wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 10:25 am GMT

PDB ID	:	6TP3
Title	:	Crystal structure of the Orexin-1 receptor in complex with daridorexant
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	:	2019-12-12
Resolution	:	3.04 Å(reported)

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

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

The 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:

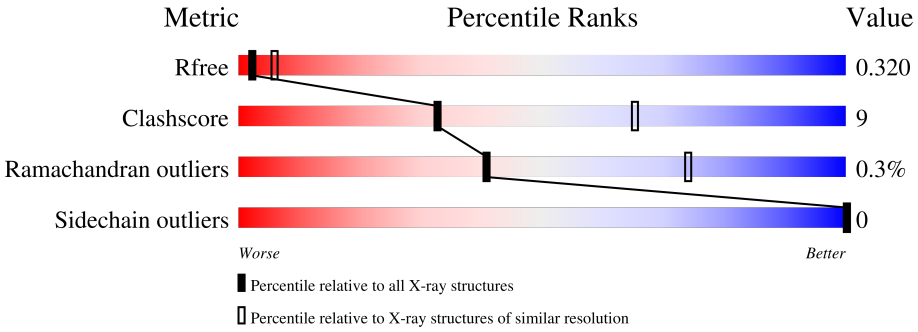
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)

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	368	73% 11% • 15%
1	B	368	73% 11% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5445 atoms, of which 46 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2515	1669	421	408	17			
1	B	307	Total	C	N	O	S	0	0	0
			2467	1640	405	405	17			

There are 52 discrepancies between the modelled and reference sequences:

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

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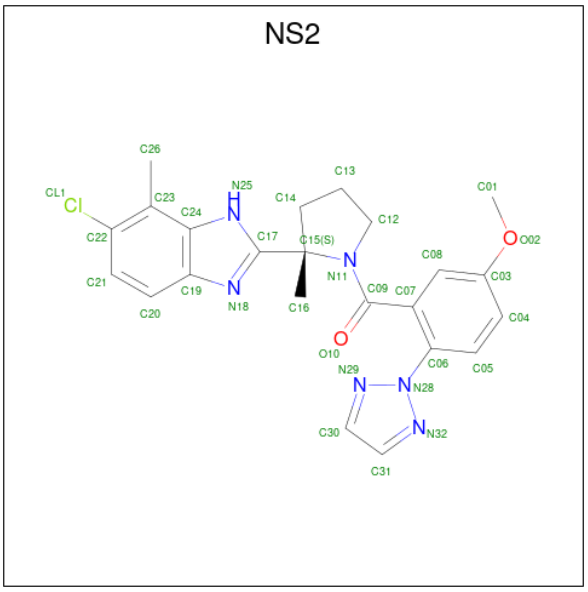
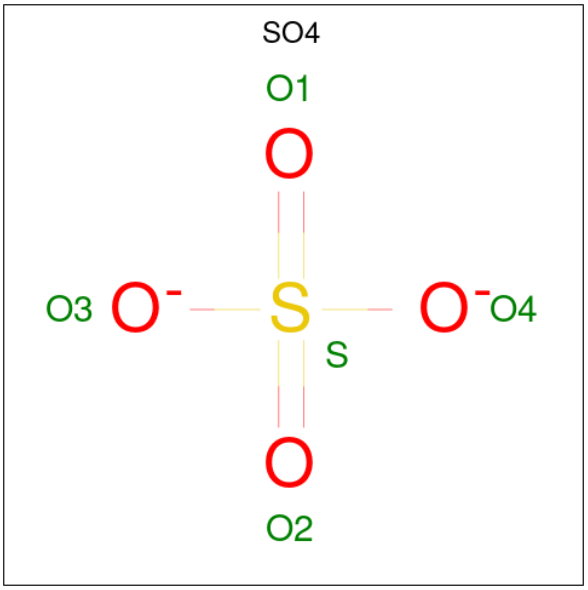
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered mutation	UNP O43613
B	162	LEU	ARG	engineered mutation	UNP O43613
B	194	ALA	ASN	engineered mutation	UNP O43613
B	198	ALA	LEU	engineered mutation	UNP O43613
B	211	ALA	TYR	engineered mutation	UNP O43613
B	304	VAL	LEU	engineered mutation	UNP O43613
B	339	ALA	CYS	engineered mutation	UNP O43613
B	375	TRP	CYS	engineered mutation	UNP O43613
B	376	TRP	CYS	engineered mutation	UNP O43613
B	381	ALA	-	expression tag	UNP O43613
B	382	ALA	-	expression tag	UNP O43613
B	383	ALA	-	expression tag	UNP O43613
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is [(2 {S})-2-(6-chloranyl-7-methyl-1 {H}-benzimidazol-2-yl)-2-methyl-pyrrolidin -1-yl]-[5-methoxy-2-(1,2,3-triazol-2-yl)phenyl]methanone (three-letter code: NS2) (formula: $C_{23}H_{23}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			55	23	1	23	6	2		
2	B	1	Total	C	Cl	H	N	O	0	0
			55	23	1	23	6	2		

