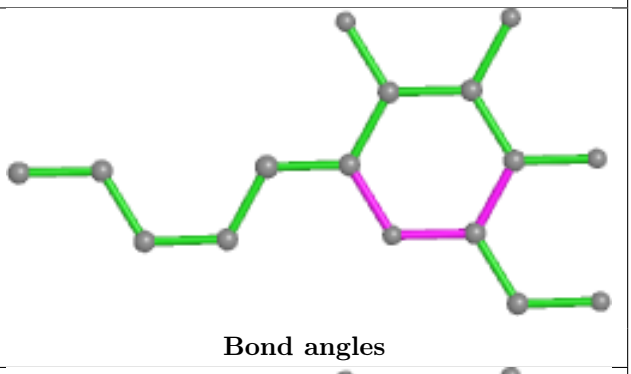
Ligand SOG A 411



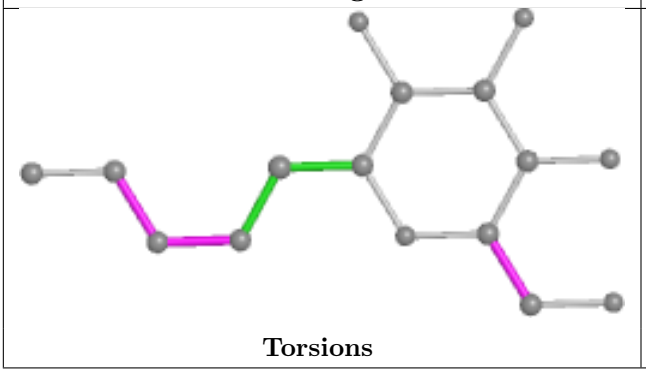
Ligand SOG A 408



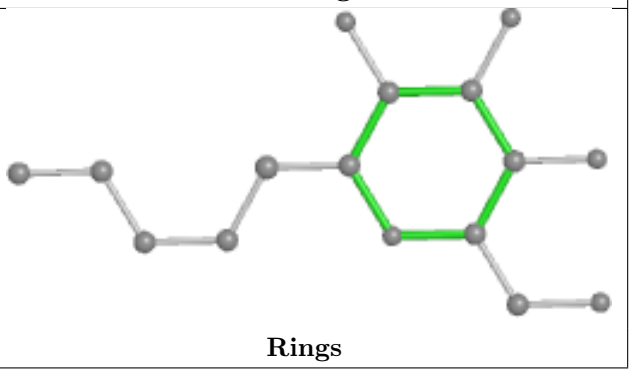
Bond lengths



Bond angles

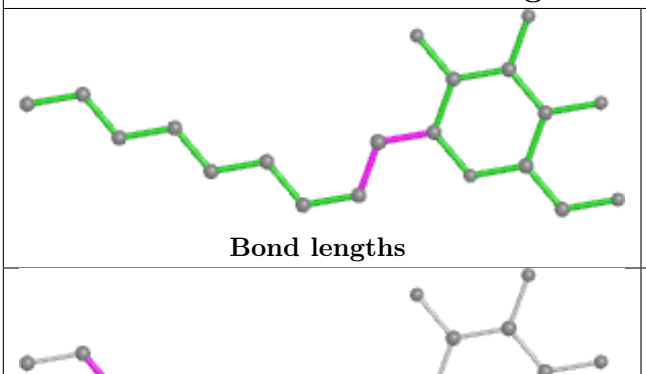


Torsions

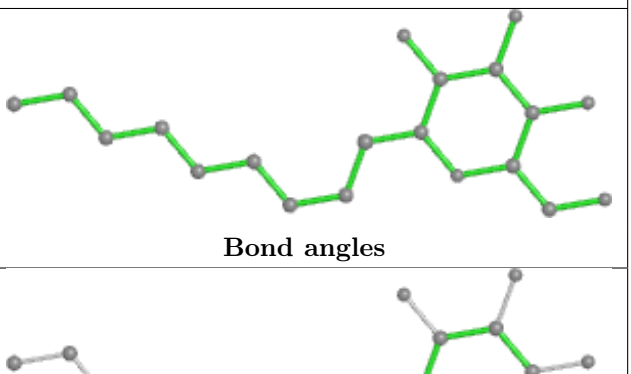


Rings

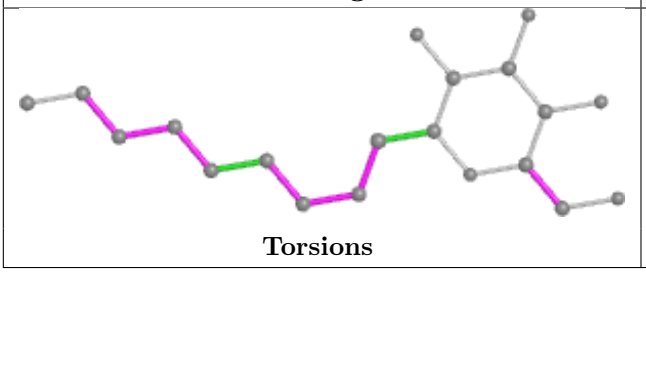
Ligand SOG B 408



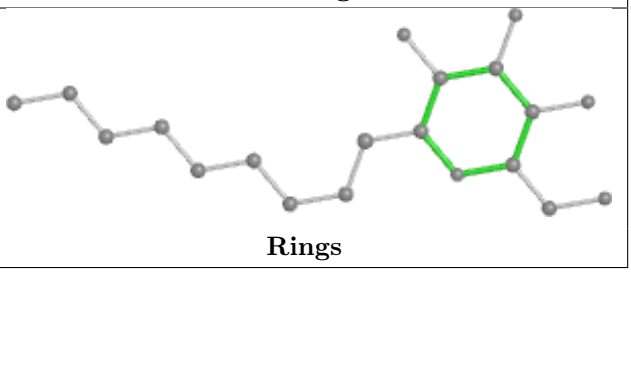
Bond lengths



Bond angles

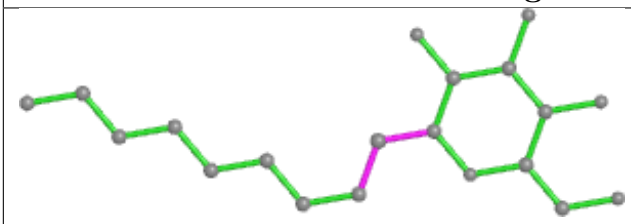


Torsions

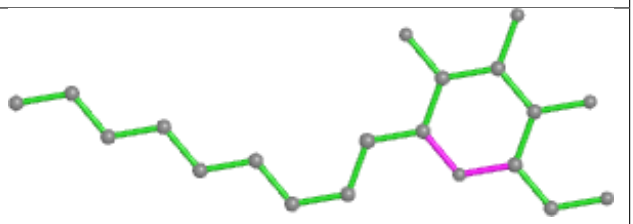


Rings

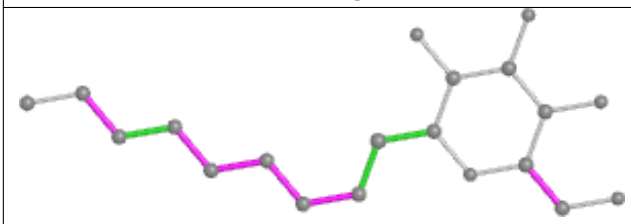
Ligand SOG B 407



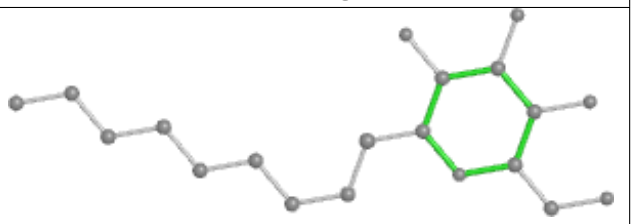
Bond lengths



Bond angles

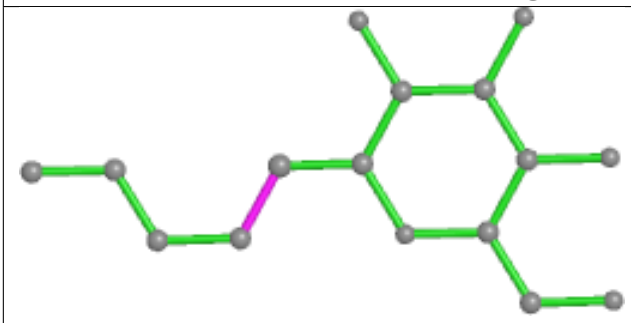


Torsions

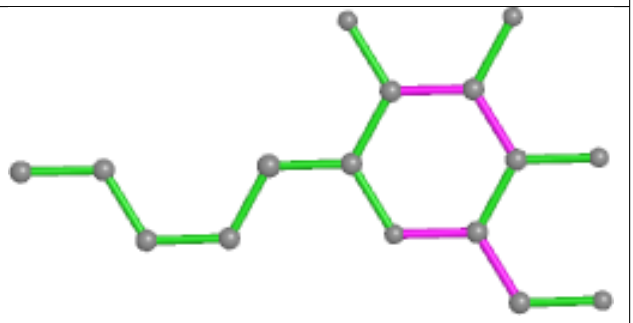


Rings

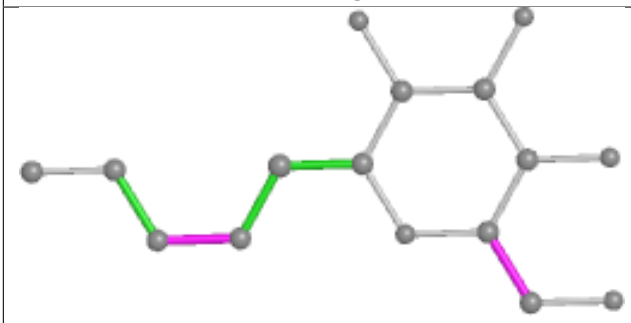
Ligand SOG B 413



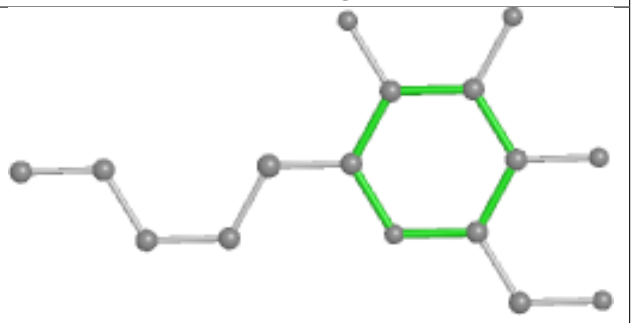
Bond lengths



Bond angles

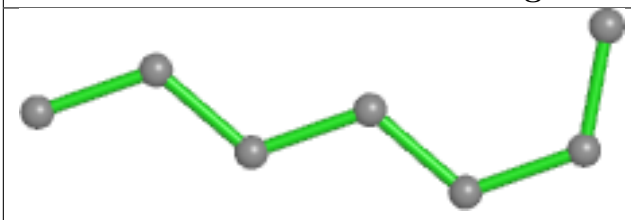


Torsions

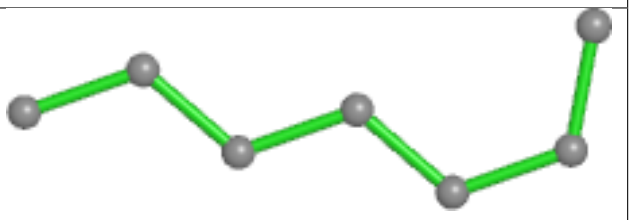


Rings

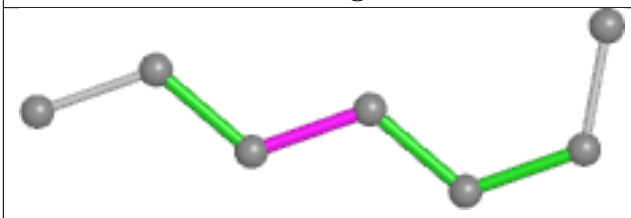
Ligand SOG B 427



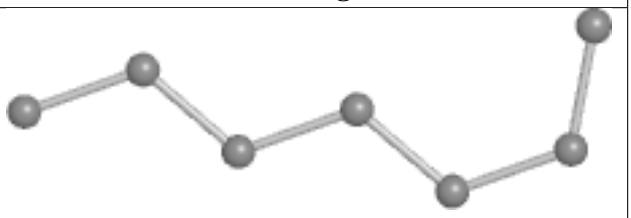
Bond lengths



Bond angles

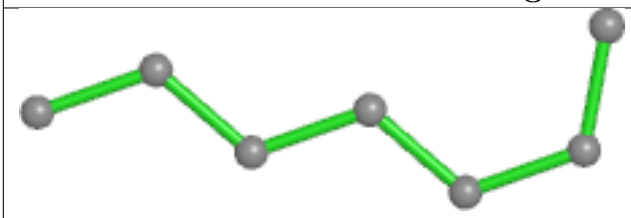


Torsions

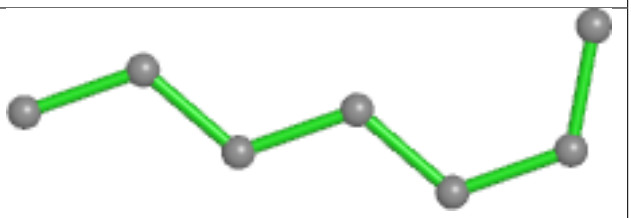


Rings

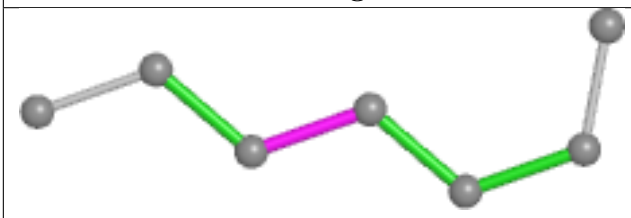
Ligand SOG B 428



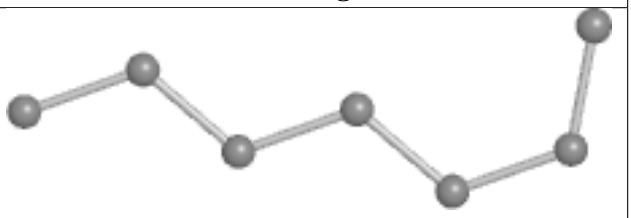
Bond lengths



Bond angles

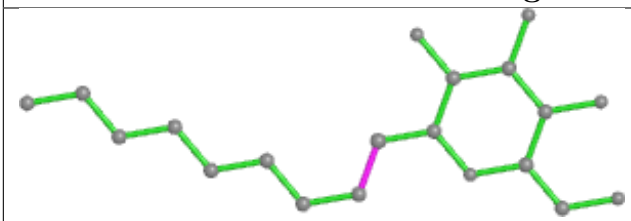


Torsions

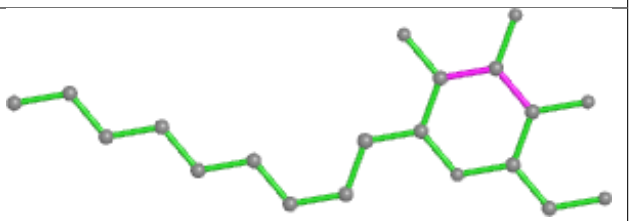


Rings

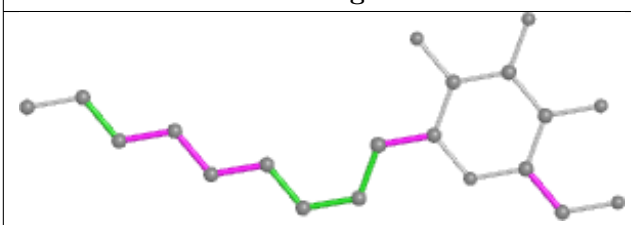
Ligand SOG A 409



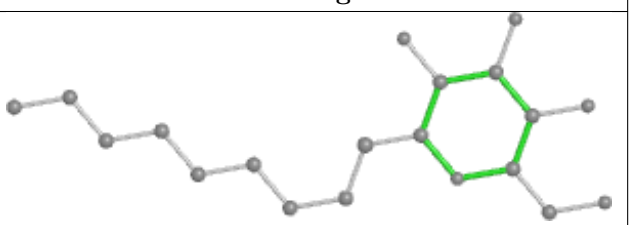
Bond lengths



Bond angles

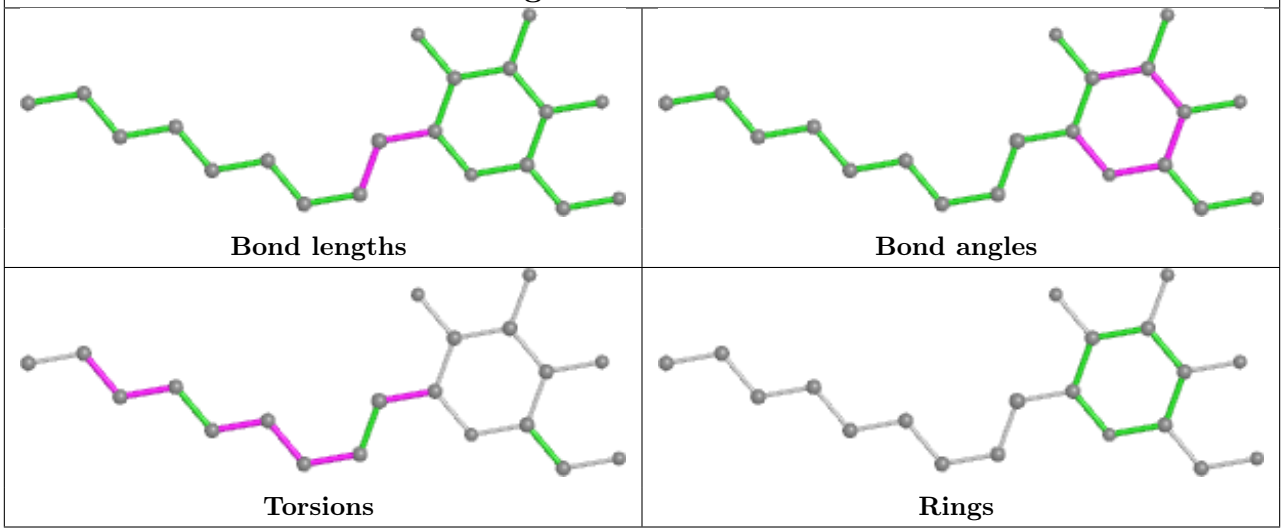


Torsions

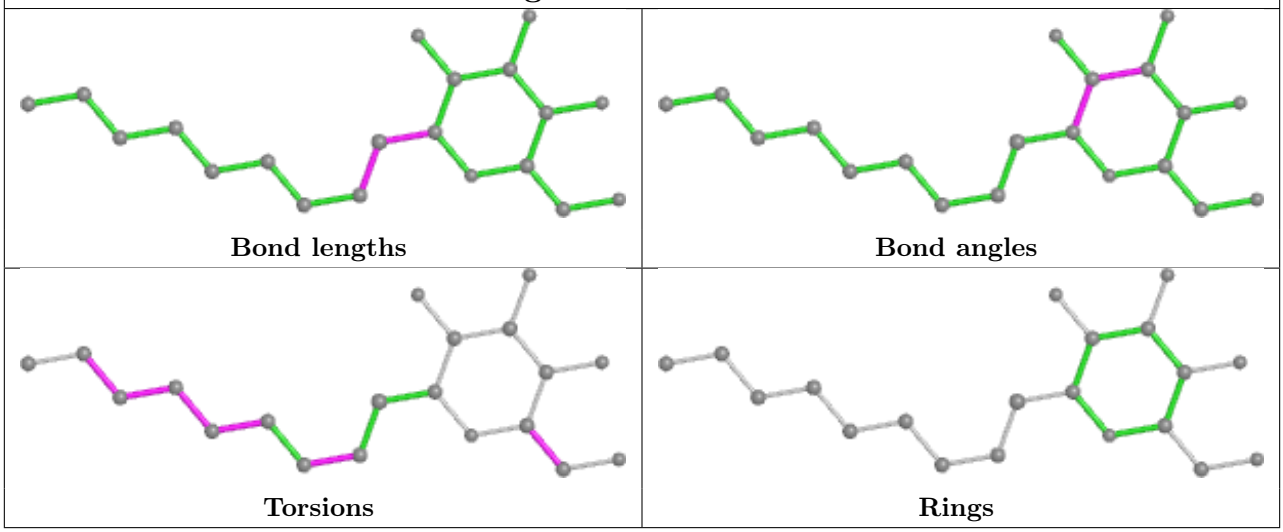


Rings

Ligand SOG A 417



Ligand SOG A 416



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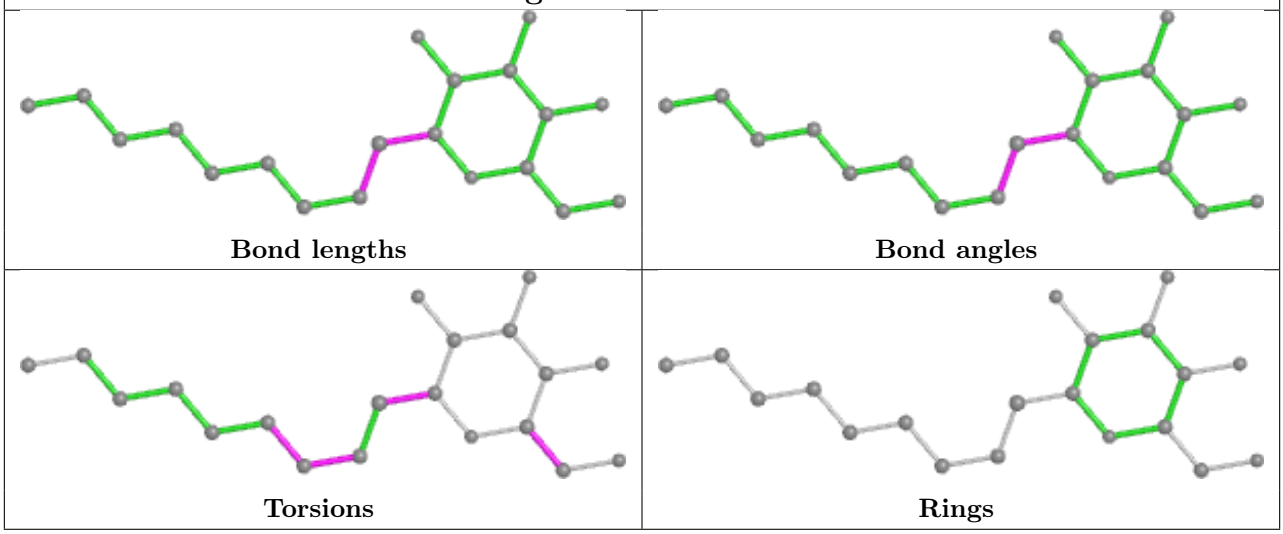
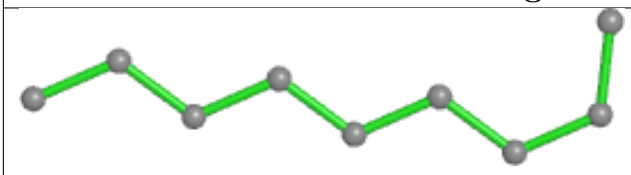
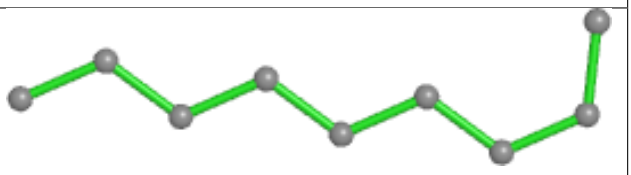