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



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

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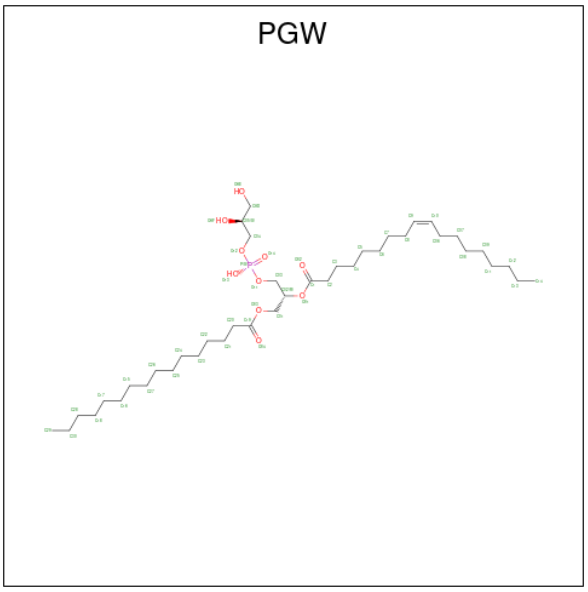
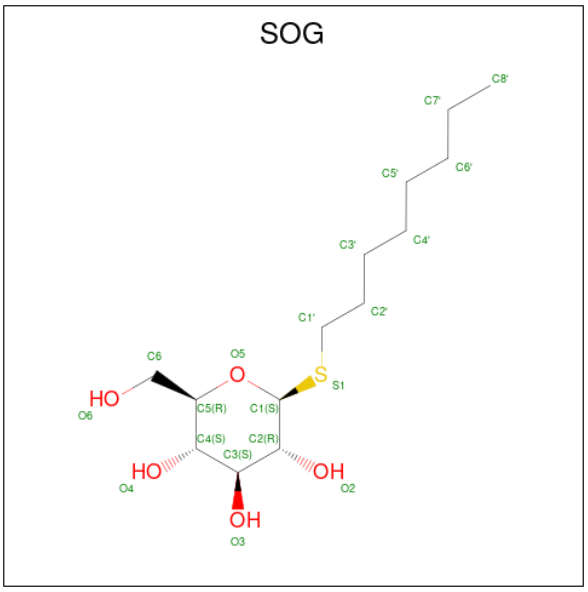
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 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
4	A	1	Total C O P 51 40 10 1	0	0
4	B	1	Total C O P 51 40 10 1	0	0

- Molecule 5 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula: $C_{14}H_{28}O_5S$).



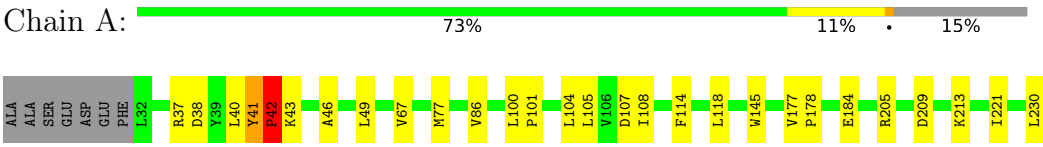
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C O S 14 8 5 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	A	1	Total C O S 20 14 5 1	0	0
5	B	1	Total C O S 20 14 5 1	0	0
5	B	1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

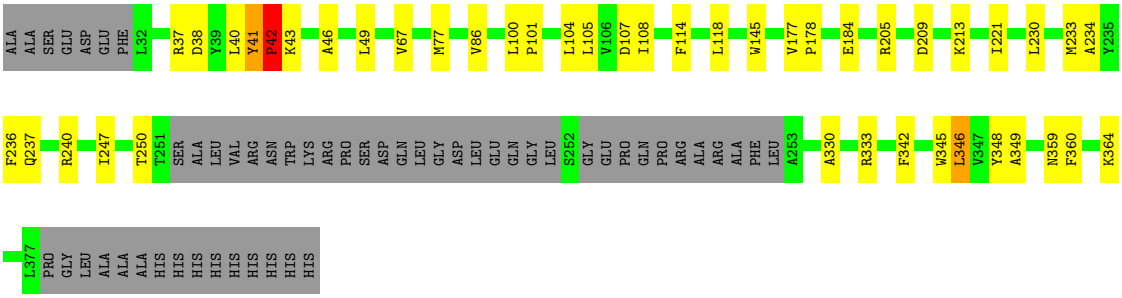
3 Residue-property plots (i)

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

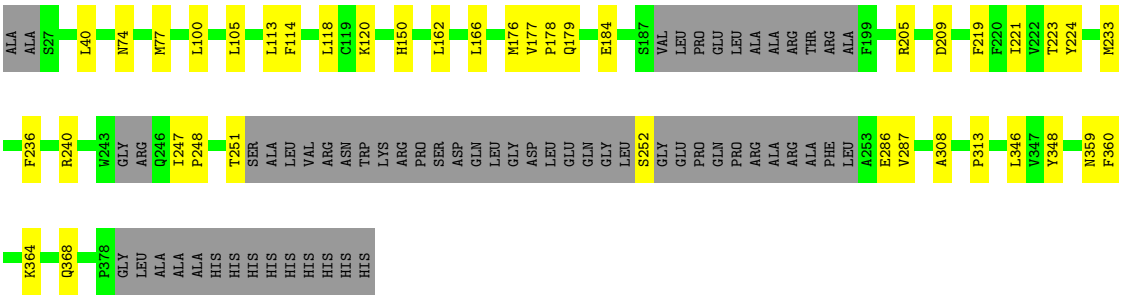
Chain A:





• Molecule 1: Orexin receptor type 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.22Å 146.42Å 73.60Å 90.00° 109.55° 90.00°	Depositor
Resolution (Å)	25.86 – 3.04 73.21 – 3.02	Depositor EDS
% Data completeness (in resolution range)	58.6 (25.86-3.04) 77.4 (73.21-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.15 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.205 , 0.230 0.254 , 0.320	Depositor DCC
R_{free} test set	1173 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	84.5	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 71.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5445	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: SO4, PGW, NS2, SOG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.50	0/2587	0.63	2/3529 (0.1%)
1	B	0.50	0/2538	0.60	0/3460
All	All	0.50	0/5125	0.61	2/6989 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	PRO	CA-N-CD	5.57	119.50	111.70
1	A	346	LEU	CB-CA-C	-5.12	100.48	110.20

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	2515	0	2581	59	2
1	B	2467	0	2508	40	2
2	A	32	23	0	1	0
2	B	32	23	0	1	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	51	0	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	51	0	76	1	0
5	A	134	0	181	6	0
5	B	102	0	121	6	0
All	All	5399	46	5543	95	2

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 9.

The worst 5 of 95 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:A:41:TYR:CD2	1:A:42:PRO:HD3	1.60	1.34
1:A:345:TRP:HE3	1:A:346:LEU:HD12	1.16	1.11
1:A:41:TYR:CG	1:A:42:PRO:HD3	1.89	1.08
1:A:345:TRP:CE3	1:A:346:LEU:HD12	1.90	1.06
1:A:41:TYR:HB3	1:A:42:PRO:CD	1.92	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:CE1	1:B:40:LEU:CD2[2_445]	1.22	0.98
1:A:41:TYR:CD1	1:B:40:LEU:CD2[2_445]	2.06	0.14

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	312/368 (85%)	306 (98%)	4 (1%)	2 (1%)	25 60
1	B	301/368 (82%)	294 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	613/736 (83%)	600 (98%)	11 (2%)	2 (0%)	41 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	A	41	TYR

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	263/305 (86%)	263 (100%)	0	100 100
1	B	260/305 (85%)	260 (100%)	0	100 100
All	All	523/610 (86%)	523 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	75	HIS
1	B	75	HIS
1	B	150	HIS

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)

21 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	SO4	B	402	-	4,4,4	0.06	0	6,6,6	0.24	0
5	SOG	A	405	-	20,20,20	1.12	1 (5%)	24,25,25	1.41	4 (16%)
4	PGW	A	404	-	50,50,50	1.03	2 (4%)	53,56,56	1.09	4 (7%)
2	NS2	B	401	-	32,36,36	2.09	10 (31%)	31,54,54	2.62	11 (35%)
3	SO4	A	402	-	4,4,4	0.38	0	6,6,6	0.43	0
4	PGW	B	403	-	50,50,50	1.09	2 (4%)	53,56,56	1.03	3 (5%)
5	SOG	A	409	-	20,20,20	0.89	2 (10%)	24,25,25	1.49	5 (20%)
2	NS2	A	401	-	32,36,36	2.18	11 (34%)	31,54,54	2.51	11 (35%)
5	SOG	B	407	-	4,4,20	0.41	0	2,3,25	0.56	0
5	SOG	B	408	-	11,12,20	1.10	0	15,17,25	1.43	3 (20%)
5	SOG	B	409	-	11,12,20	0.95	0	15,17,25	1.76	2 (13%)
5	SOG	A	406	-	20,20,20	1.12	1 (5%)	24,25,25	1.56	4 (16%)
5	SOG	B	404	-	20,20,20	1.07	1 (5%)	24,25,25	2.00	5 (20%)
5	SOG	A	410	-	20,20,20	1.14	2 (10%)	24,25,25	0.98	1 (4%)
5	SOG	B	405	-	20,20,20	0.97	1 (5%)	24,25,25	1.75	4 (16%)
5	SOG	A	408	-	14,14,20	0.91	0	18,19,25	1.24	2 (11%)
5	SOG	A	407	-	20,20,20	1.13	2 (10%)	24,25,25	1.66	5 (20%)
5	SOG	B	410	-	20,20,20	0.93	1 (5%)	24,25,25	1.14	2 (8%)
3	SO4	A	403	-	4,4,4	0.13	0	6,6,6	0.19	0
5	SOG	A	411	-	20,20,20	1.03	1 (5%)	24,25,25	1.43	5 (20%)
5	SOG	B	406	-	12,13,20	0.83	0	16,18,25	0.95	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	B	404	-	-	9/11/31/31	0/1/1/1
5	SOG	B	406	-	-	2/4/24/31	0/1/1/1
4	PGW	B	403	-	-	30/55/55/55	-
5	SOG	A	405	-	-	6/11/31/31	0/1/1/1
5	SOG	B	410	-	-	5/11/31/31	0/1/1/1
5	SOG	A	409	-	-	7/11/31/31	0/1/1/1
2	NS2	A	401	-	-	4/12/33/33	0/5/5/5
4	PGW	A	404	-	-	31/55/55/55	-
5	SOG	A	410	-	-	5/11/31/31	0/1/1/1
5	SOG	B	407	-	-	2/2/2/31	-
5	SOG	B	408	-	-	1/2/22/31	0/1/1/1
5	SOG	A	407	-	-	7/11/31/31	0/1/1/1
5	SOG	B	405	-	-	8/11/31/31	0/1/1/1
5	SOG	B	409	-	-	1/2/22/31	0/1/1/1
5	SOG	A	408	-	-	1/5/25/31	0/1/1/1
5	SOG	A	411	-	-	4/11/31/31	0/1/1/1
5	SOG	A	406	-	-	7/11/31/31	0/1/1/1
2	NS2	B	401	-	-	4/12/33/33	0/5/5/5

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NS2	C12-N11	5.93	1.54	1.47
2	B	401	NS2	C09-N11	5.65	1.44	1.35
2	A	401	NS2	C09-N11	5.57	1.44	1.35
4	B	403	PGW	O01-C1	5.06	1.48	1.34
4	B	403	PGW	O03-C19	4.88	1.47	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NS2	C23-C22-CL1	6.60	127.84	119.45
2	B	401	NS2	C21-C22-CL1	-6.59	105.19	118.41
2	A	401	NS2	C23-C22-CL1	6.32	127.48	119.45
2	A	401	NS2	C21-C22-CL1	-6.01	106.34	118.41
5	B	404	SOG	C1-O5-C5	5.52	122.77	112.58

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NS2	C07-C09-N11-C12
2	A	401	NS2	C07-C09-N11-C15
2	A	401	NS2	O10-C09-N11-C12
2	A	401	NS2	O10-C09-N11-C15
2	B	401	NS2	C07-C09-N11-C12