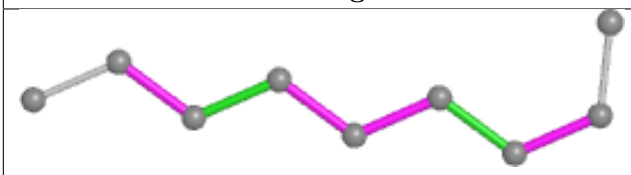
Ligand SOG B 417



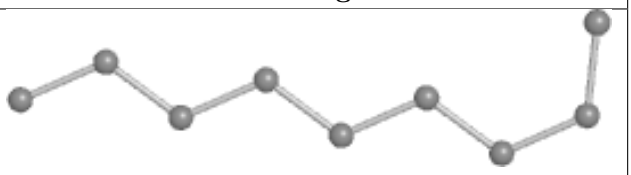
Bond lengths



Bond angles

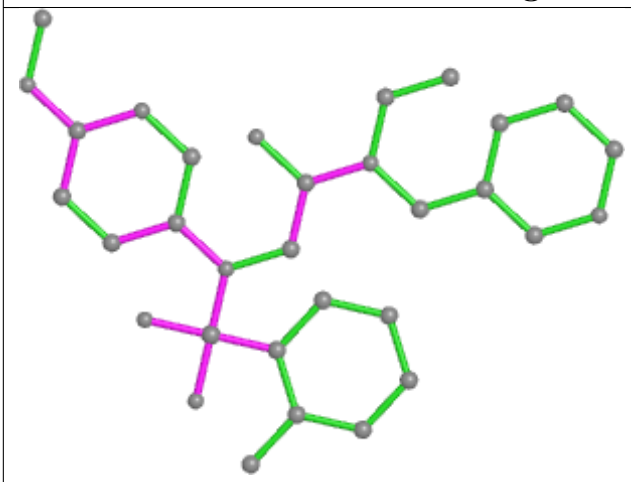


Torsions

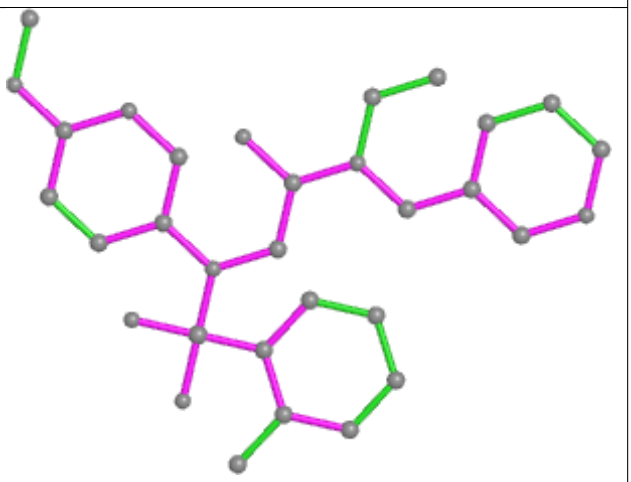


Rings

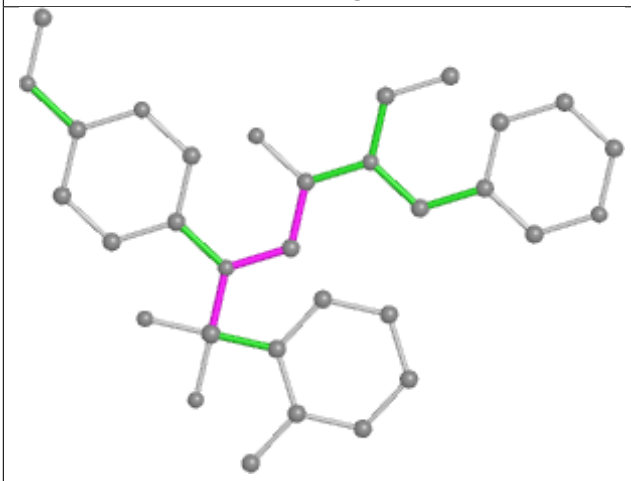
Ligand 7MA B 401



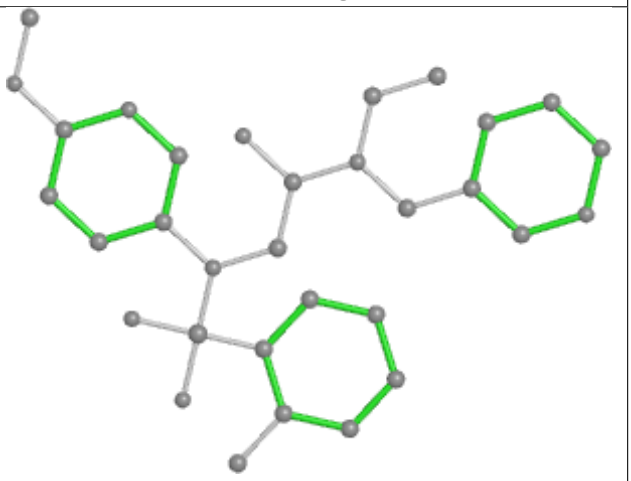
Bond lengths



Bond angles

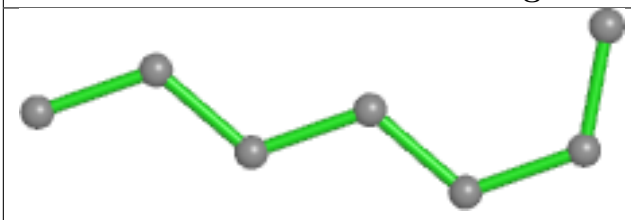


Torsions

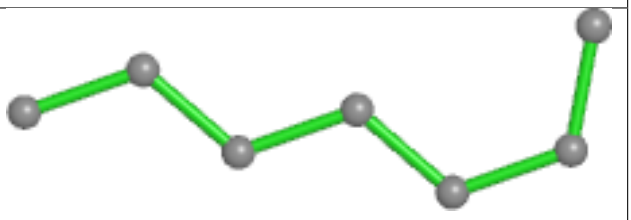


Rings

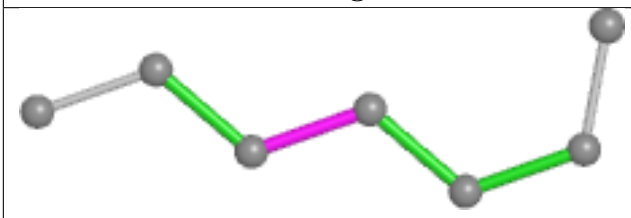
Ligand SOG A 428



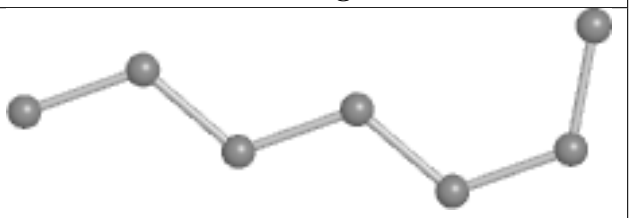
Bond lengths



Bond angles

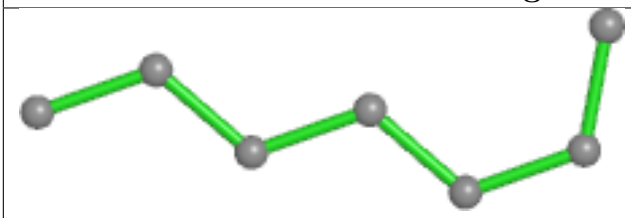


Torsions

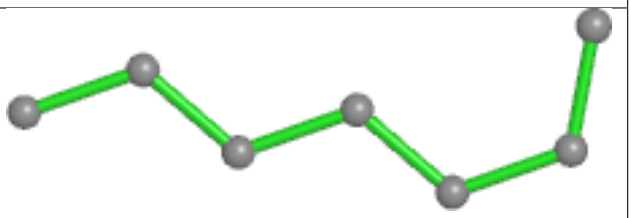


Rings

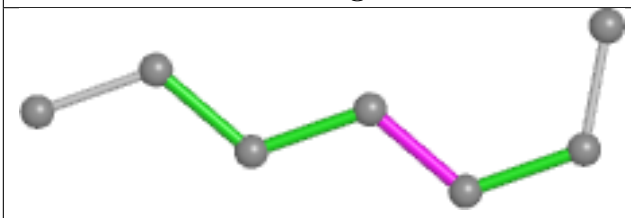
Ligand SOG A 421



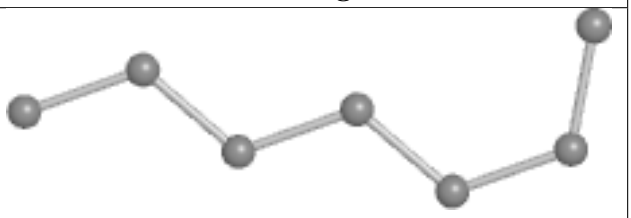
Bond lengths



Bond angles

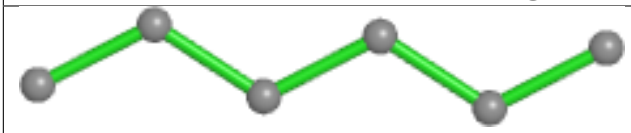


Torsions

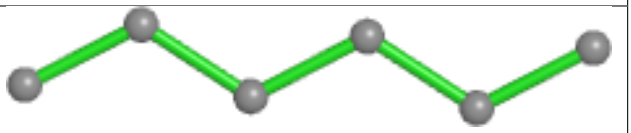


Rings

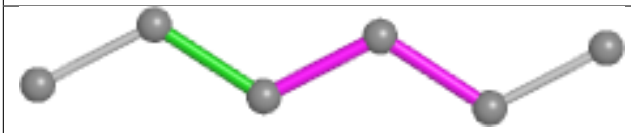
Ligand SOG B 415



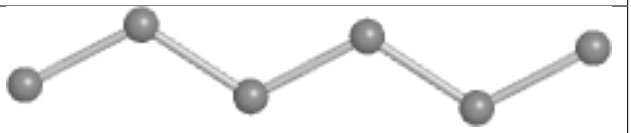
Bond lengths



Bond angles

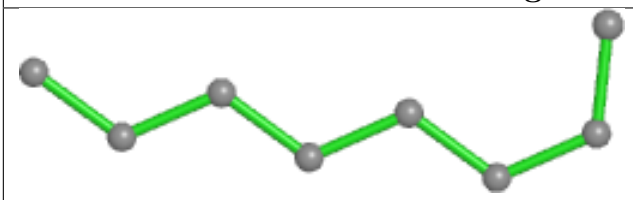


Torsions

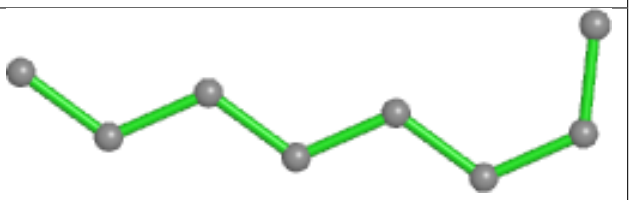


Rings

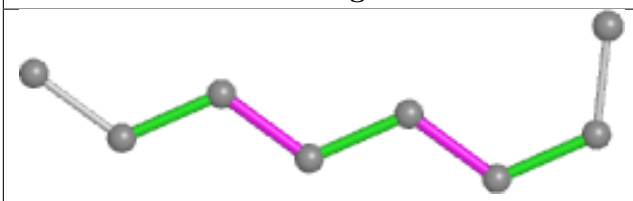
Ligand SOG B 422



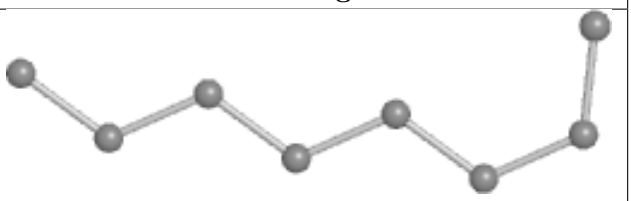
Bond lengths



Bond angles

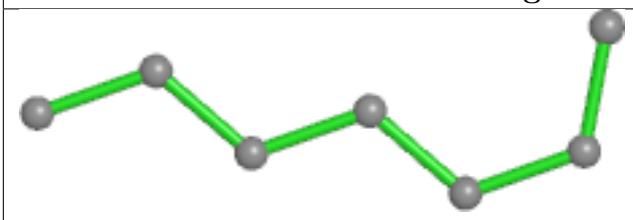


Torsions

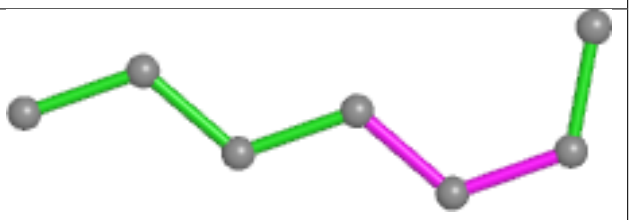


Rings

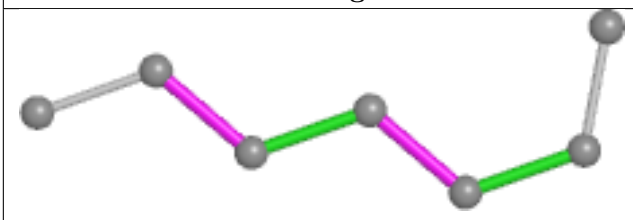
Ligand SOG A 424



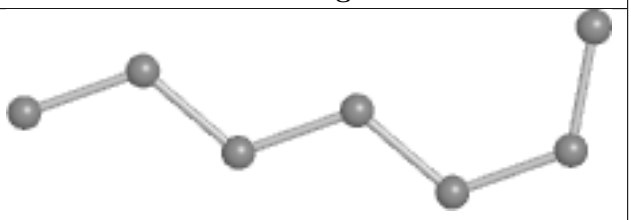
Bond lengths



Bond angles

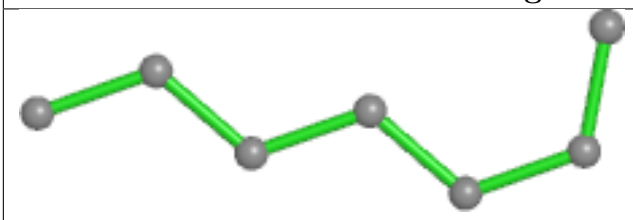


Torsions

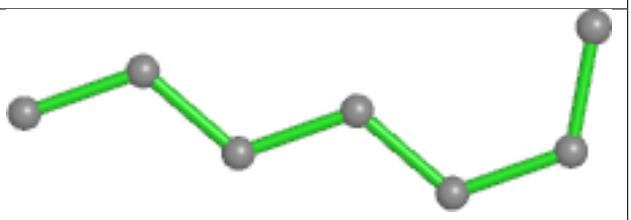


Rings

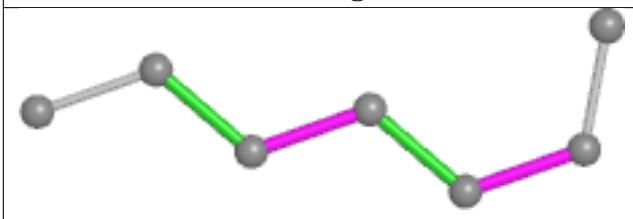
Ligand SOG B 425



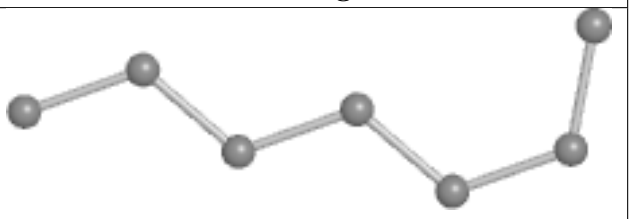
Bond lengths



Bond angles

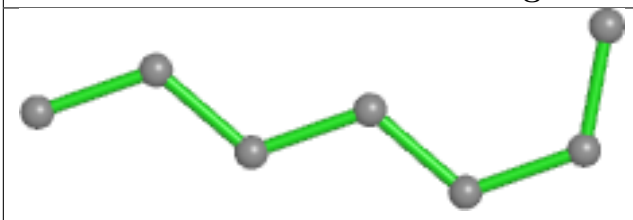


Torsions

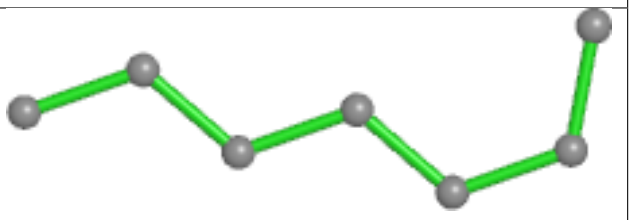


Rings

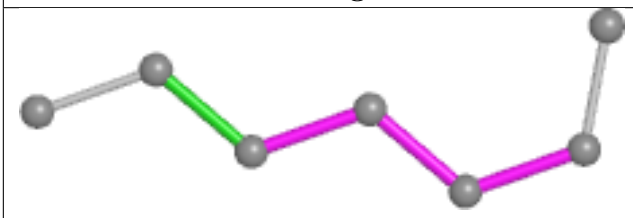
Ligand SOG A 423



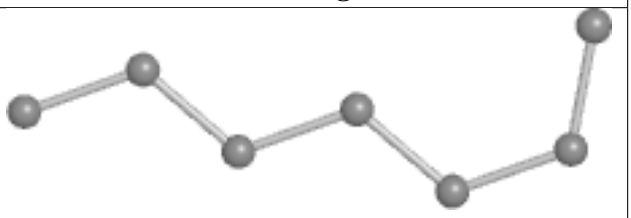
Bond lengths



Bond angles

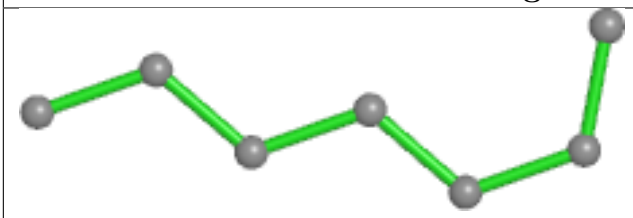


Torsions

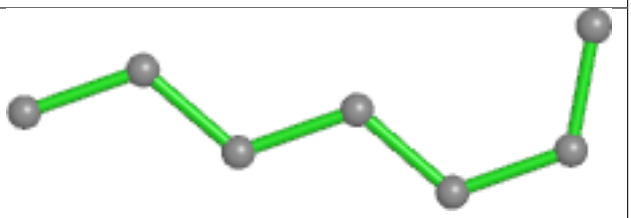


Rings

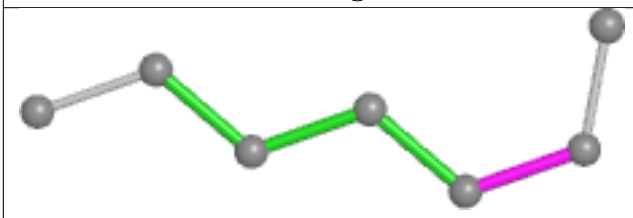
Ligand SOG A 420



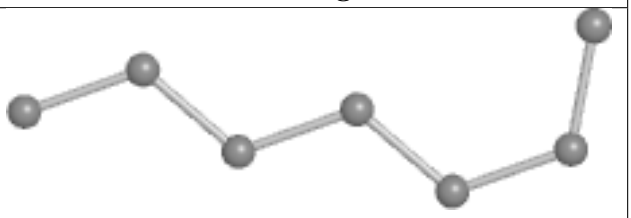
Bond lengths



Bond angles

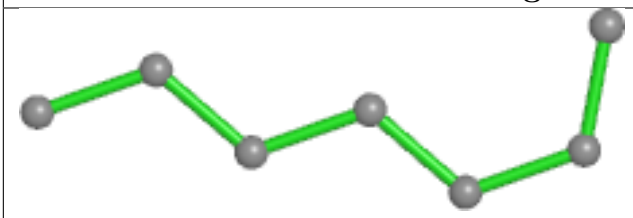


Torsions

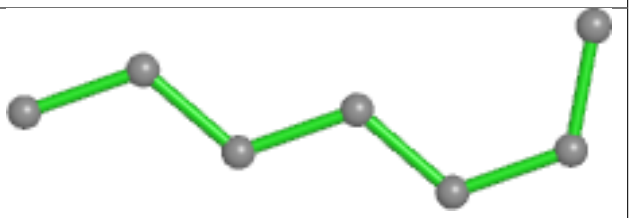


Rings

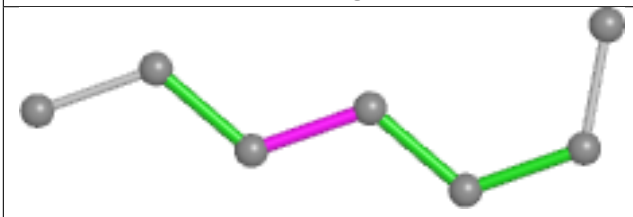
Ligand SOG A 426



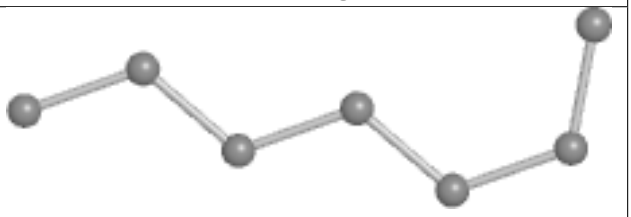
Bond lengths



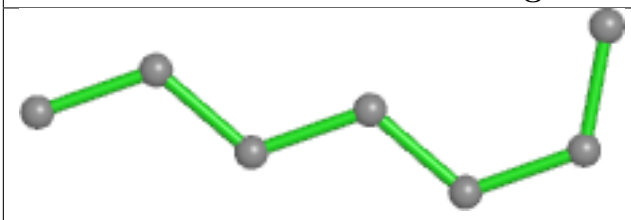
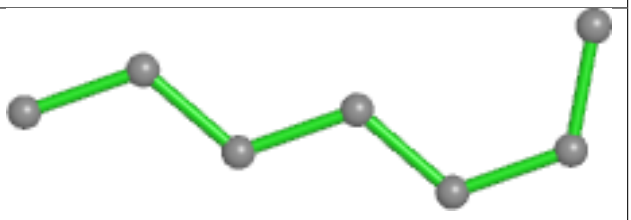
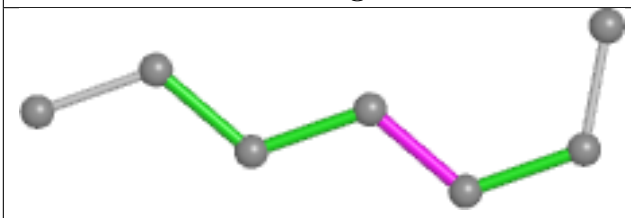
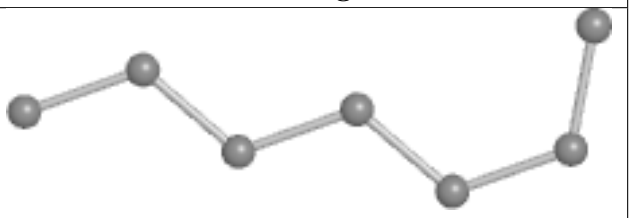
Bond angles