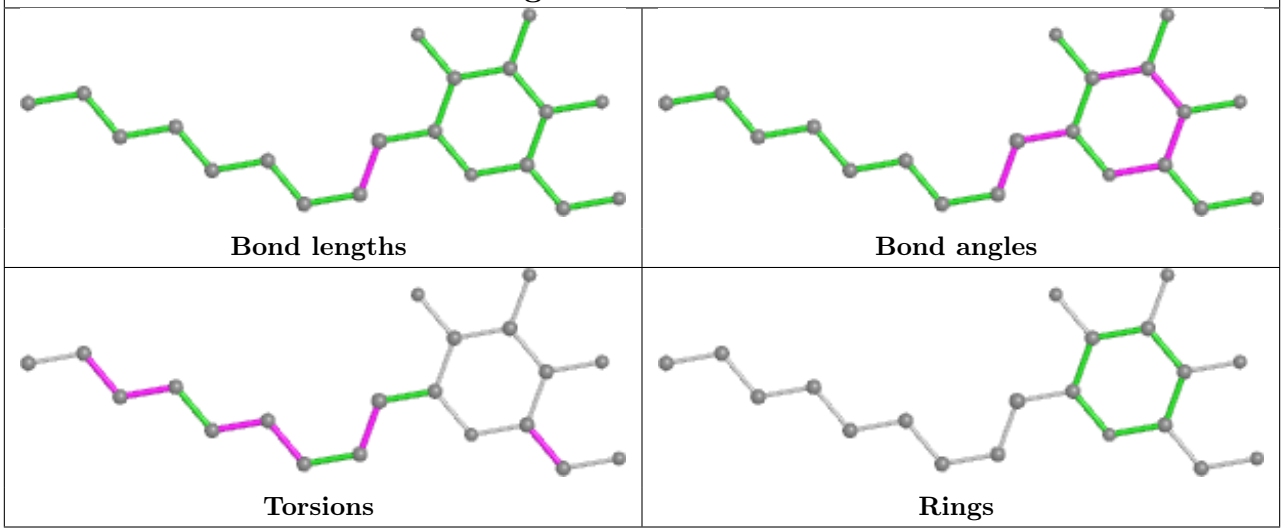
There are no ring outliers.

13 monomers are involved in 18 short contacts:

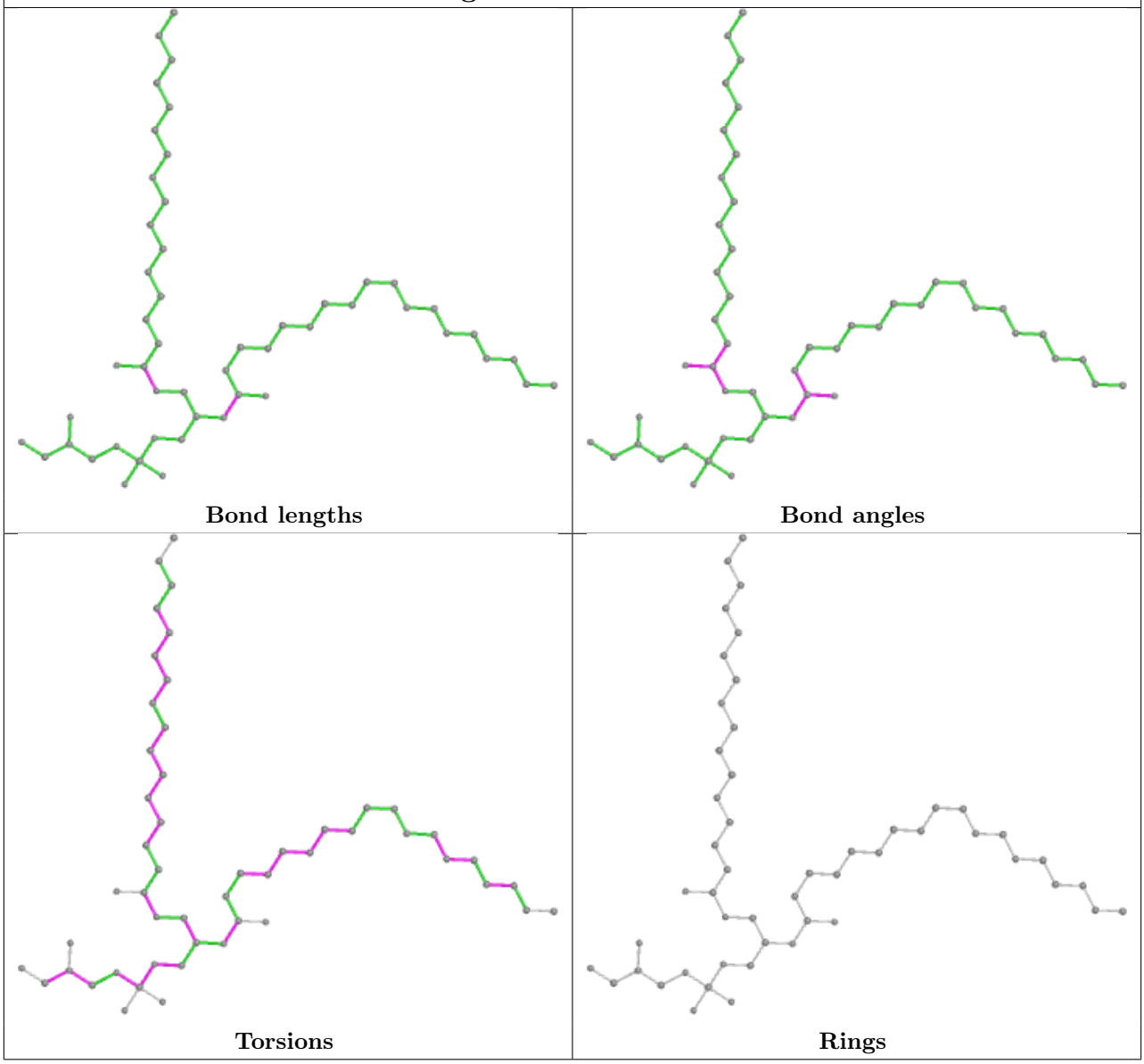
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	SOG	2	0
4	A	404	PGW	3	0
2	B	401	NS2	1	0
4	B	403	PGW	1	0
5	A	409	SOG	1	0
2	A	401	NS2	1	0
5	B	408	SOG	1	0
5	B	409	SOG	2	0
5	B	404	SOG	1	0
5	A	410	SOG	1	0
5	A	407	SOG	1	0
5	B	410	SOG	2	0
5	A	411	SOG	1	0