Torsions



Rings

Ligand SOG B 426	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

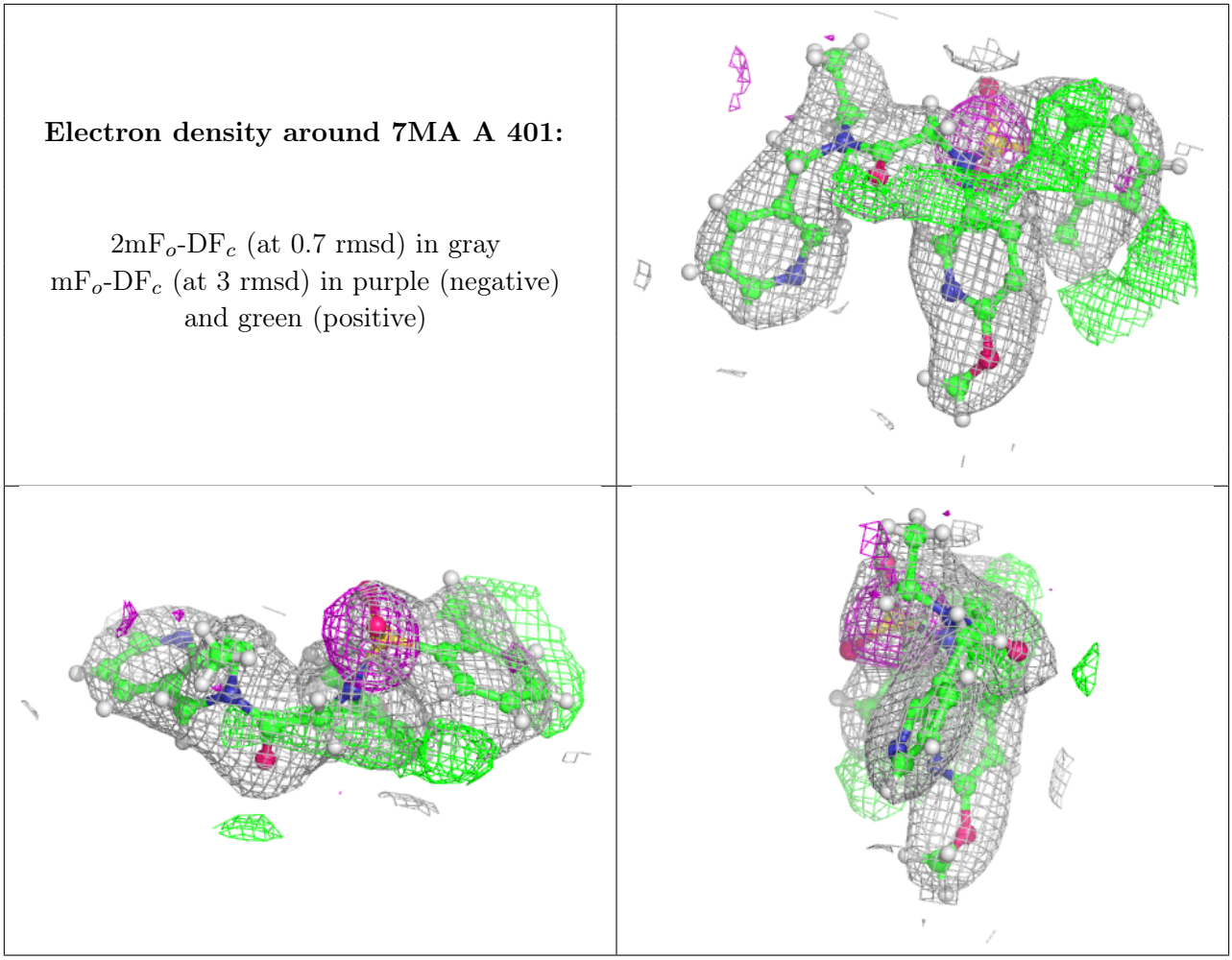
6.4 Ligands

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

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

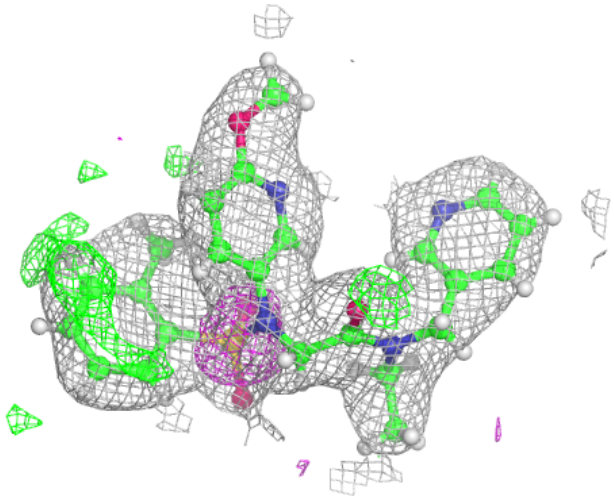
Electron density around 7MA A 401:

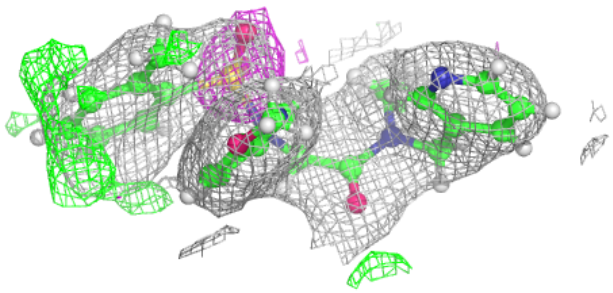
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

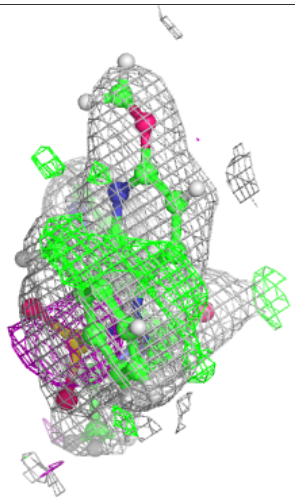


Electron density around 7MA B 401:

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

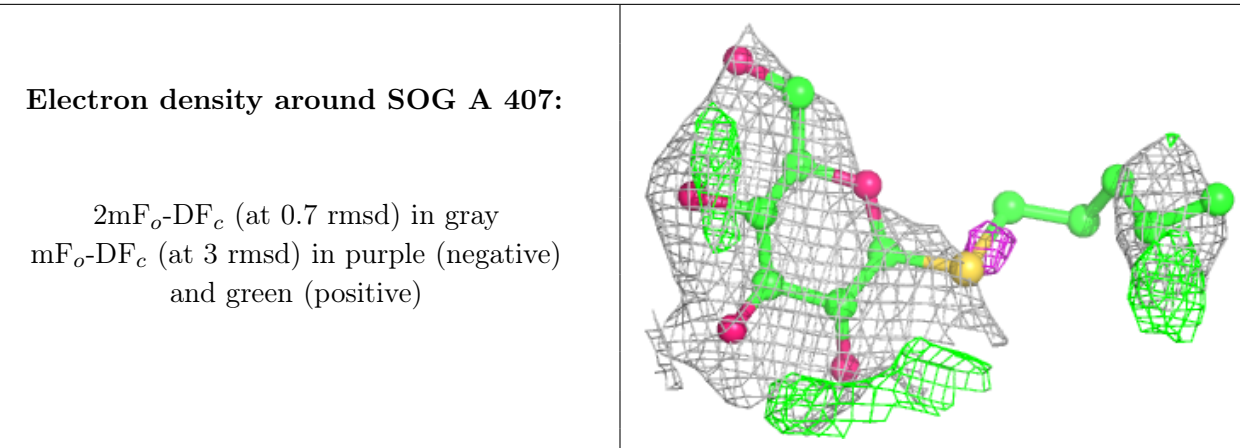






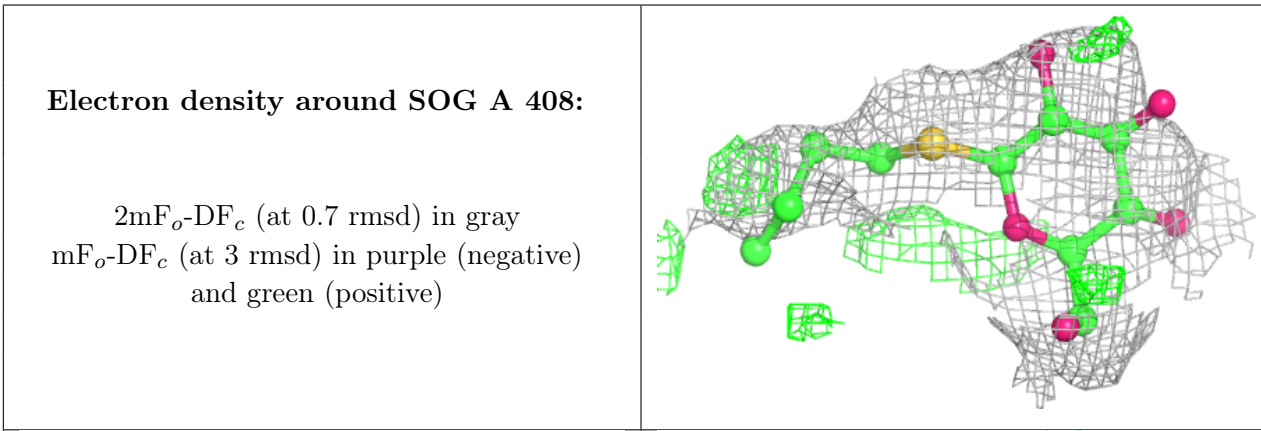
Electron density around SOG A 407:

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



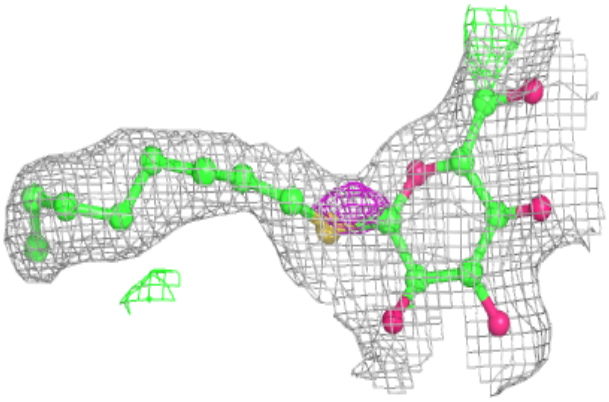
Electron density around SOG A 408:

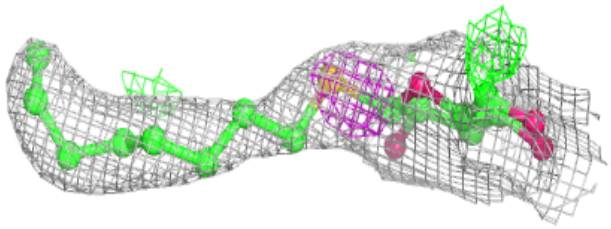
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

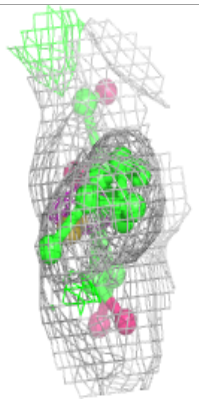


Electron density around SOG A 409:

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

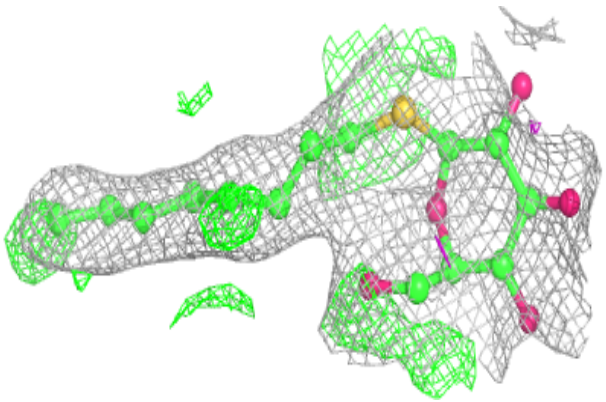


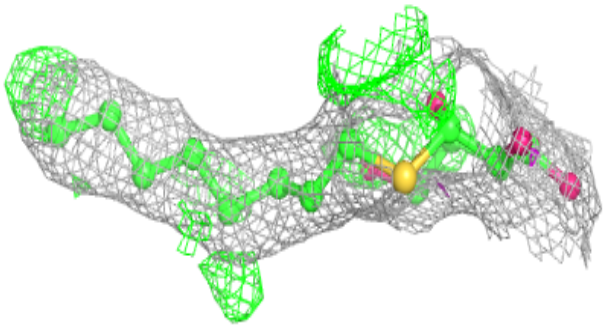


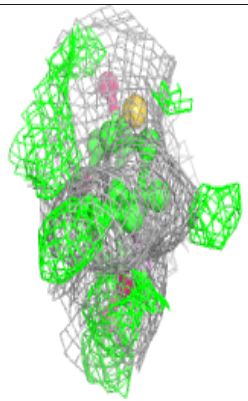


Electron density around SOG A 410:

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

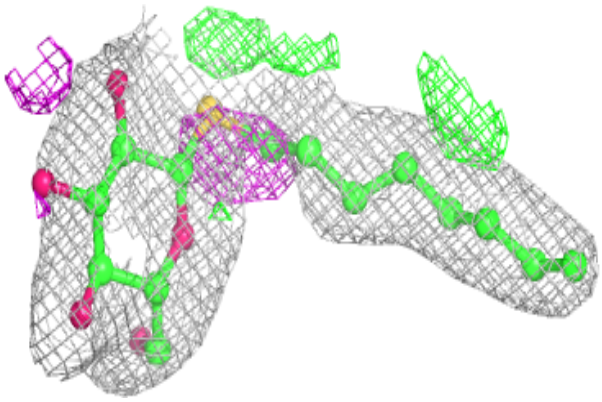


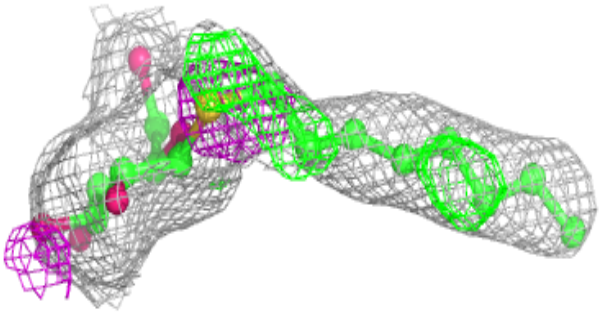


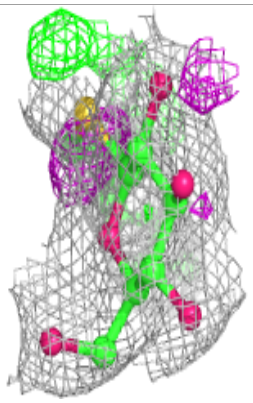


Electron density around SOG A 411:

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

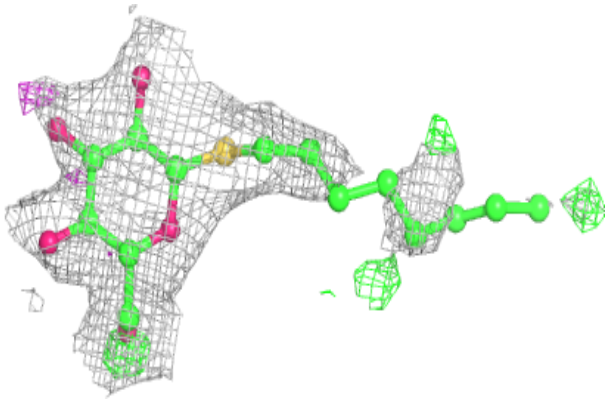


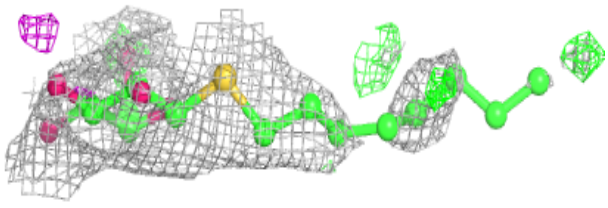


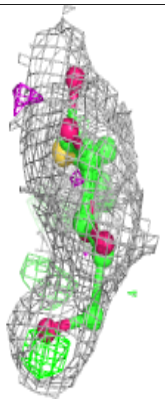


Electron density around SOG A 412:

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

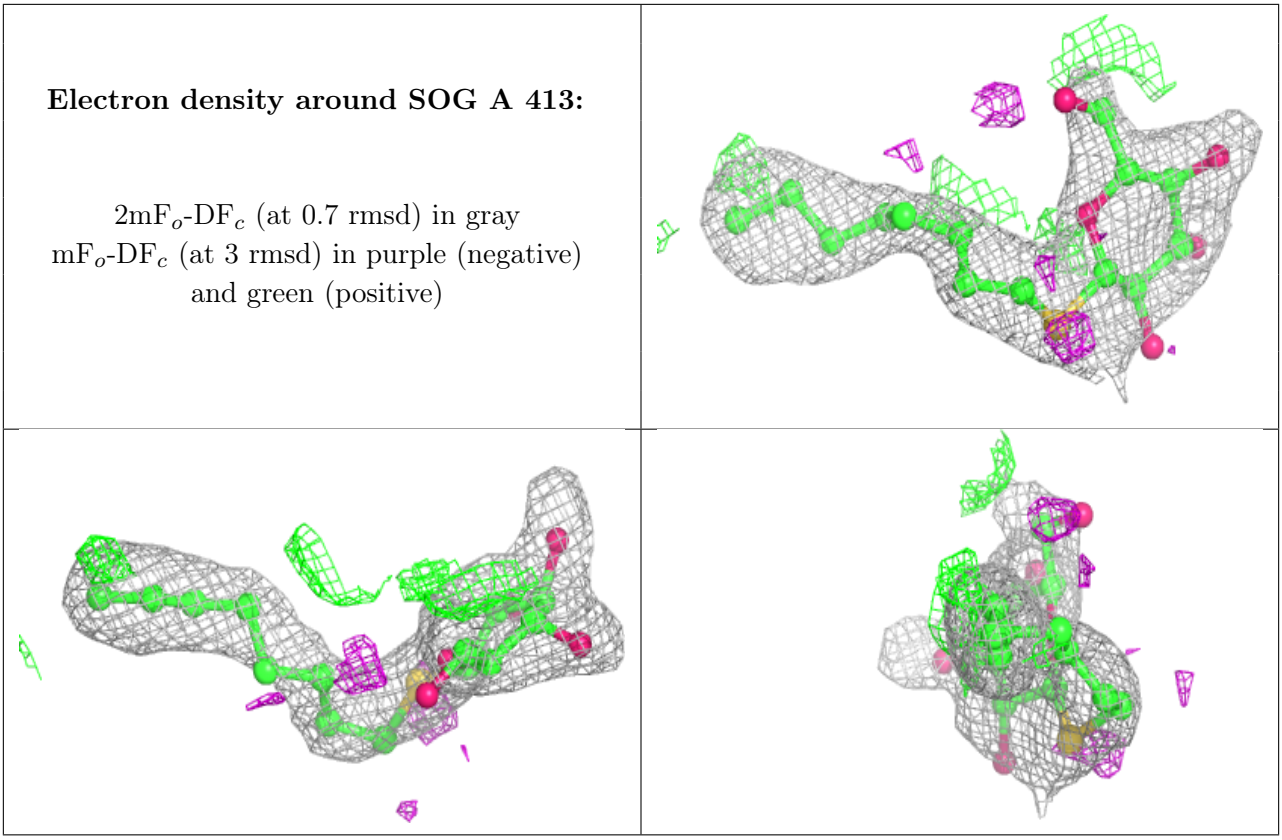






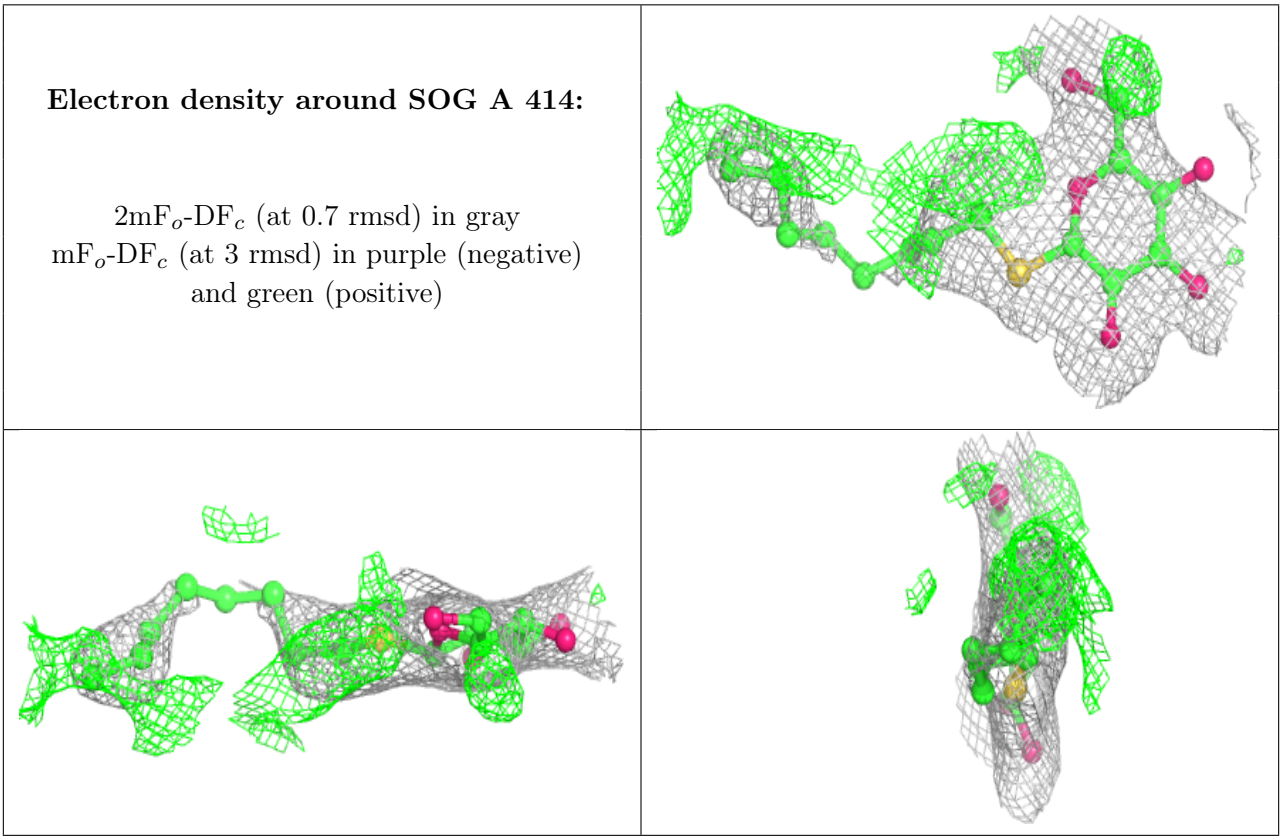
Electron density around SOG A 413:

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



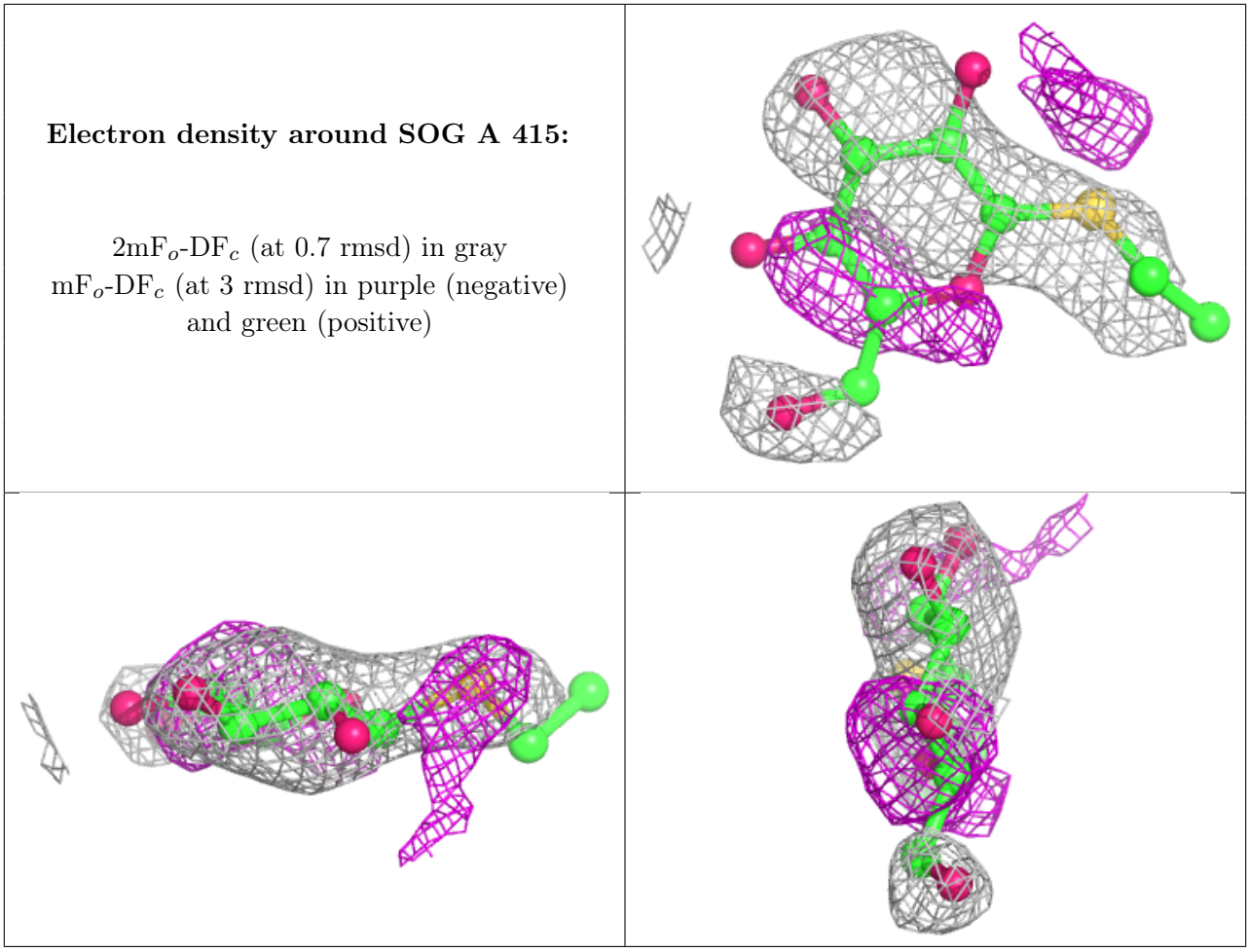
Electron density around SOG A 414:

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



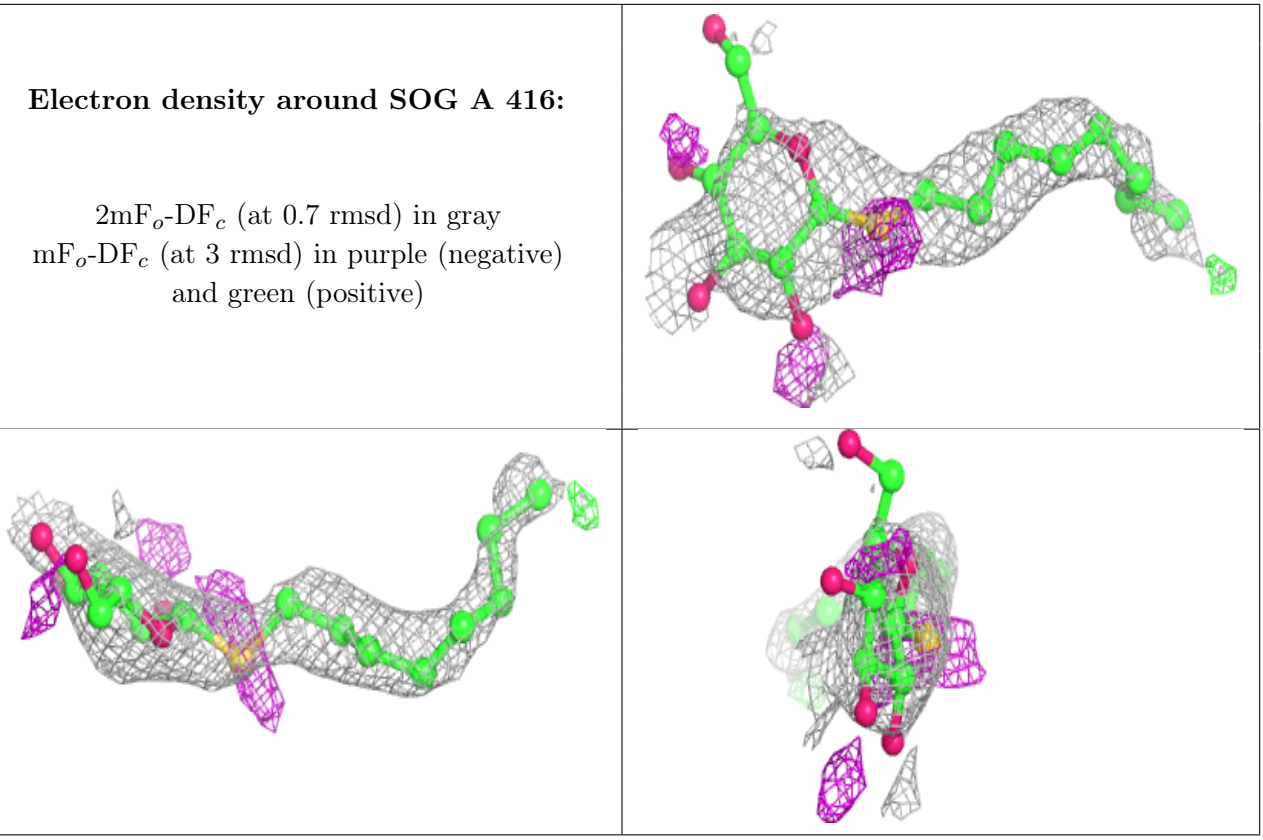
Electron density around SOG A 415:

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



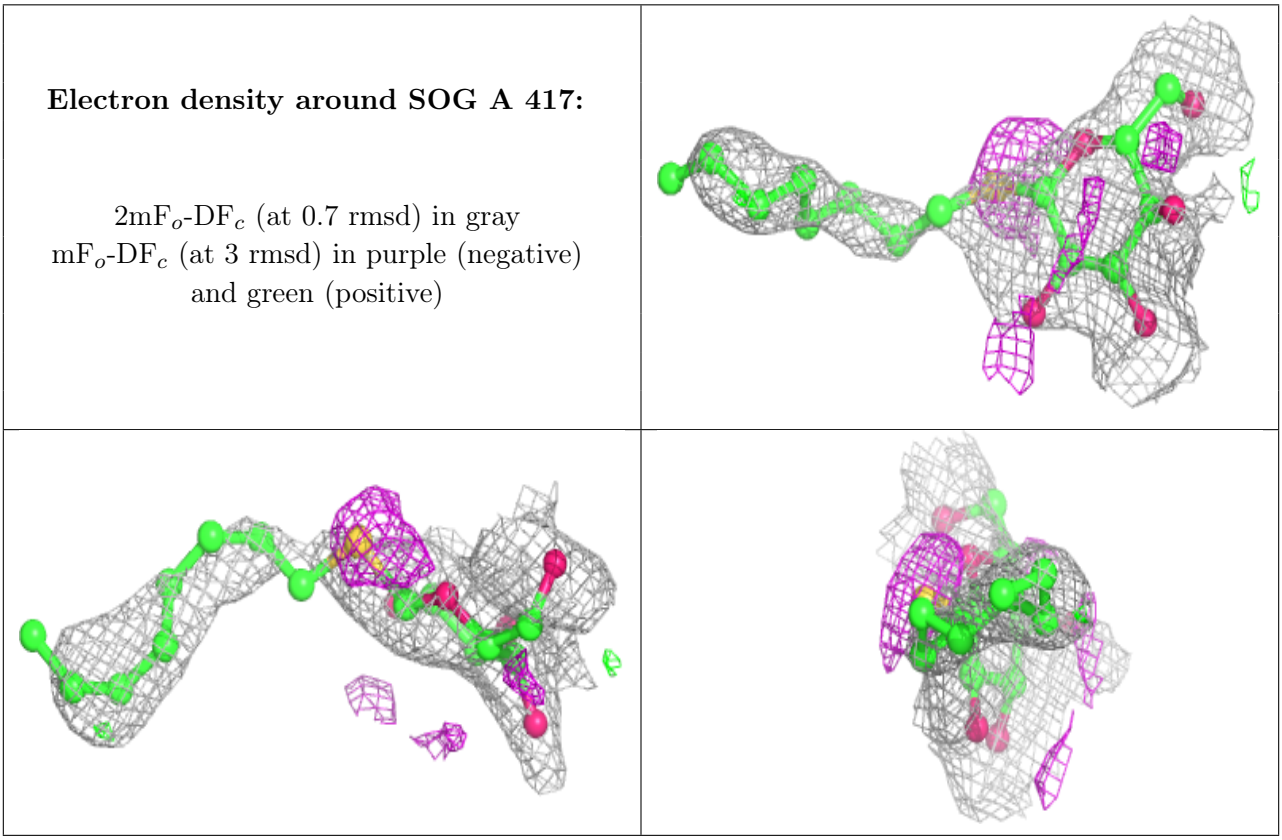
Electron density around SOG A 416:

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



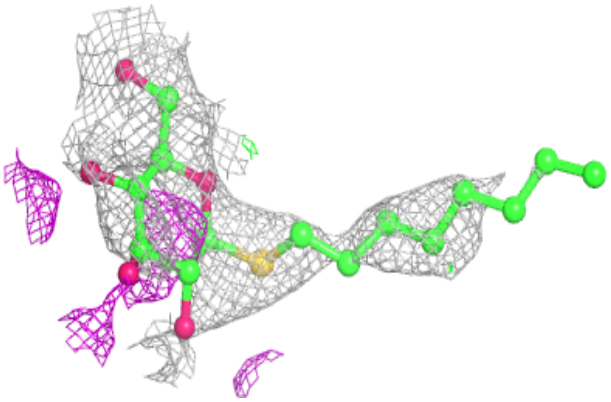
Electron density around SOG A 417:

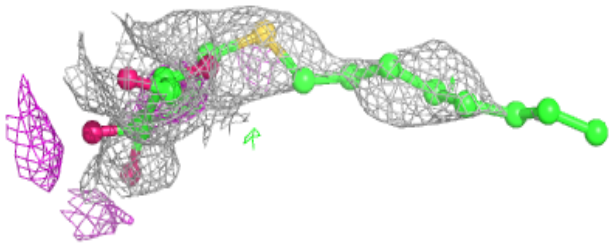
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

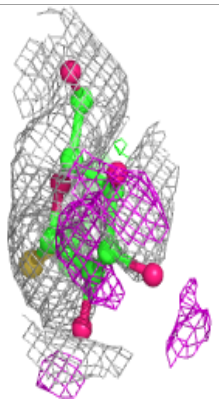


Electron density around SOG A 418:

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

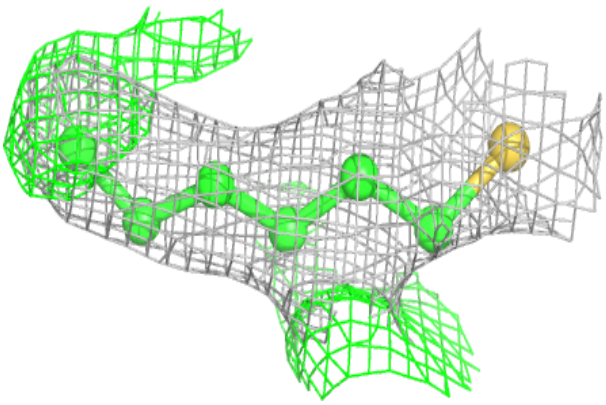


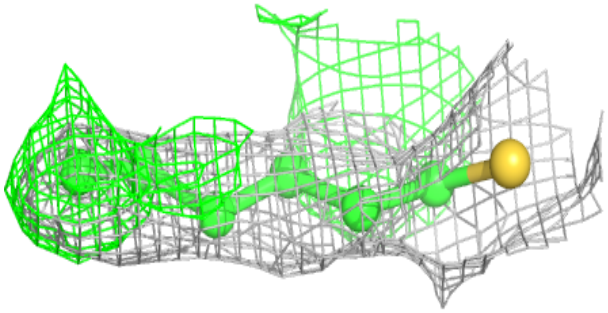


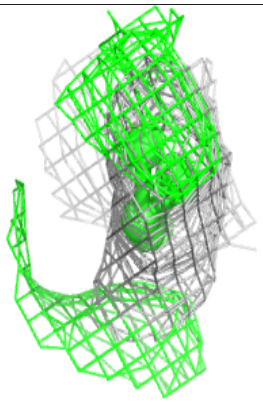


Electron density around SOG A 419:

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

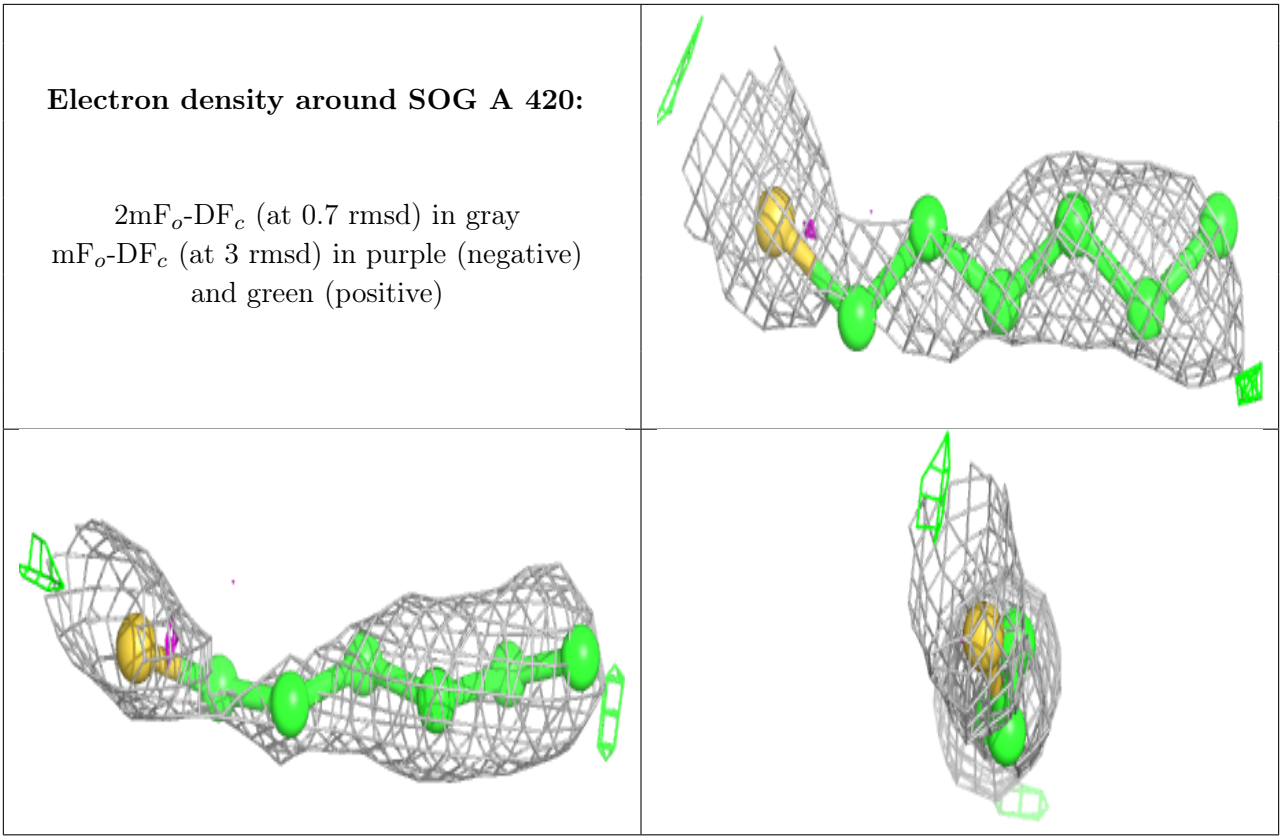






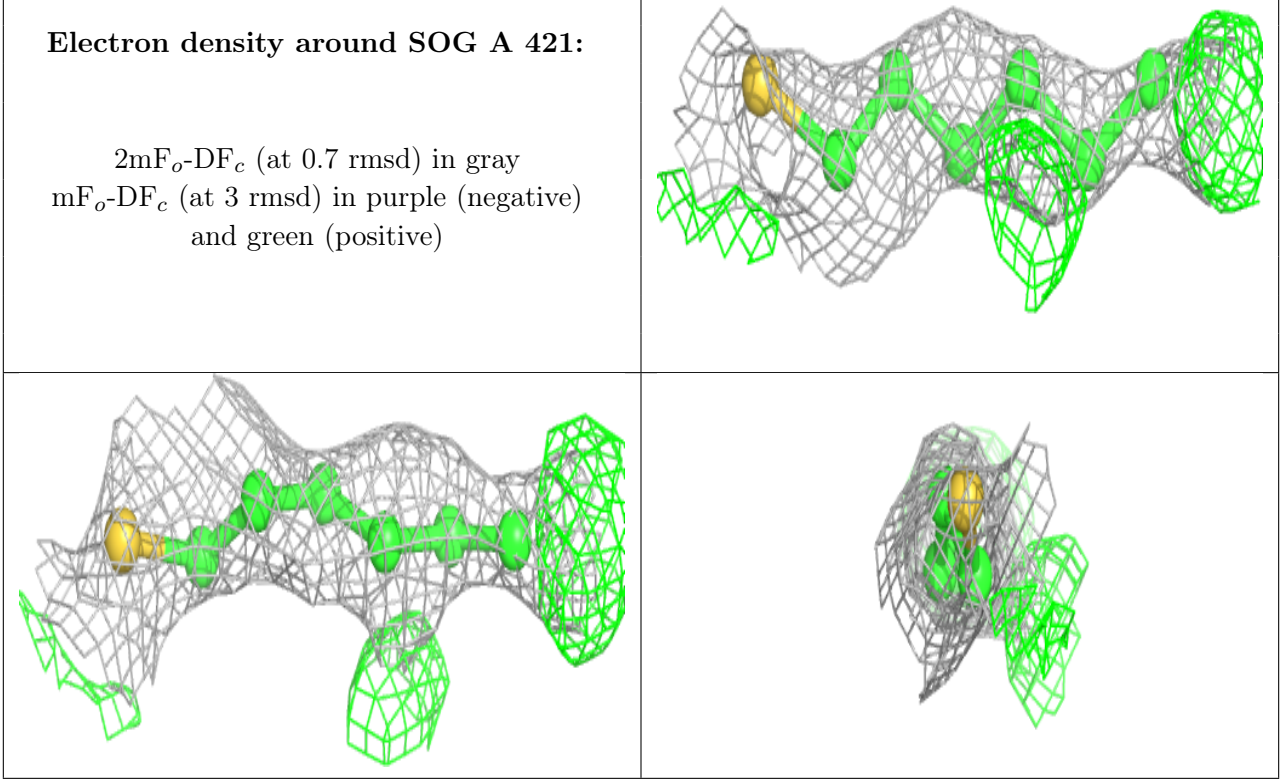
Electron density around SOG A 420:

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



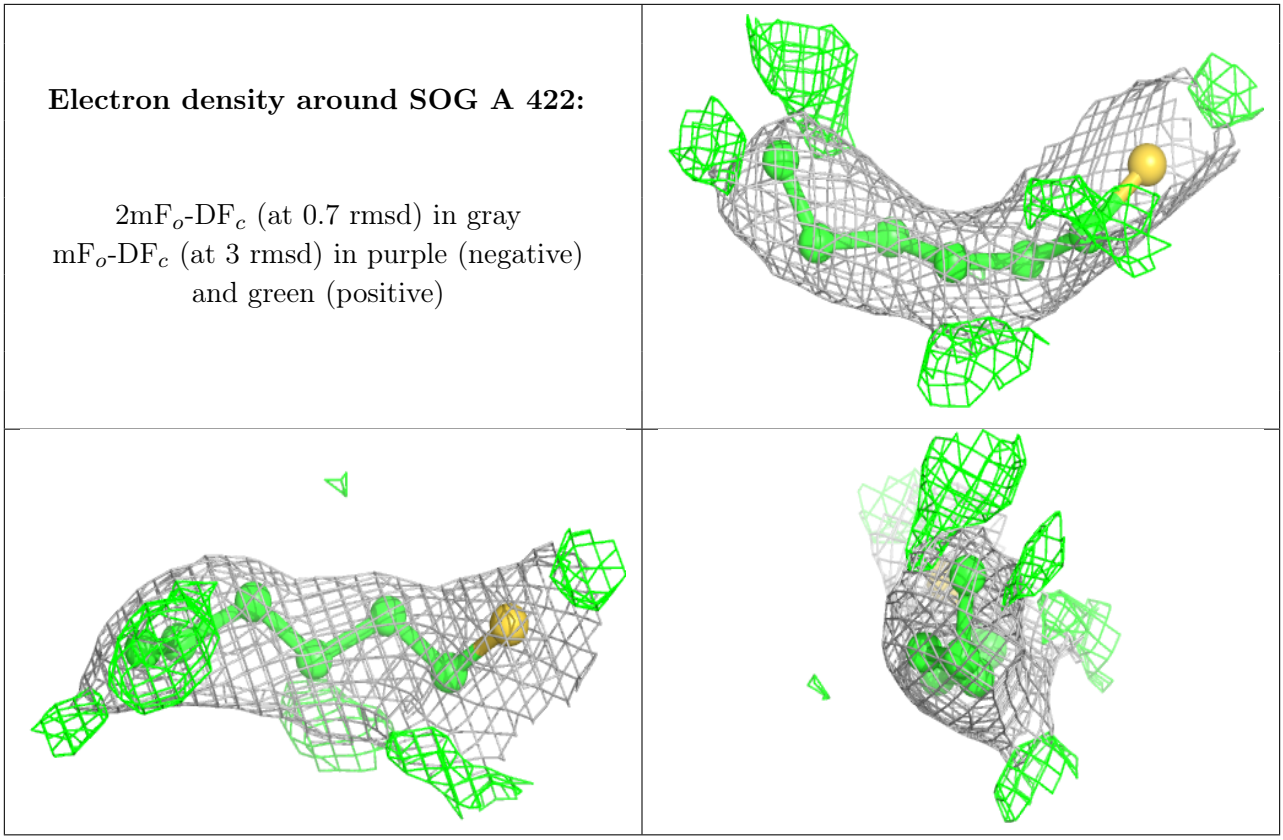
Electron density around SOG A 421:

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



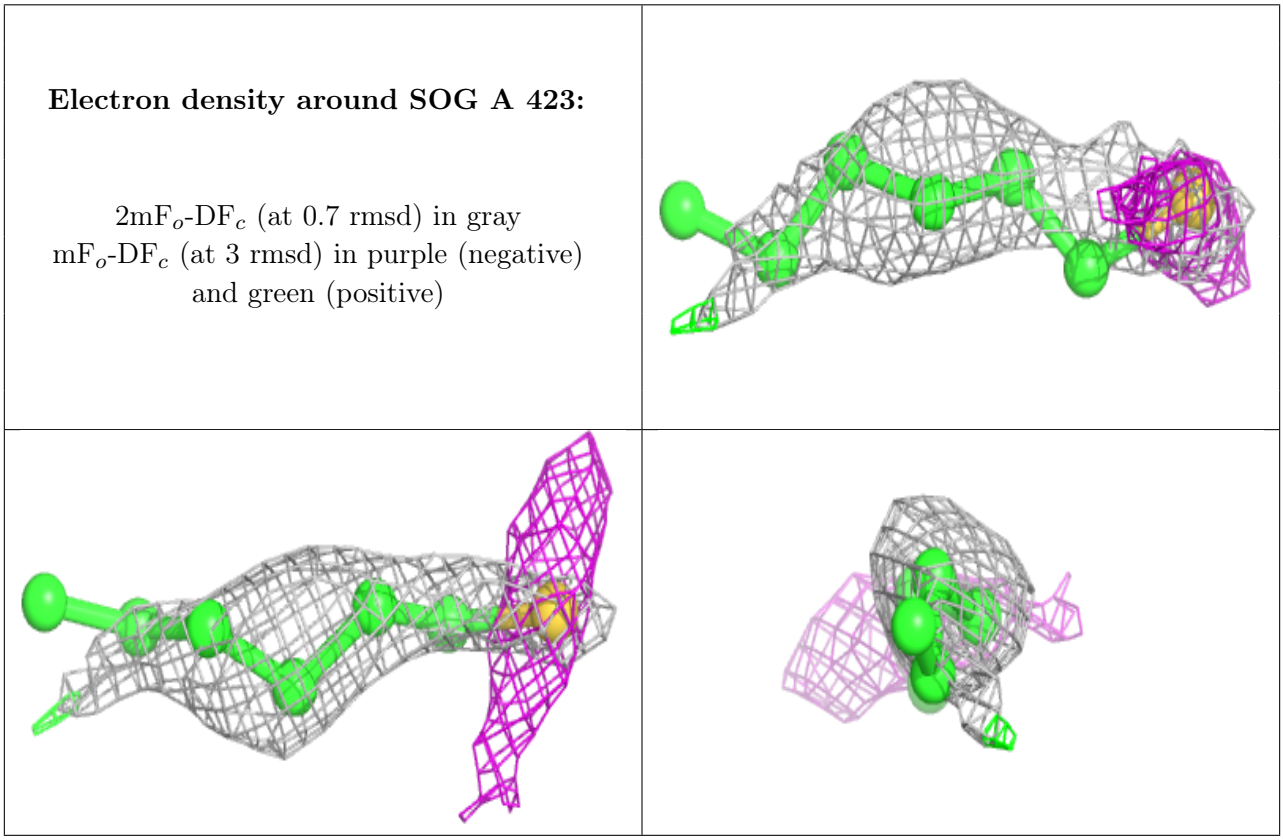
Electron density around SOG A 422:

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



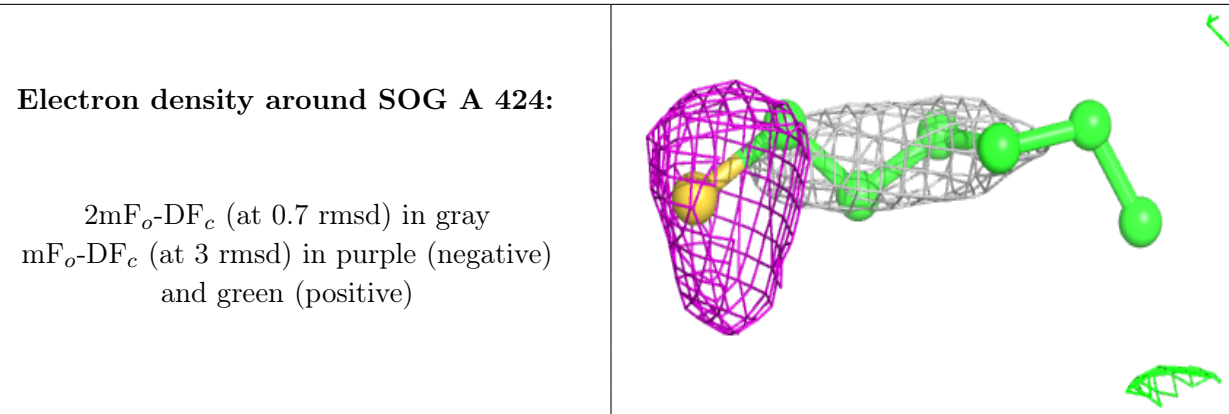
Electron density around SOG A 423:

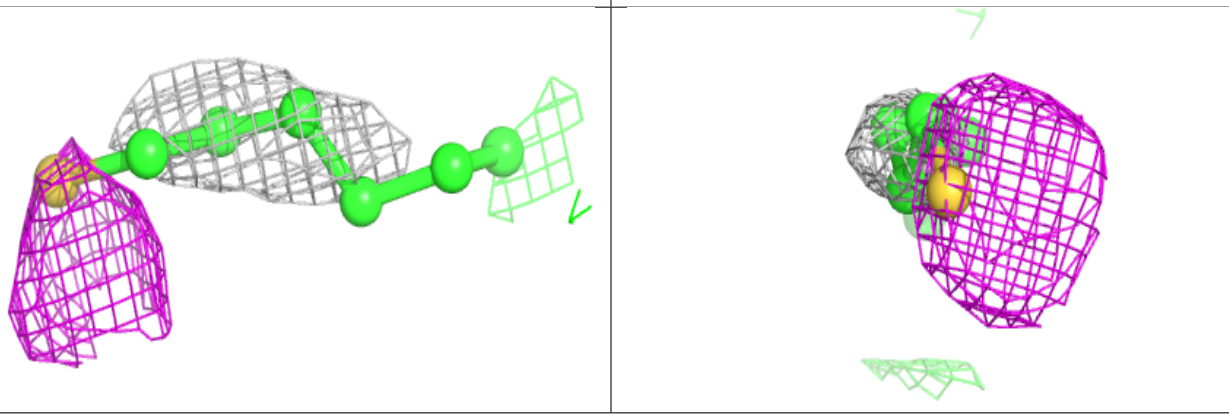
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SOG A 424:

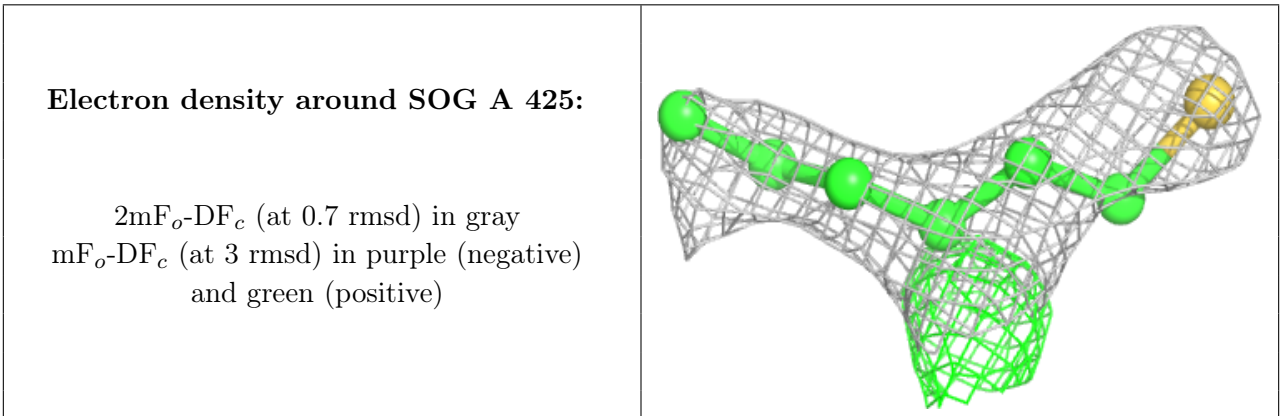
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

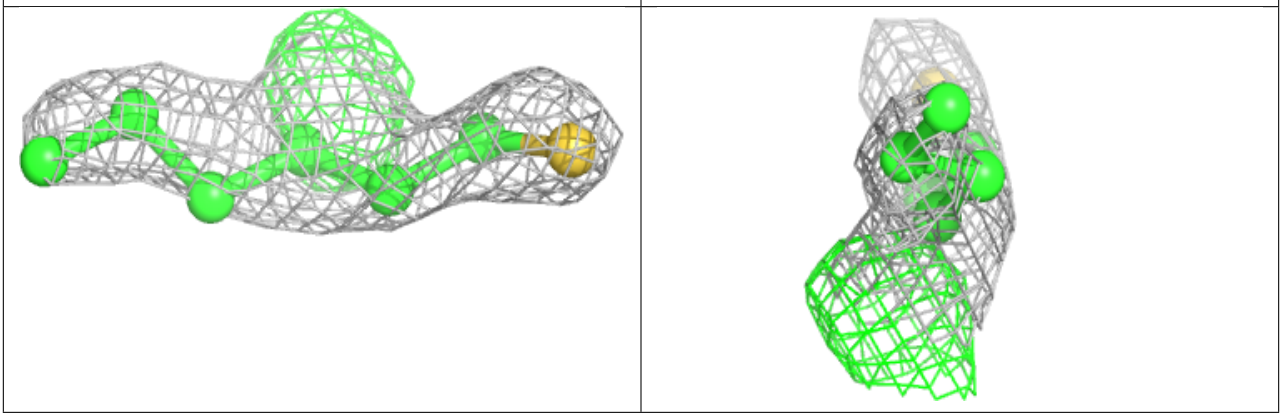




Electron density around SOG A 425:

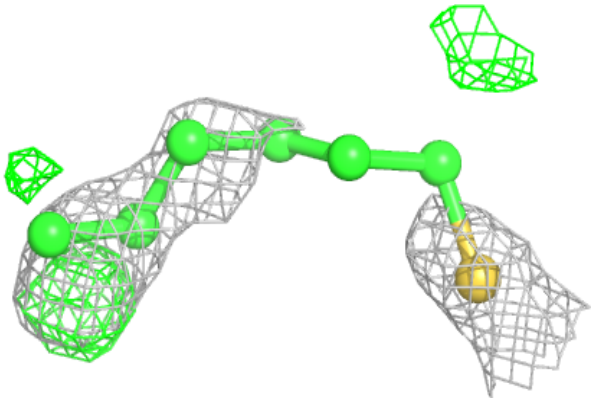
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

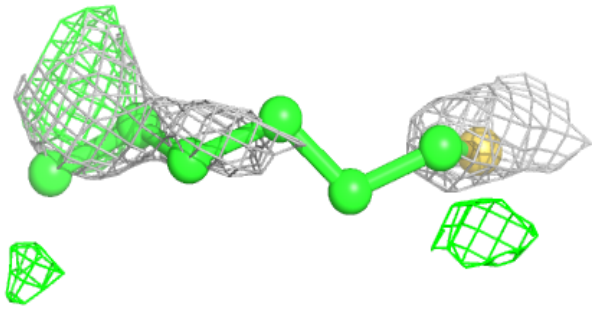


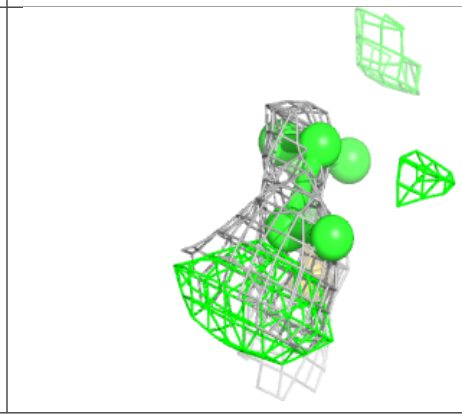


Electron density around SOG A 426:

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

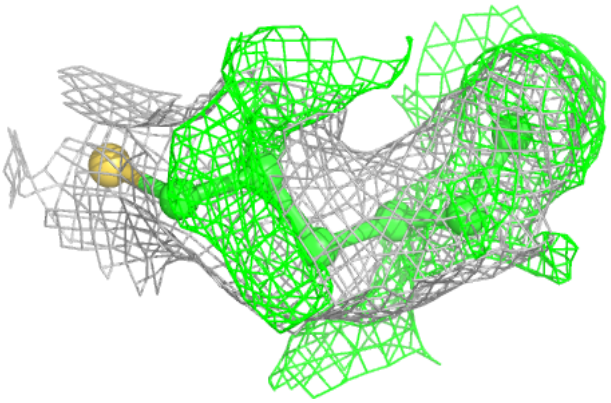


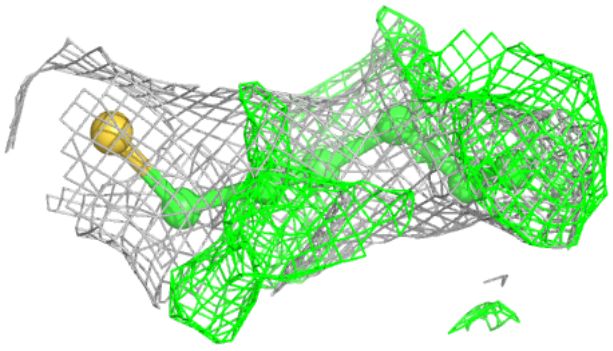


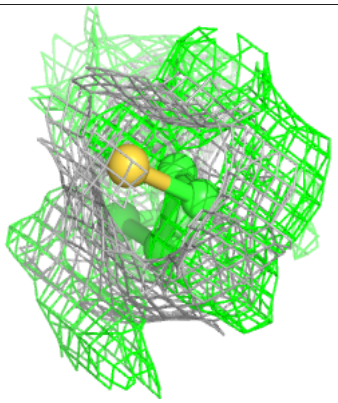


Electron density around SOG A 427:

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

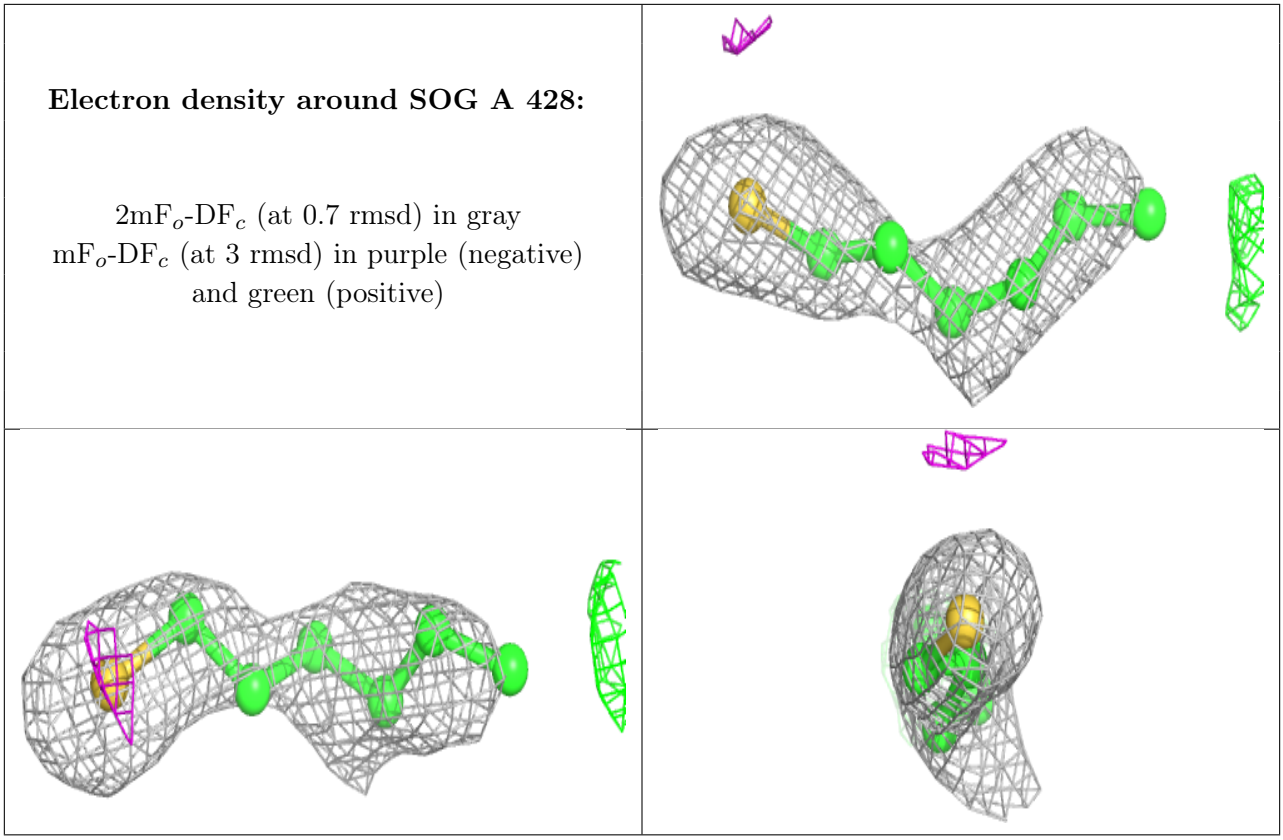






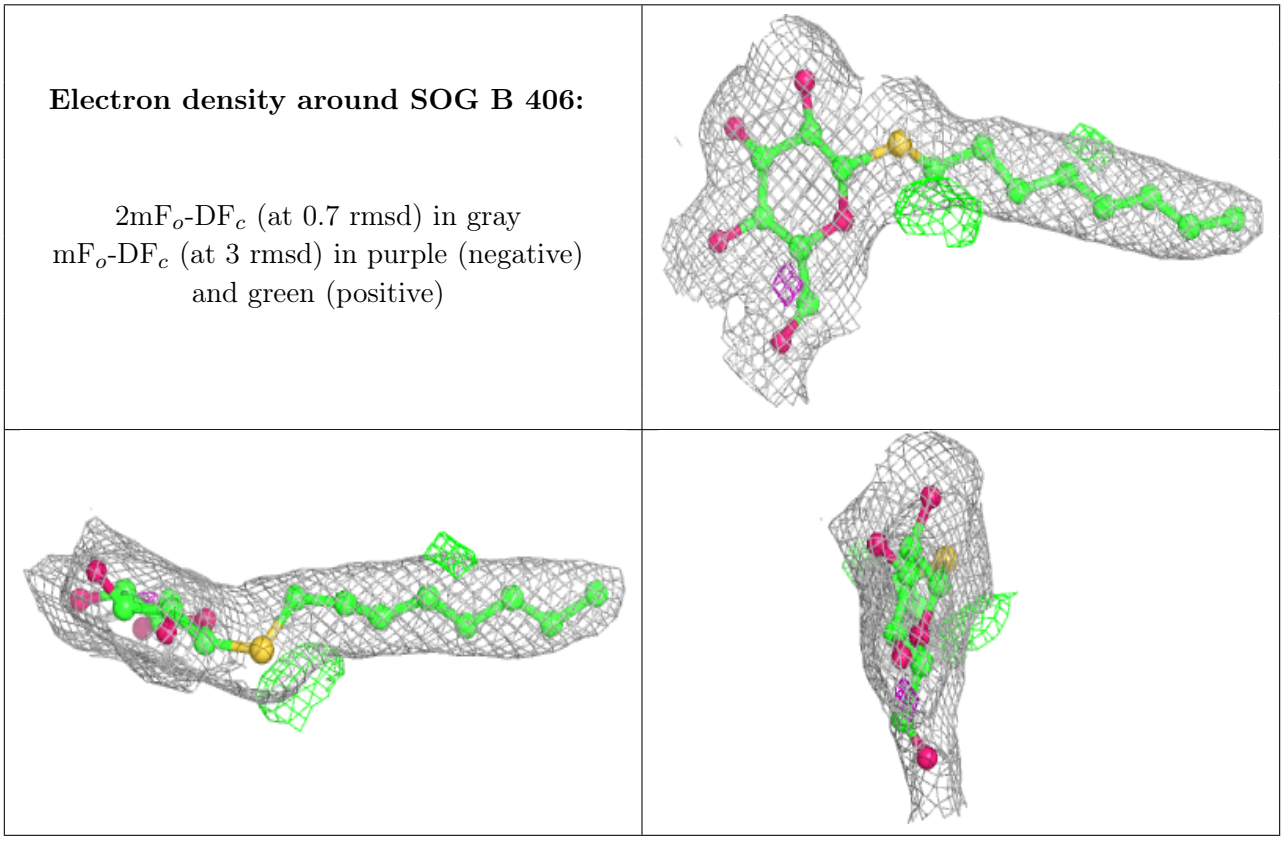
Electron density around SOG A 428:

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



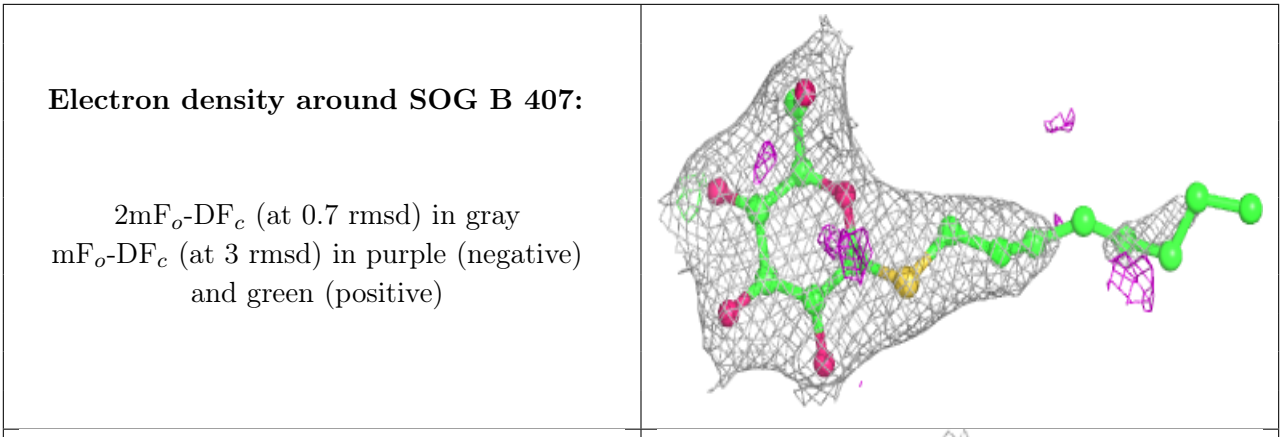
Electron density around SOG B 406:

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



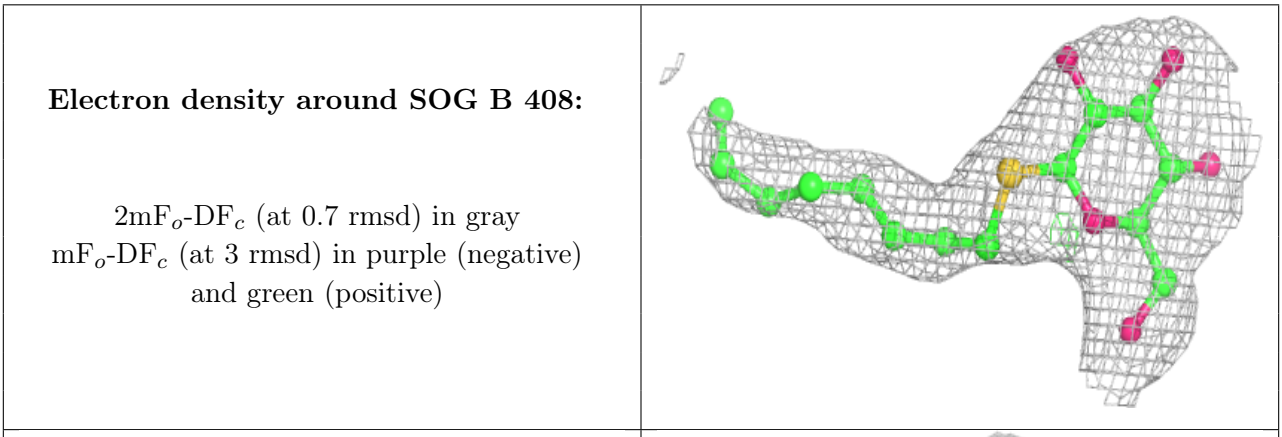
Electron density around SOG B 407:

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



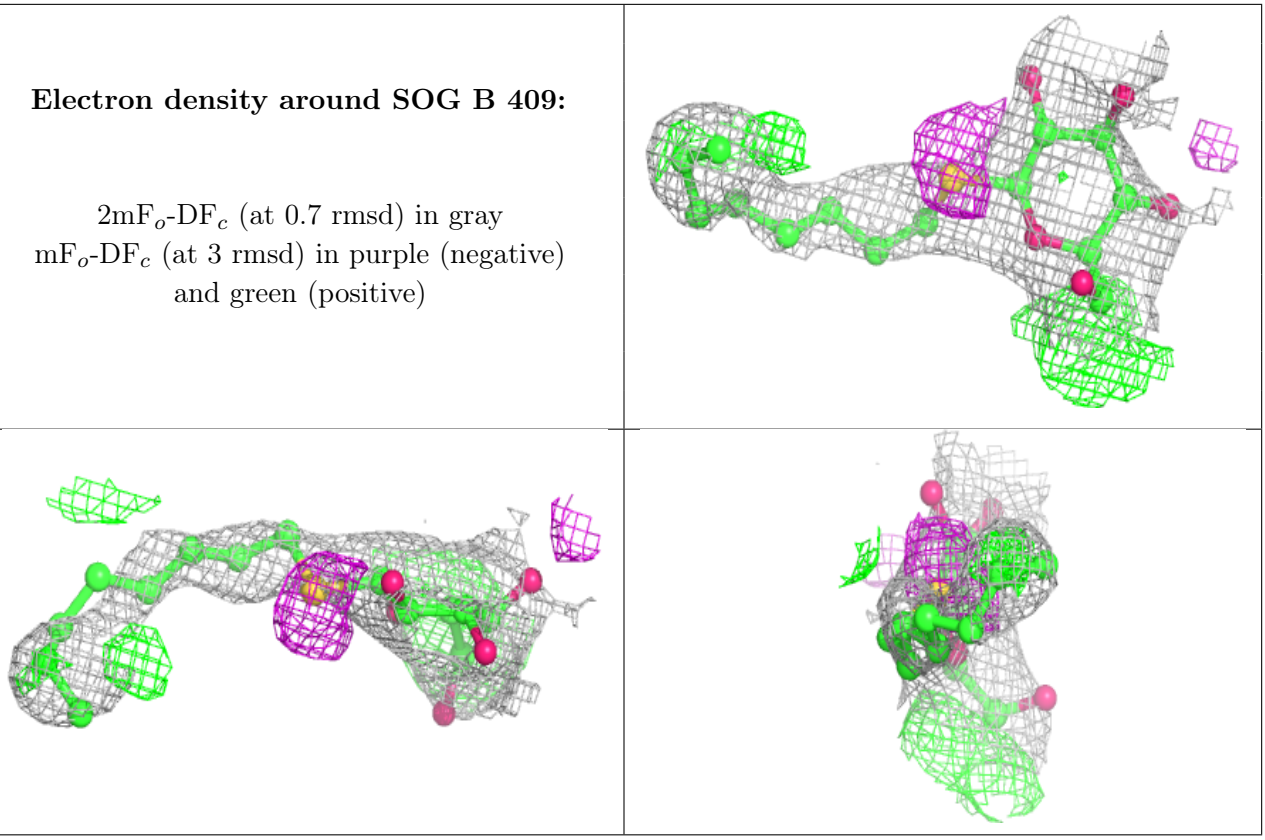
Electron density around SOG B 408:

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



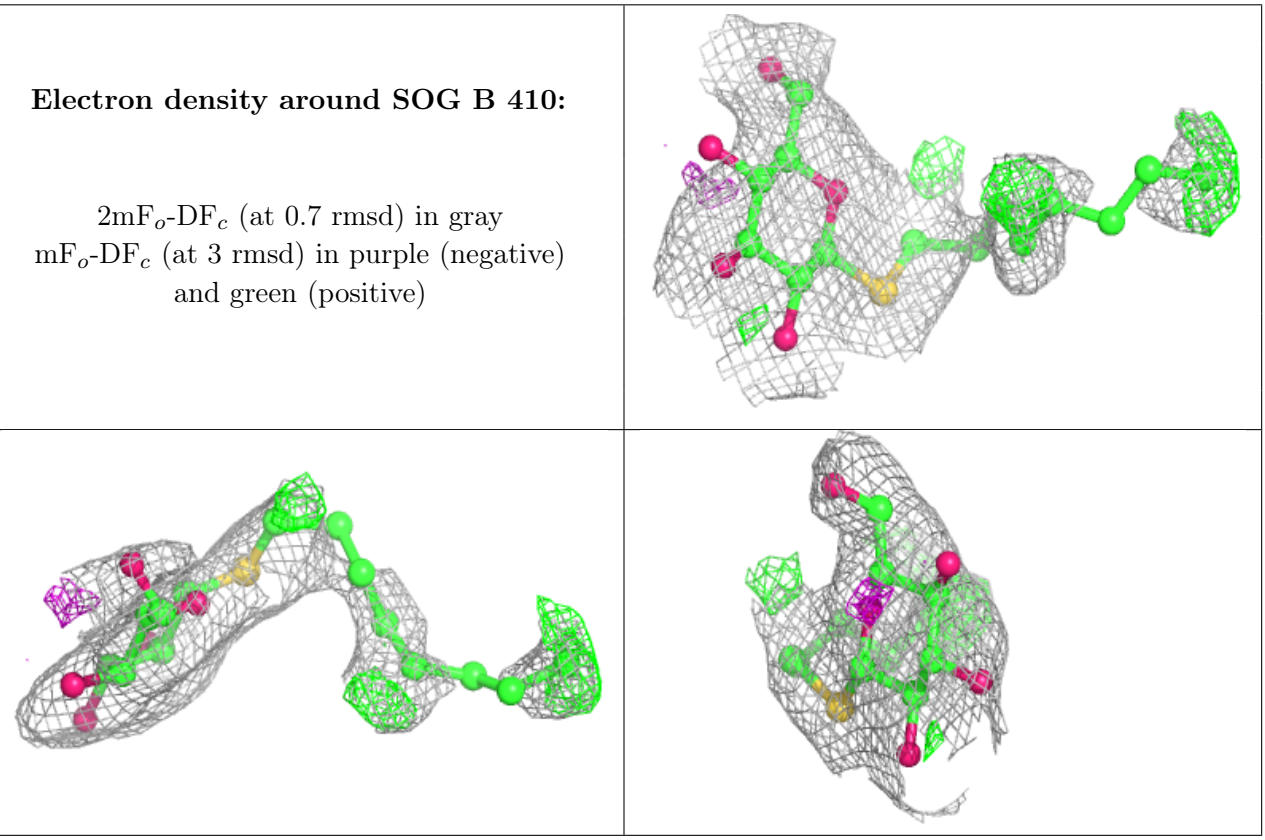
Electron density around SOG B 409:

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



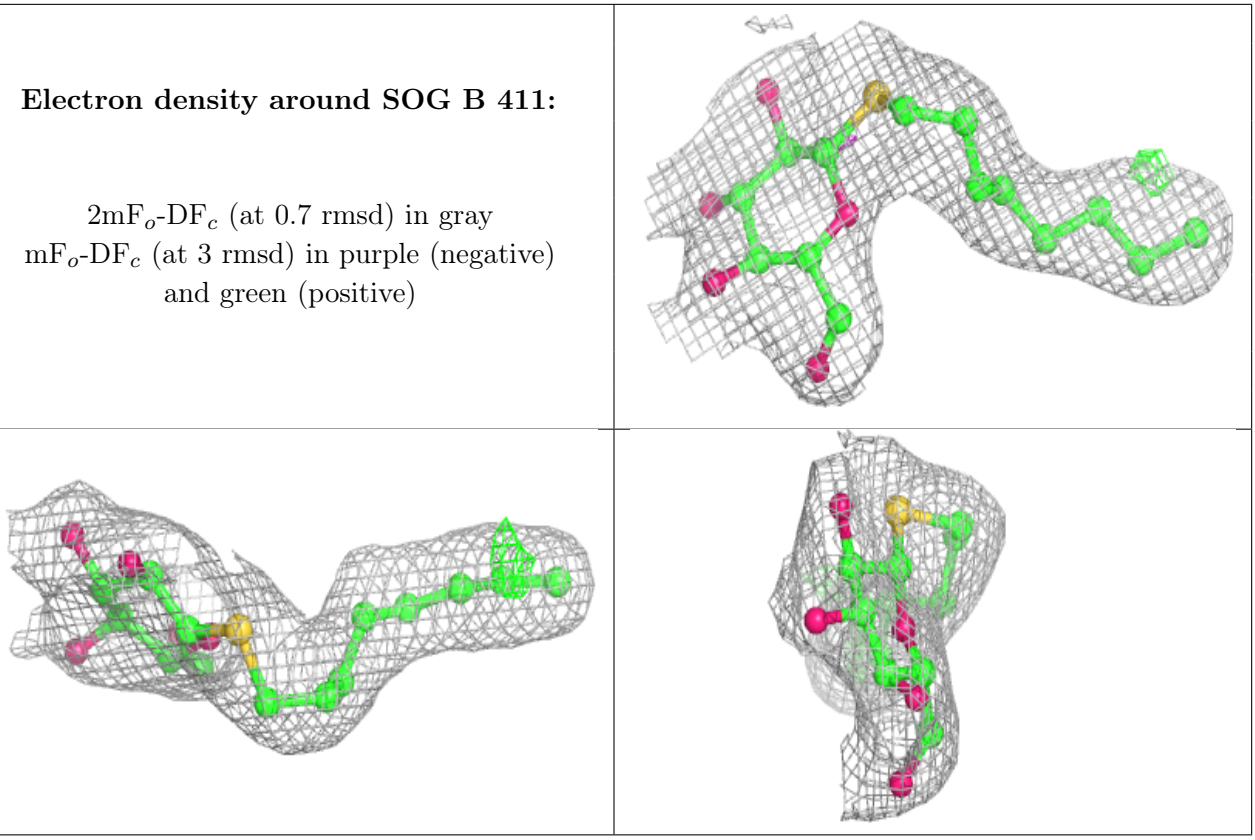
Electron density around SOG B 410:

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



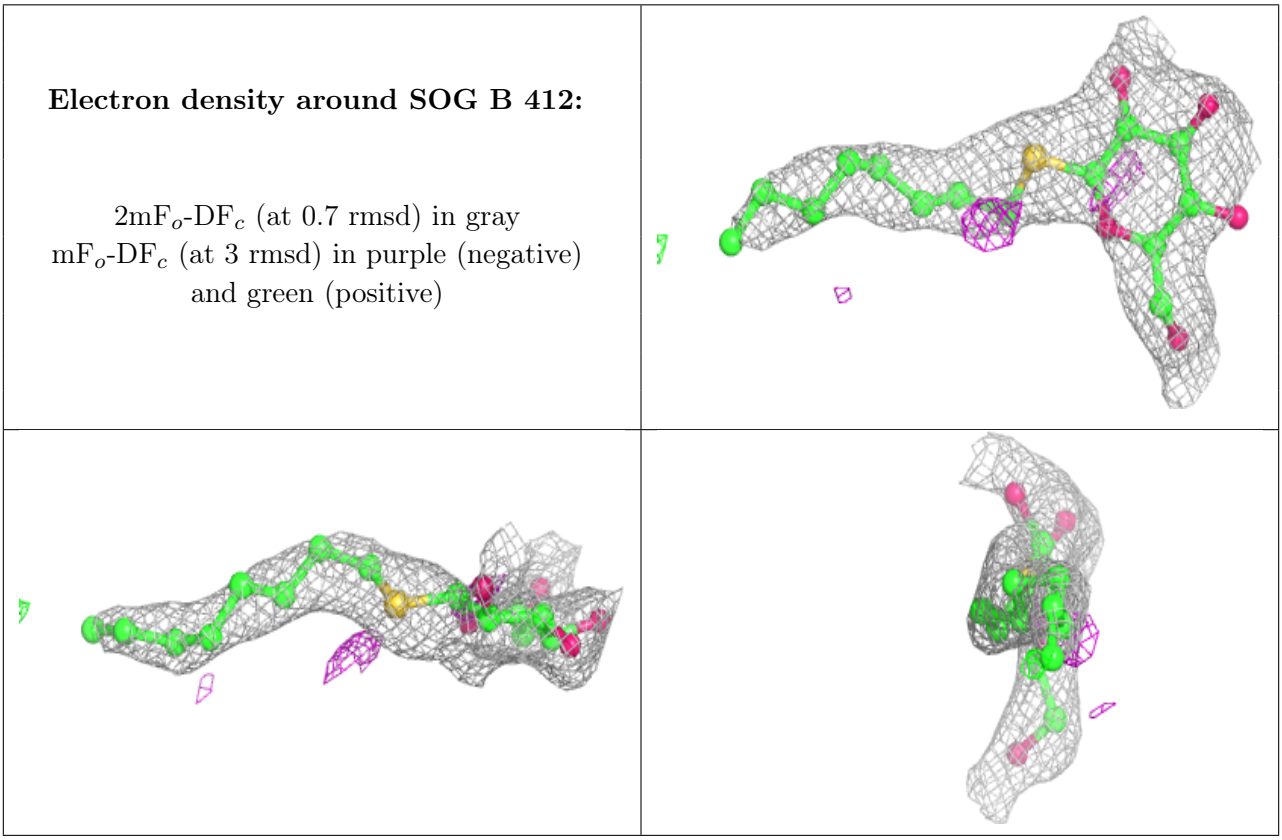
Electron density around SOG B 411:

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



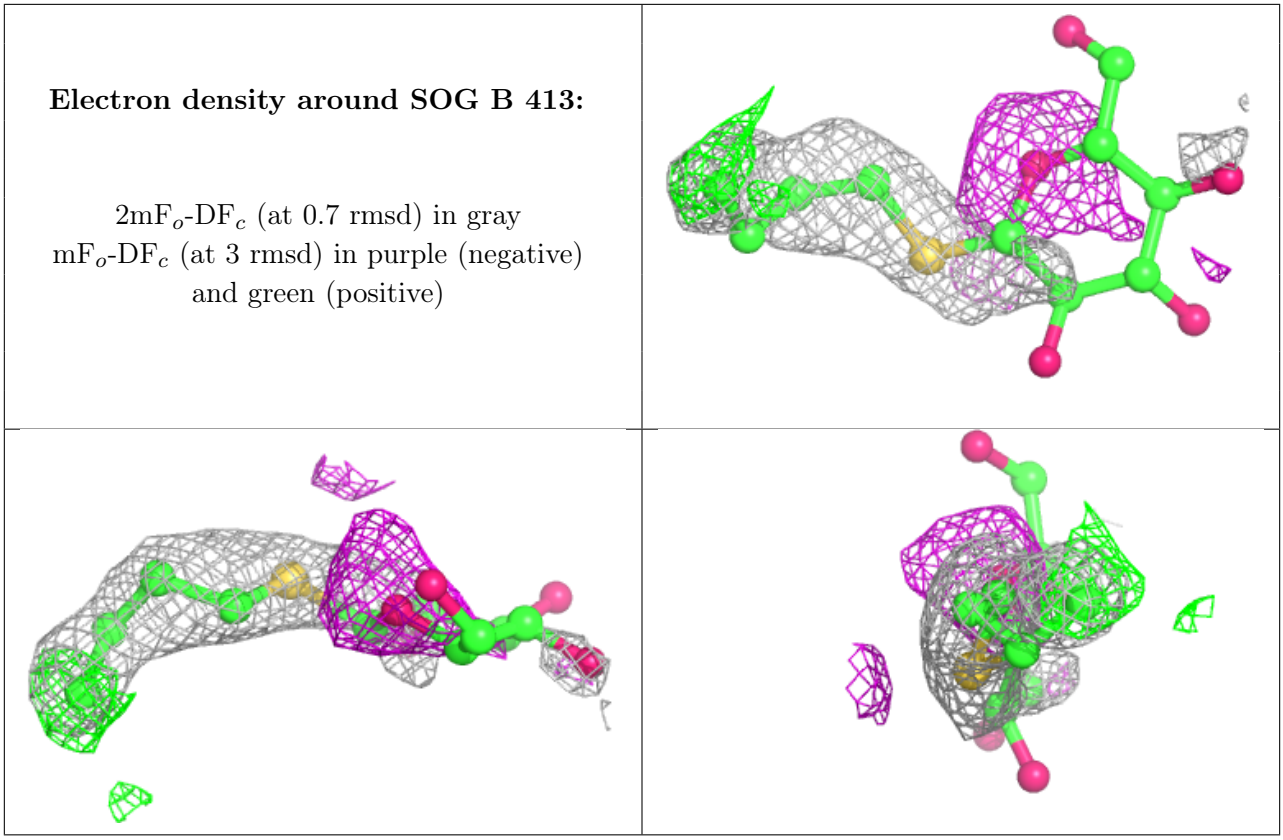
Electron density around SOG B 412:

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



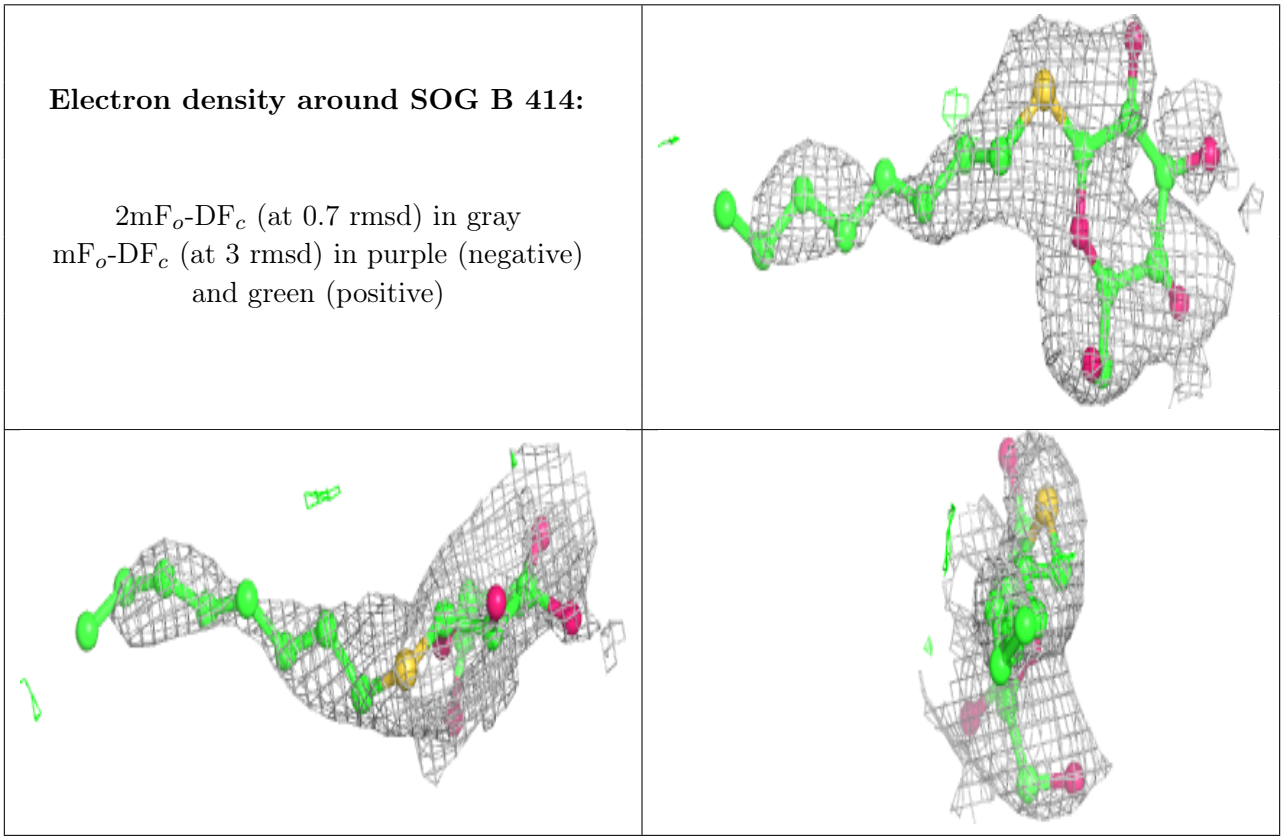
Electron density around SOG B 413:

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



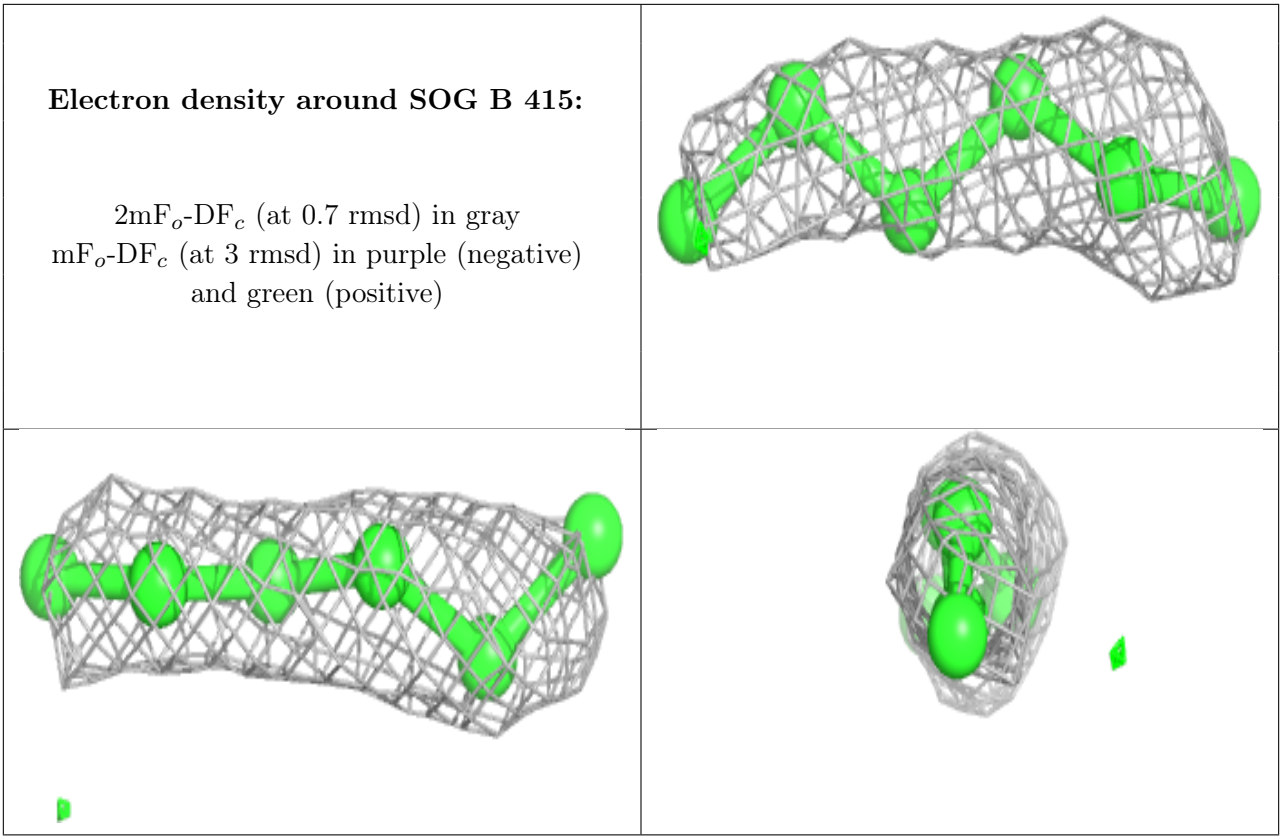
Electron density around SOG B 414:

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



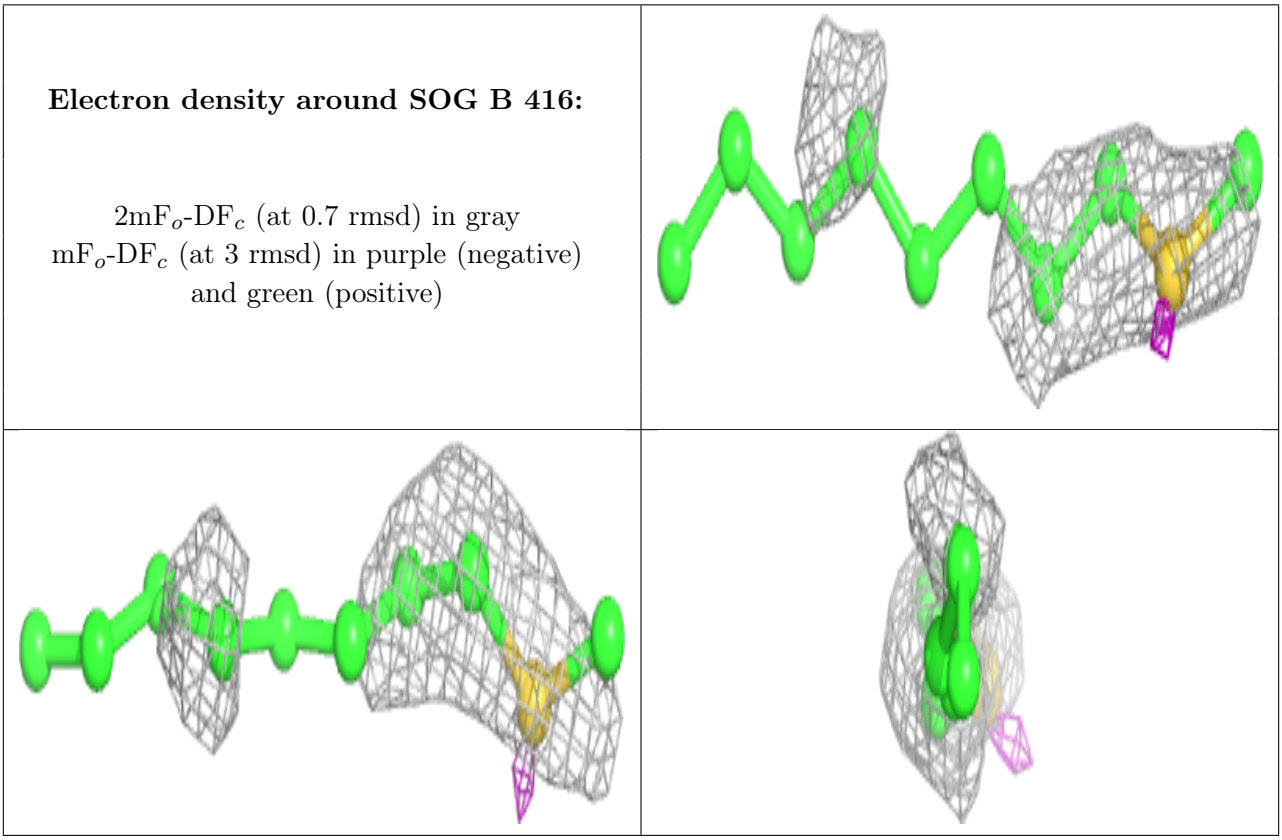
Electron density around SOG B 415:

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



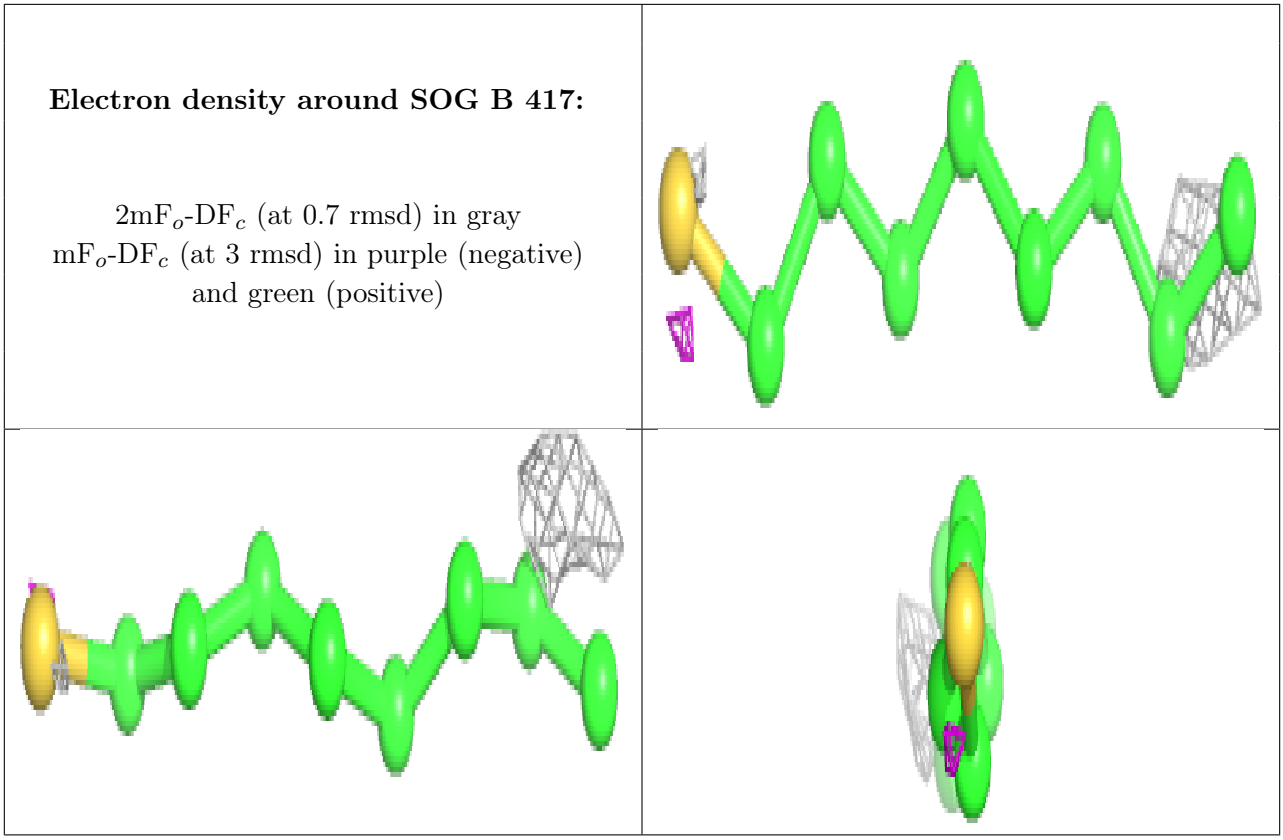
Electron density around SOG B 416:

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



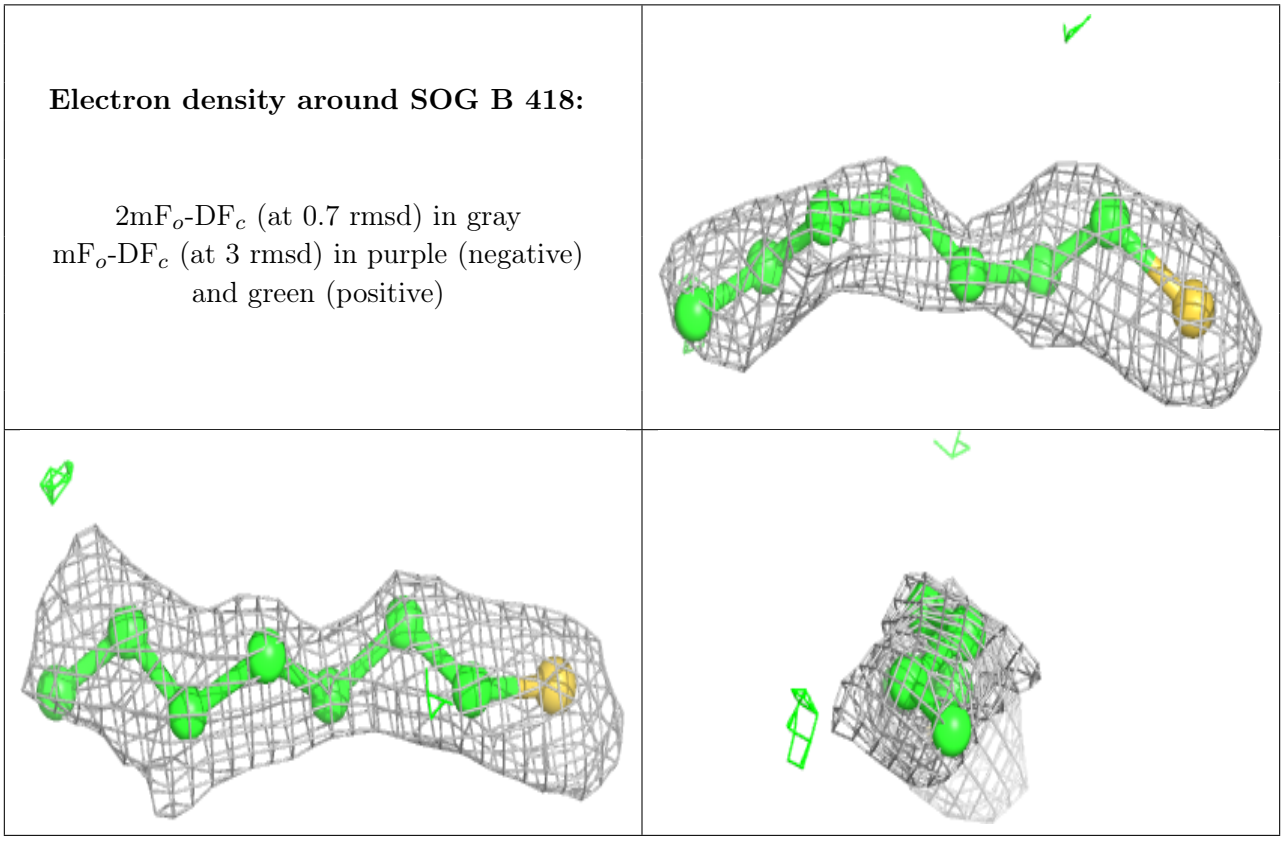
Electron density around SOG B 417:

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



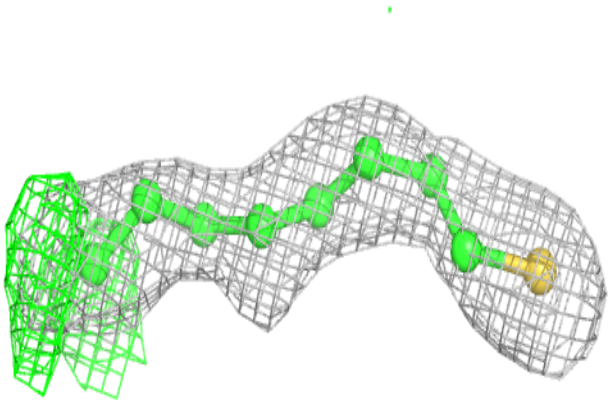
Electron density around SOG B 418:

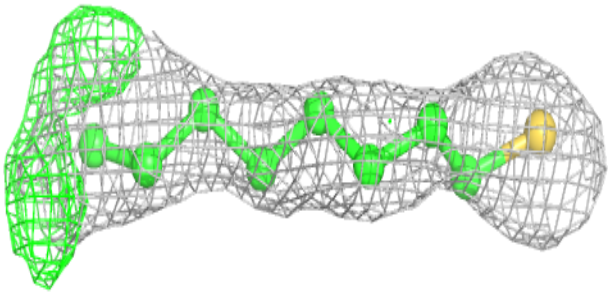
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

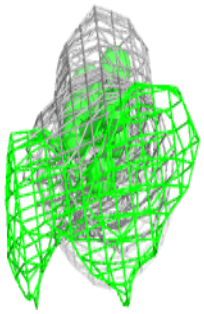


Electron density around SOG B 419:

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

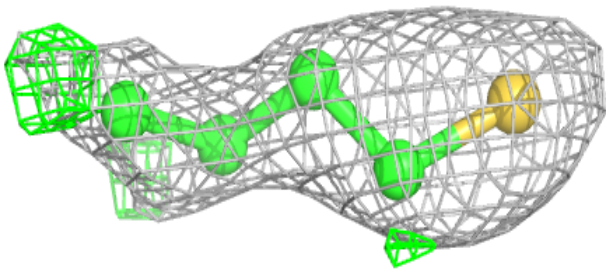


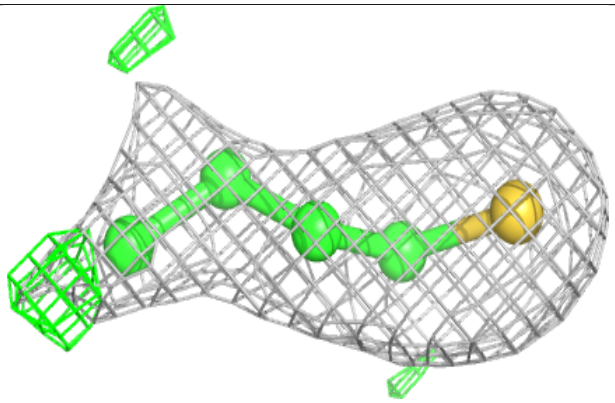


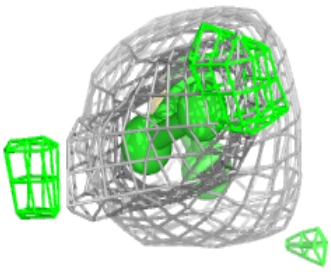


Electron density around SOG B 420:

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

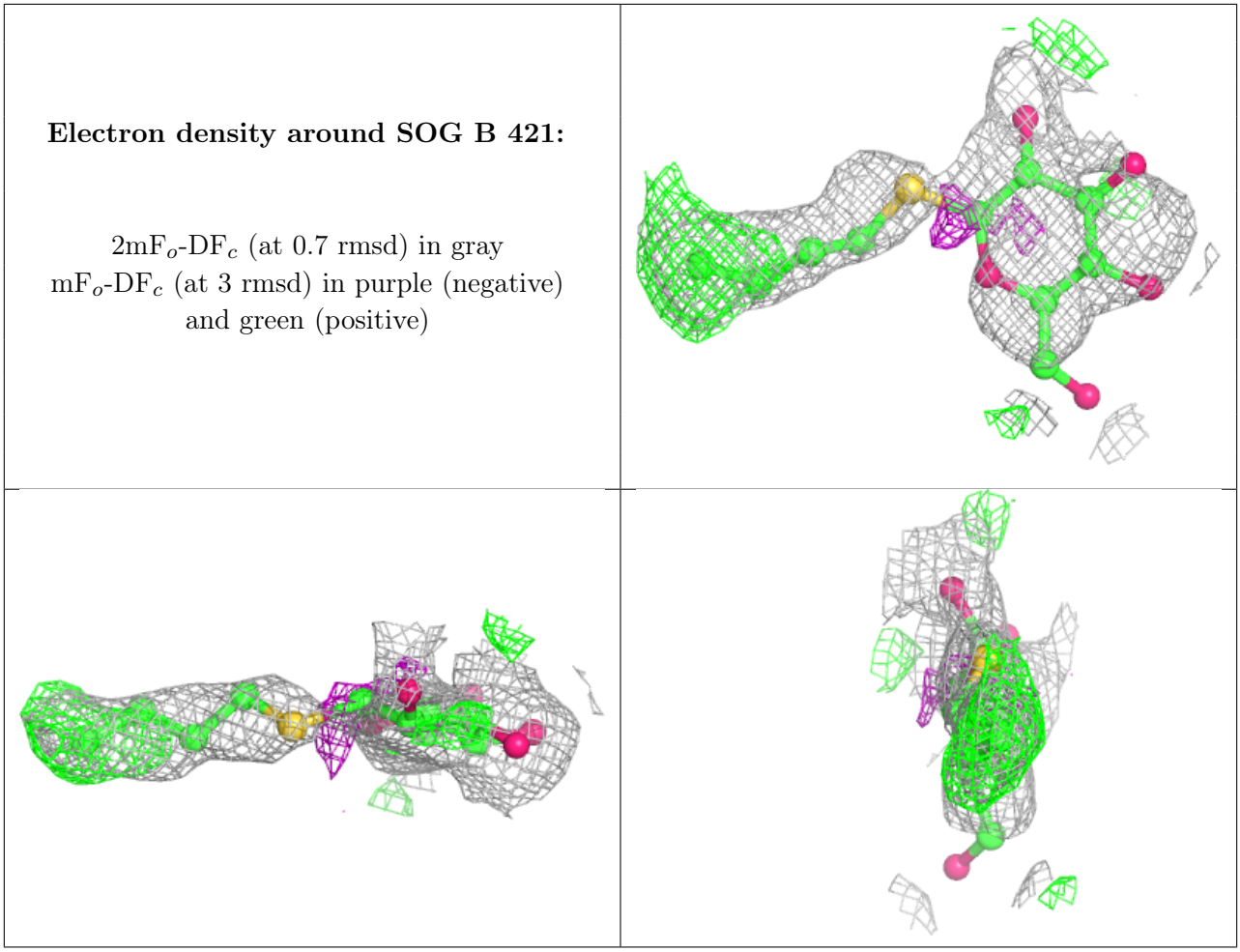






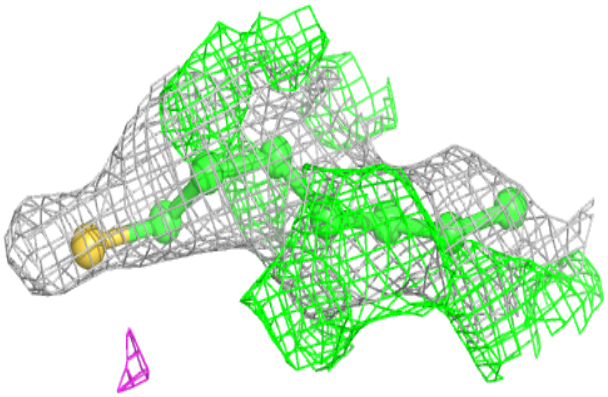
Electron density around SOG B 421:

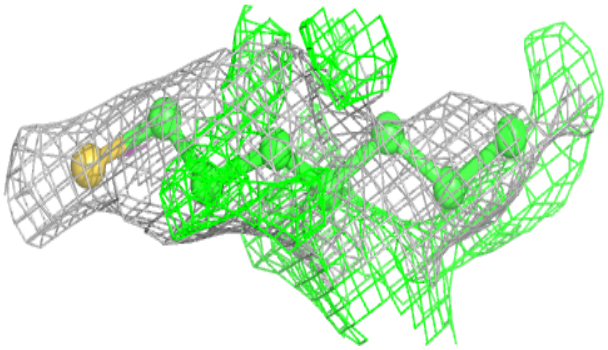
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

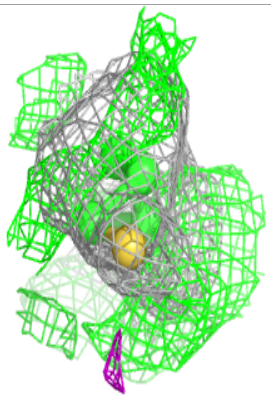


Electron density around SOG B 422:

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

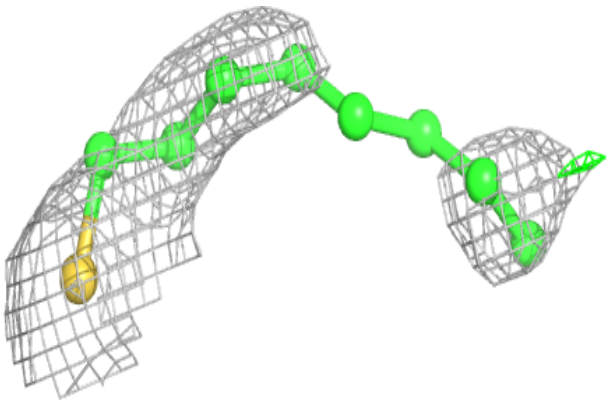


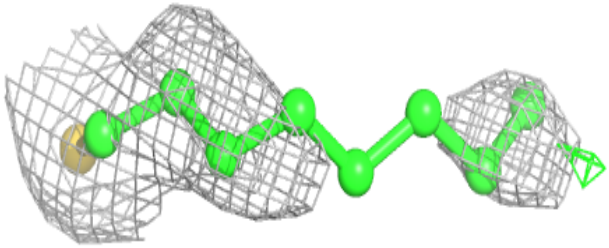


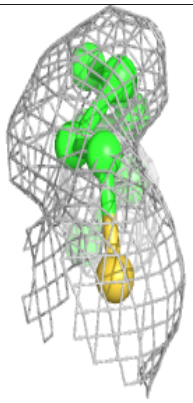


Electron density around SOG B 423:

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

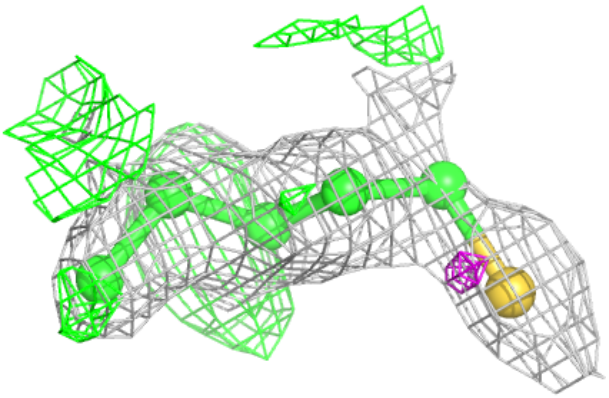


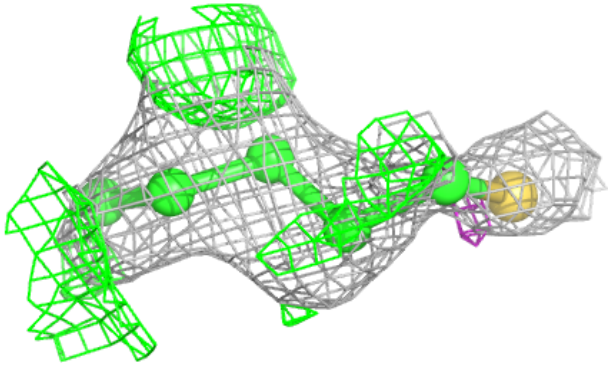


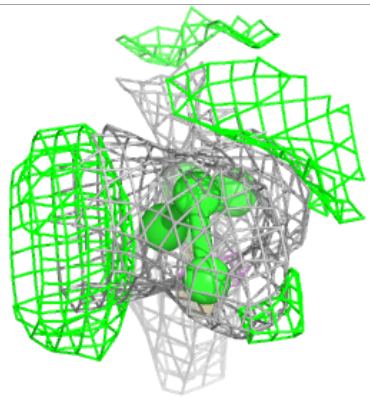


Electron density around SOG B 424:

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

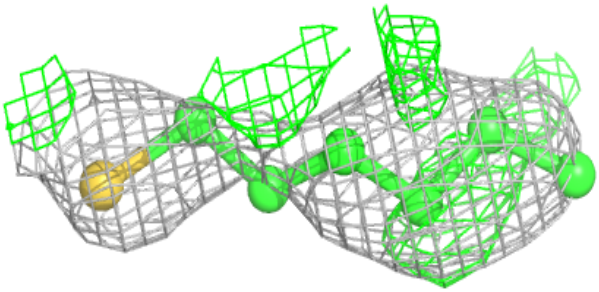


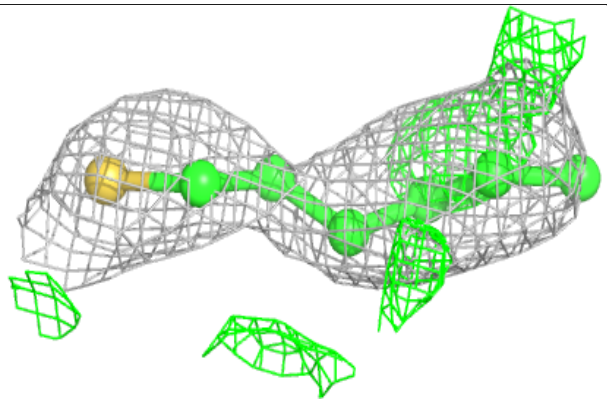


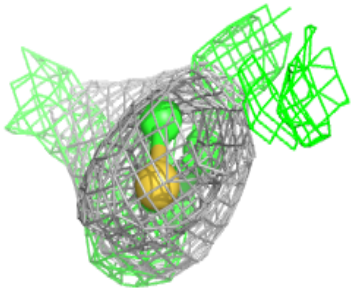


Electron density around SOG B 425:

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

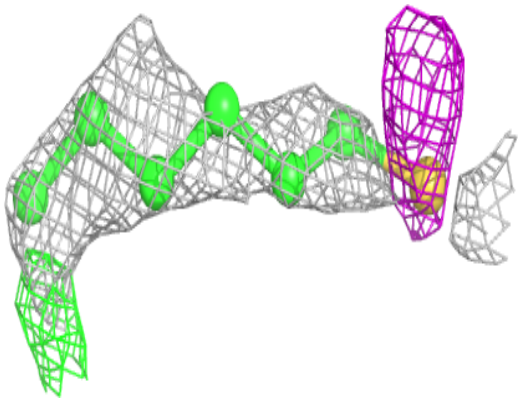


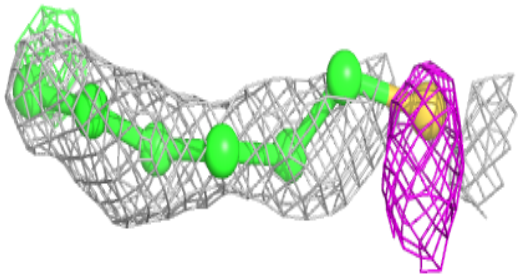


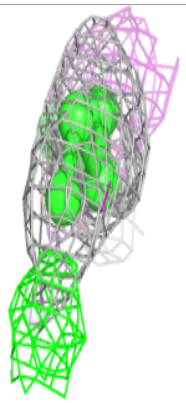


Electron density around SOG B 426:

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

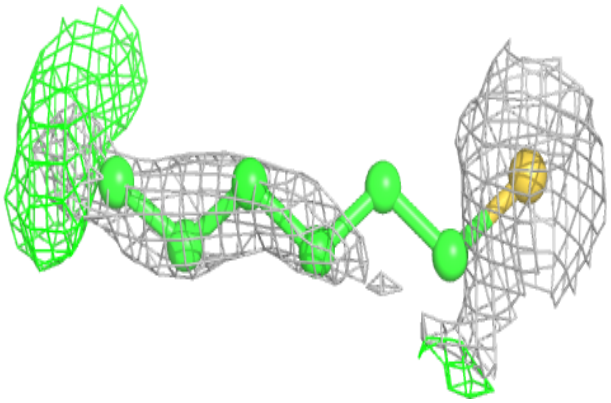


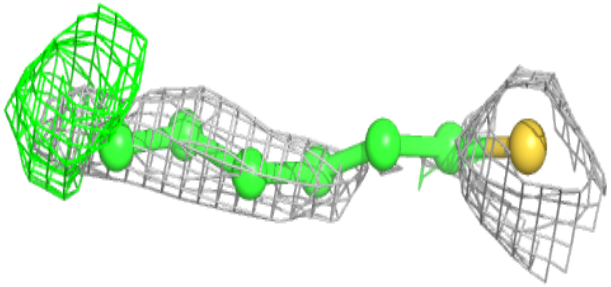


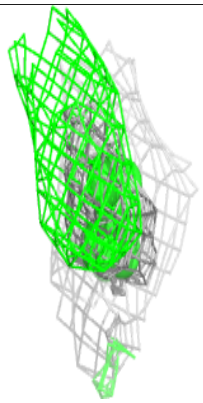


Electron density around SOG B 427:

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

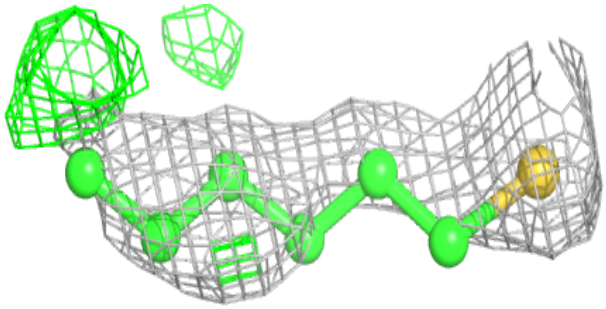


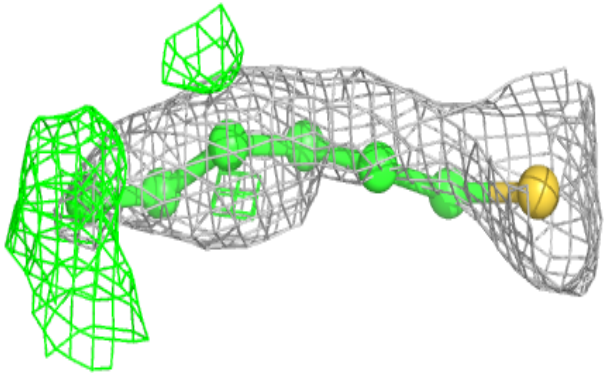


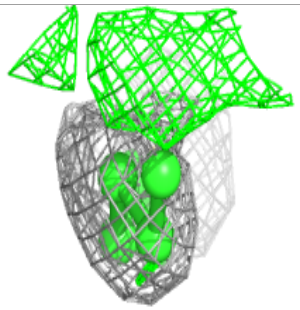


Electron density around SOG B 428:

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

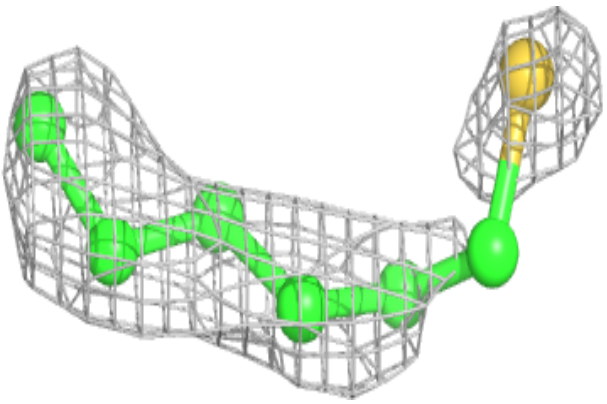


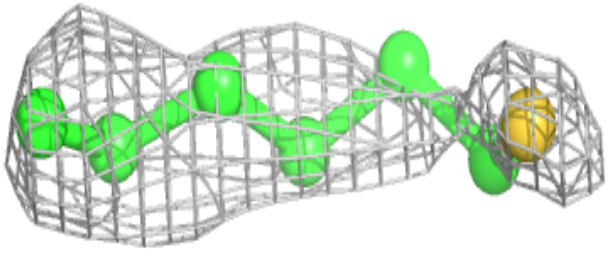


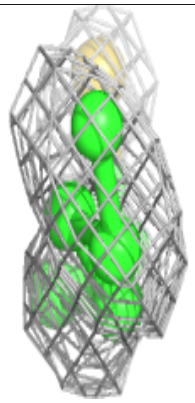


Electron density around SOG B 429:

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

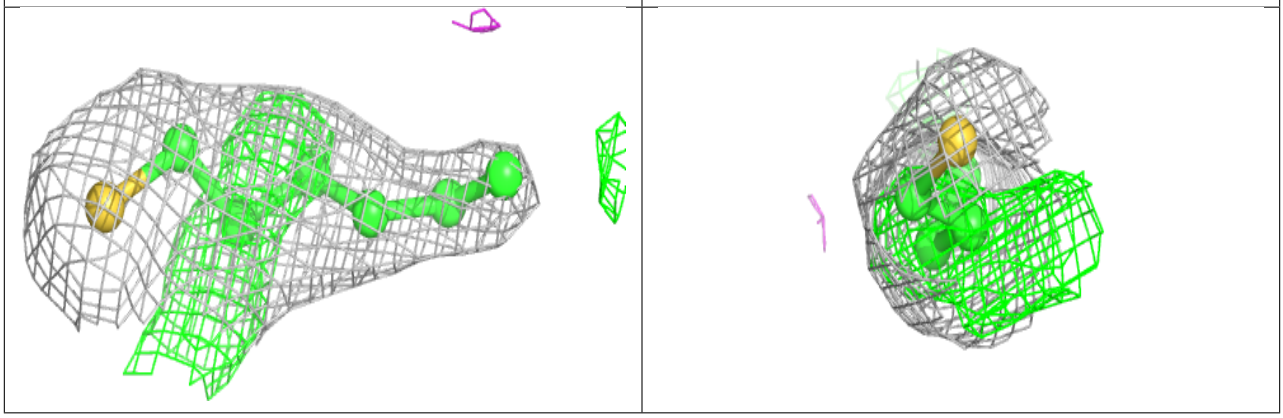






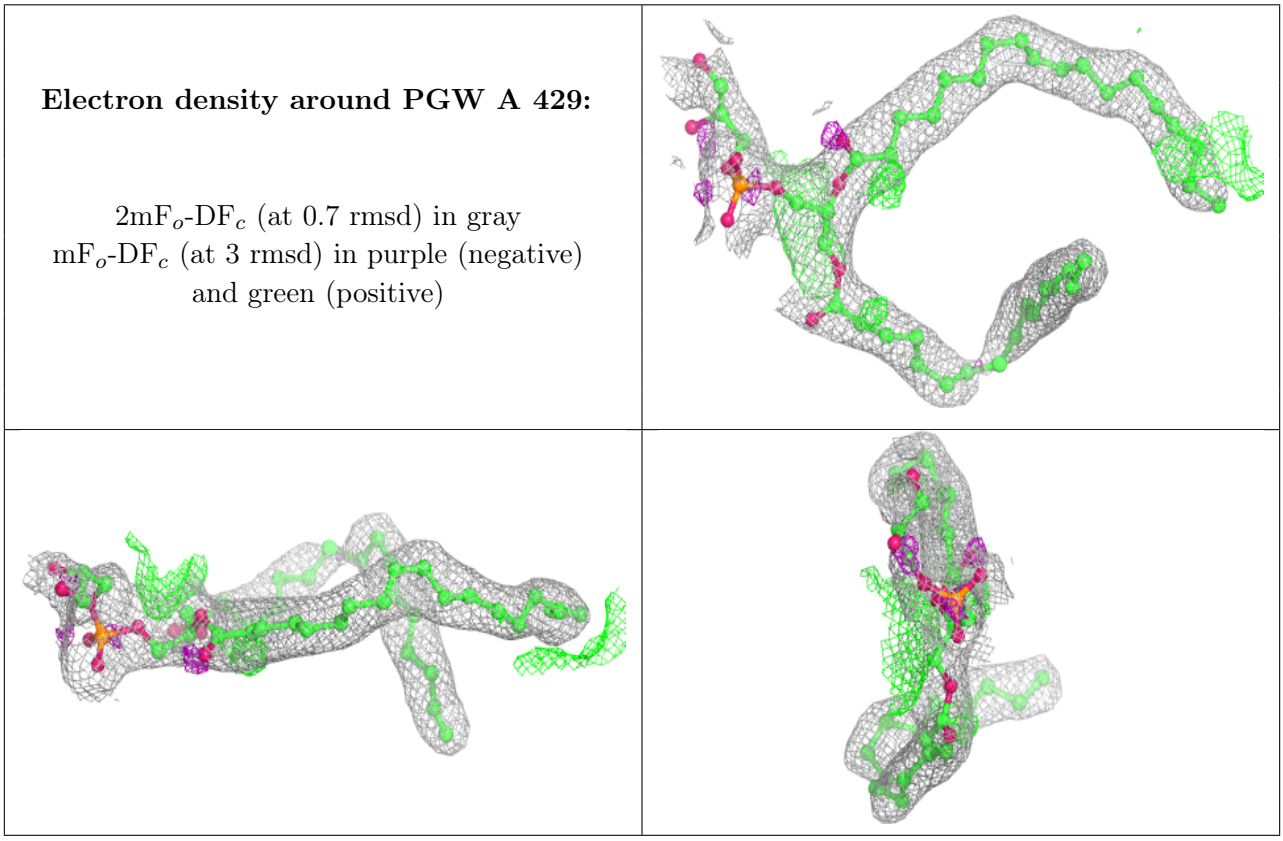
Electron density around SOG B 430:

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



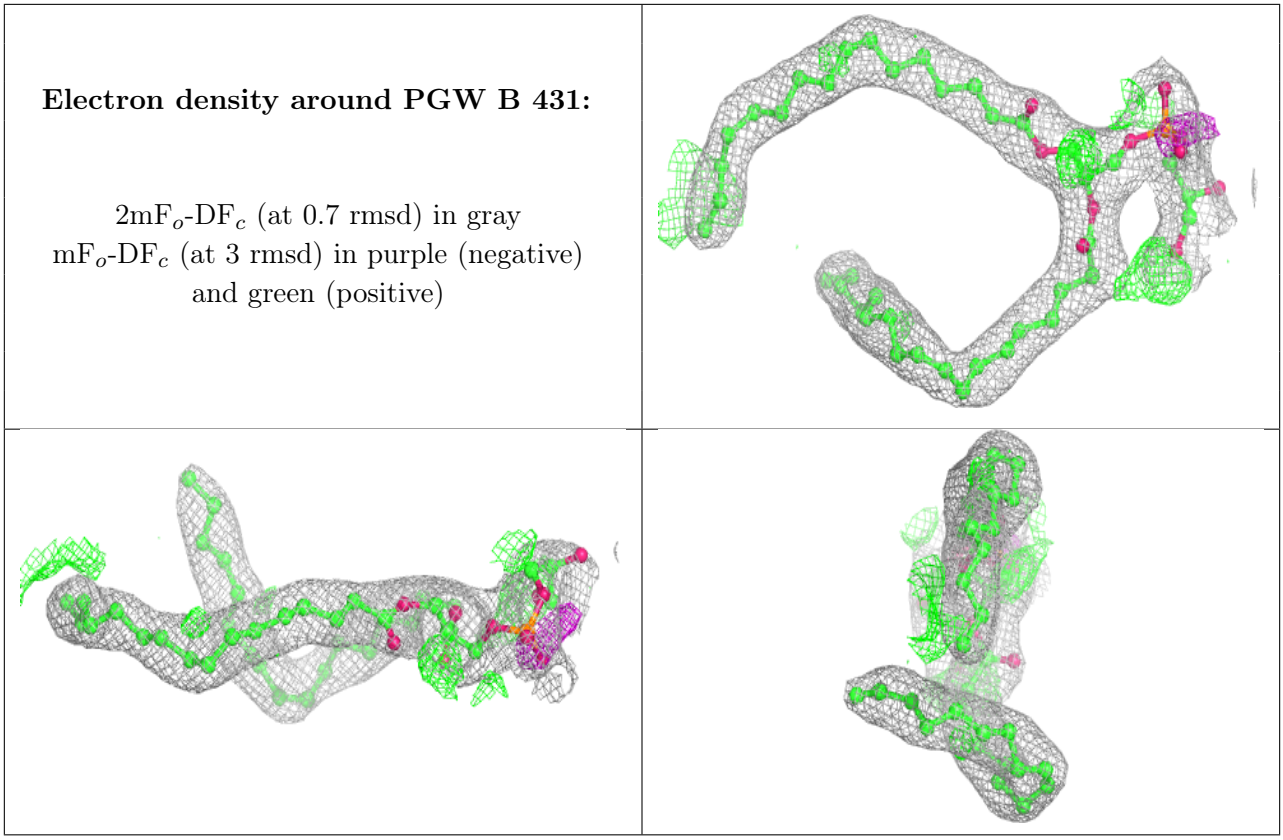
Electron density around PGW A 429:

$2mF_o$-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)



6.5 Other polymers (i)

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