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.

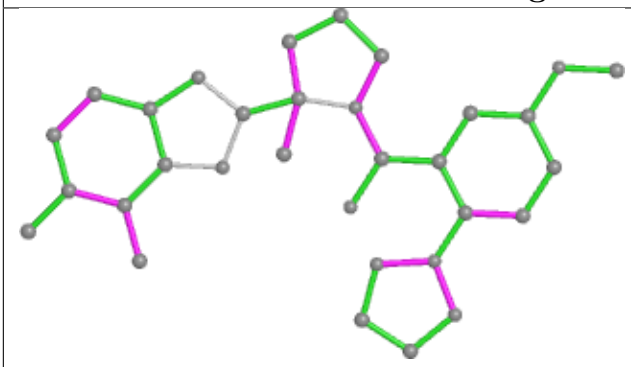
Ligand SOG A 405



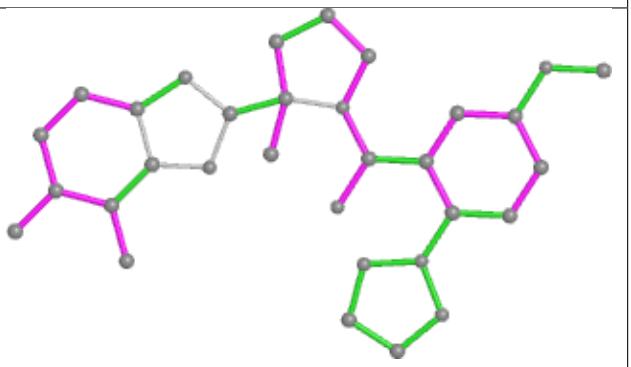
Ligand PGW A 404



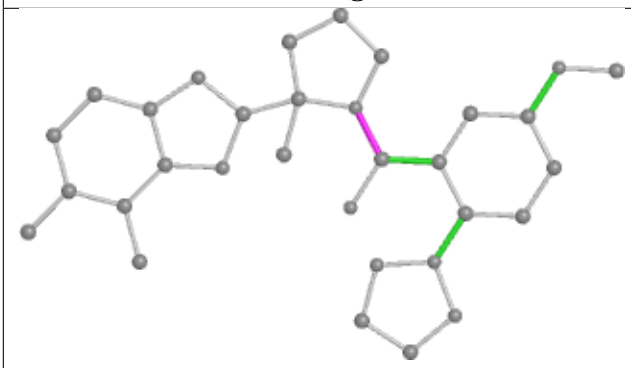
Ligand NS2 B 401



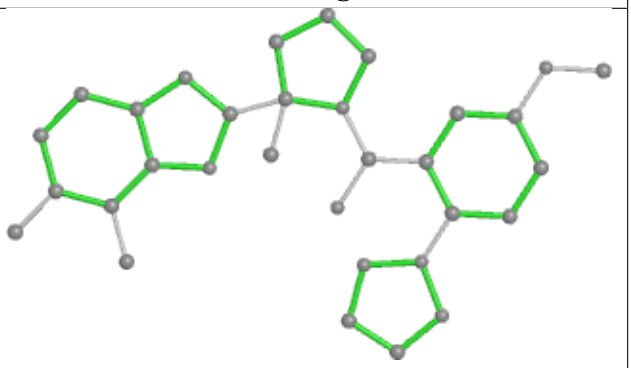
Bond lengths



Bond angles

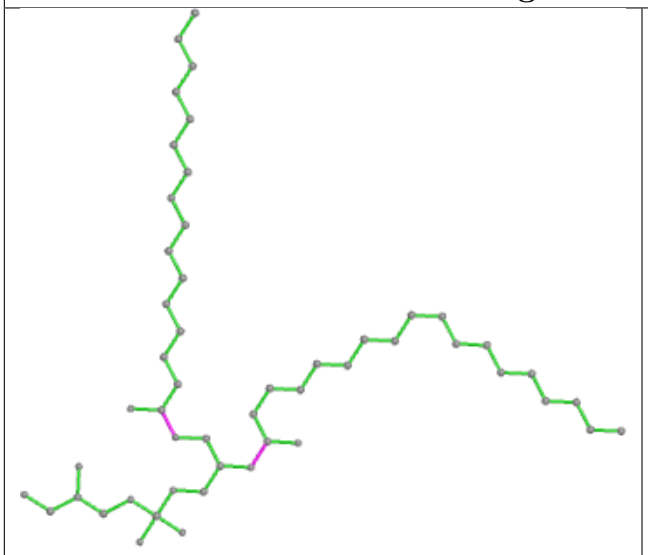


Torsions



Rings

Ligand PGW B 403



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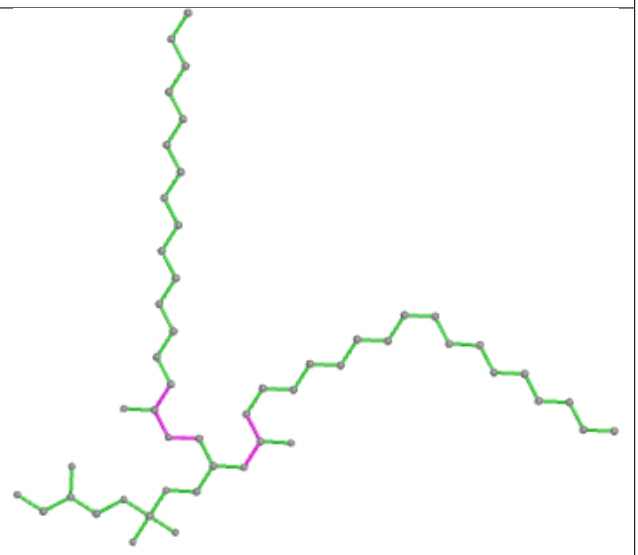

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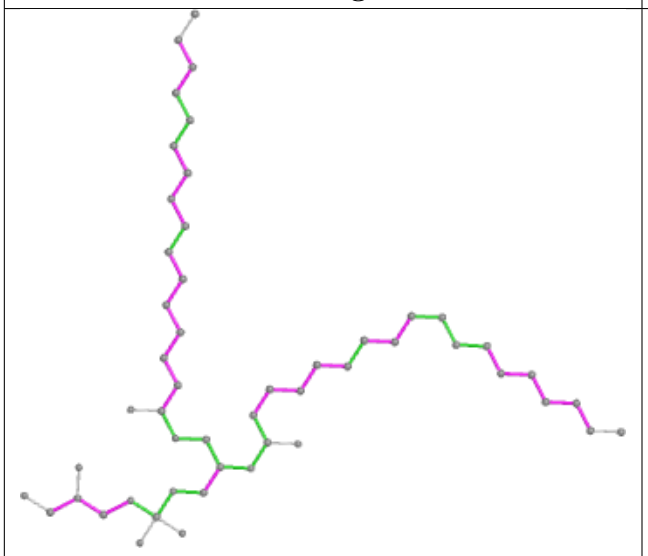

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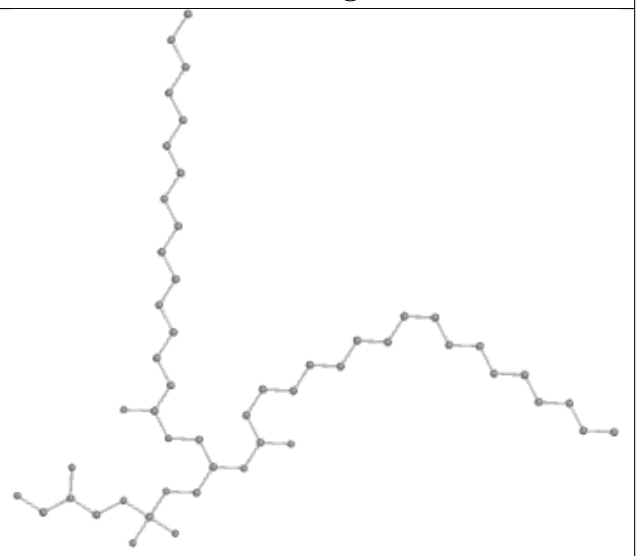
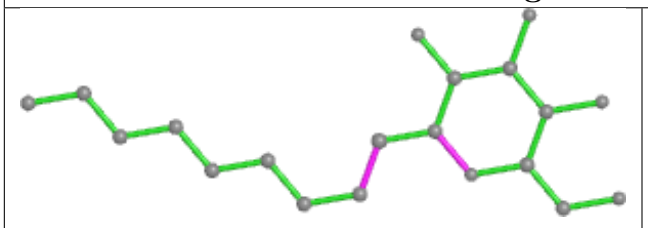
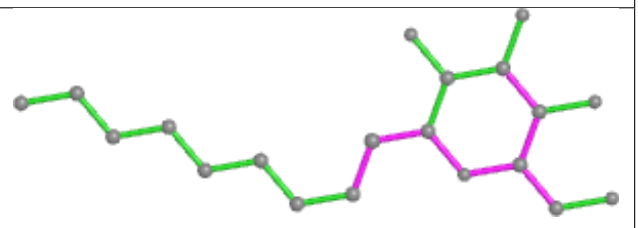


Rings

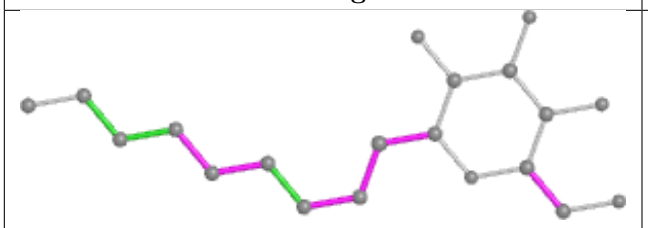
Ligand SOG A 409



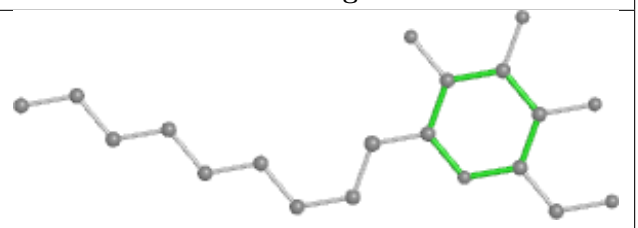
Bond lengths



Bond angles

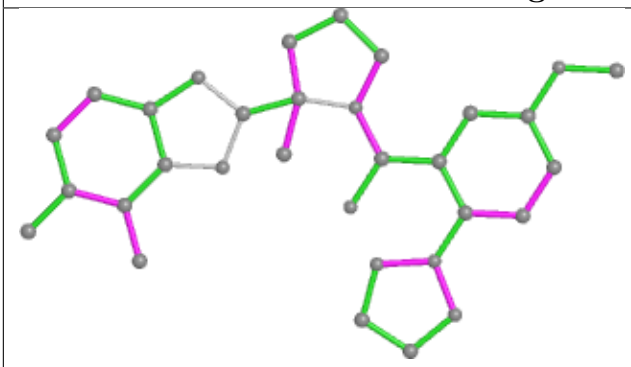


Torsions

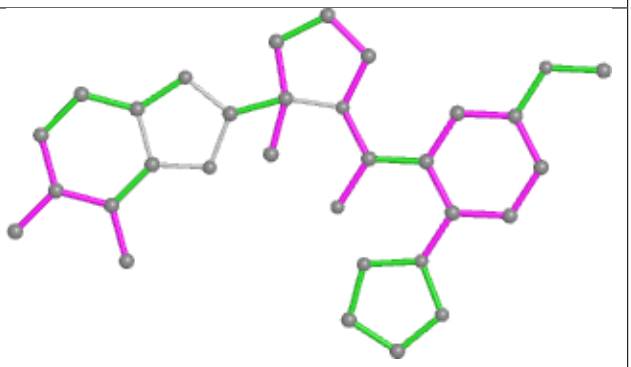


Rings

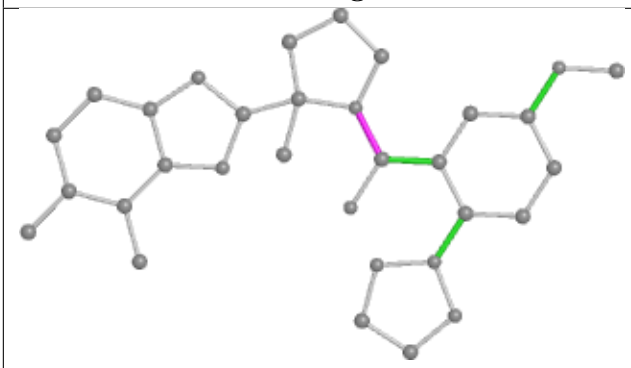
Ligand NS2 A 401



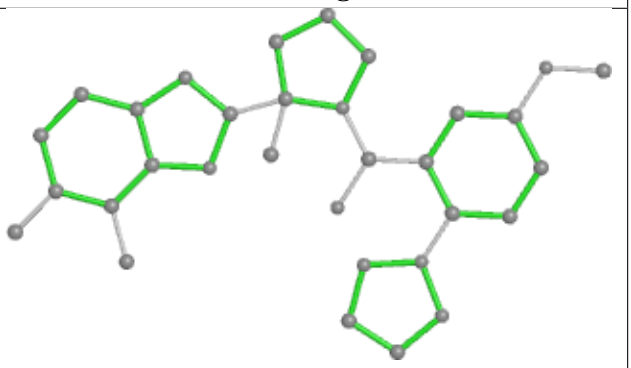
Bond lengths



Bond angles

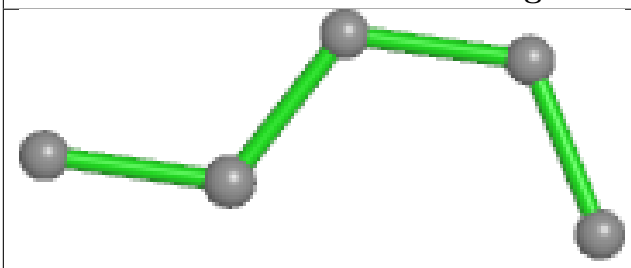


Torsions



Rings

Ligand SOG B 407



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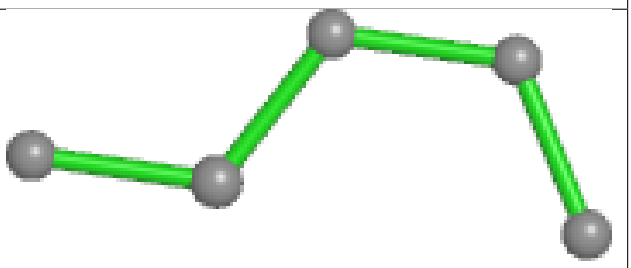

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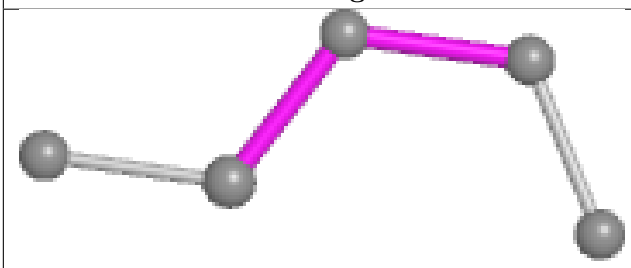

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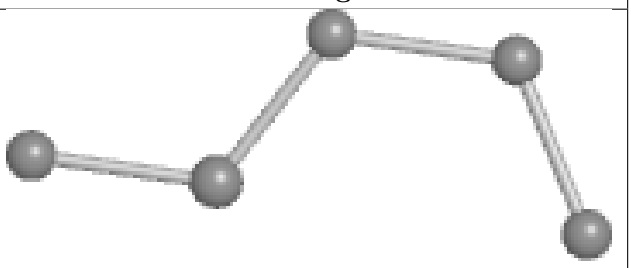

Rings

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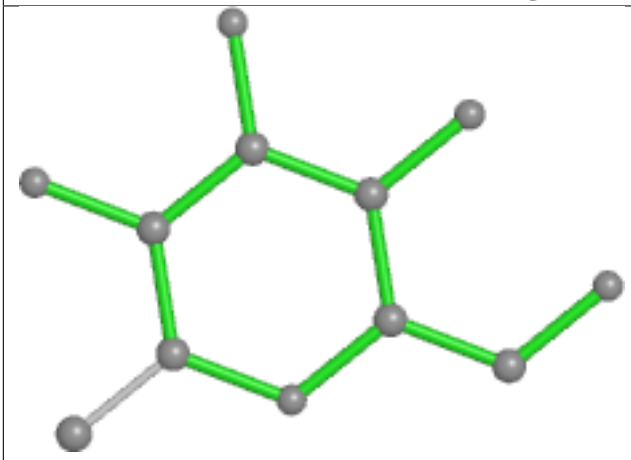

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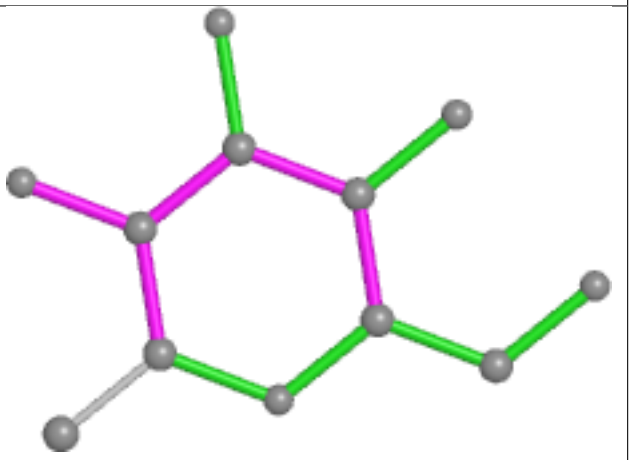

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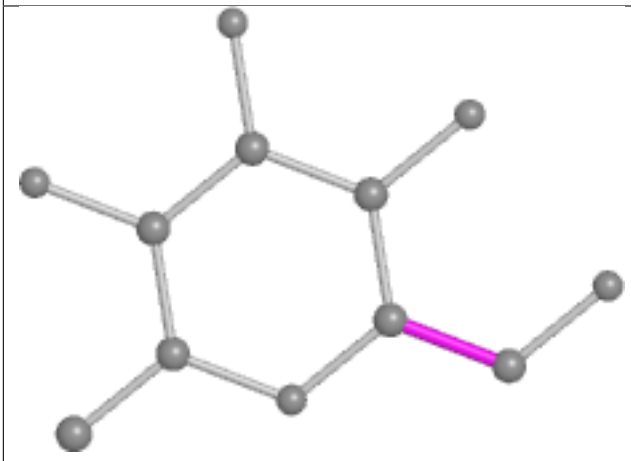

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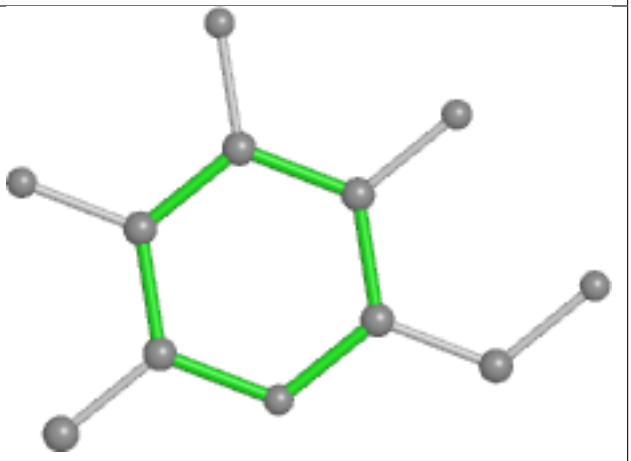
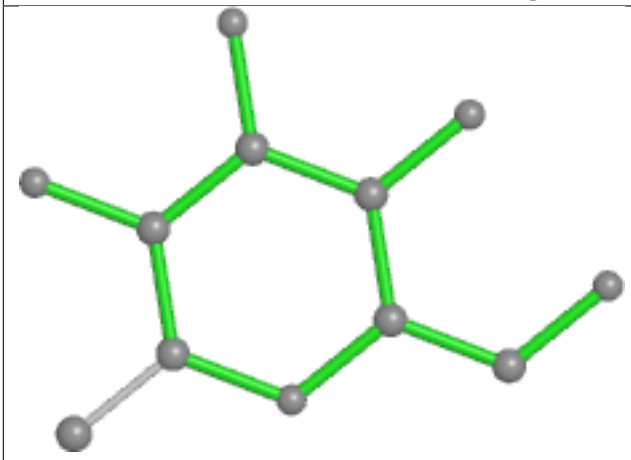


Rings

Ligand SOG B 409



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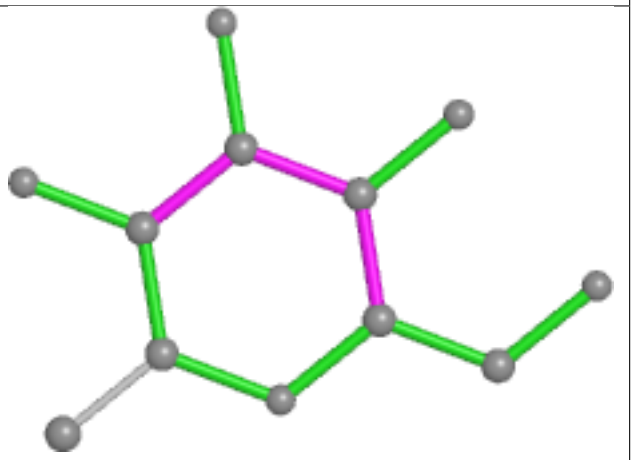

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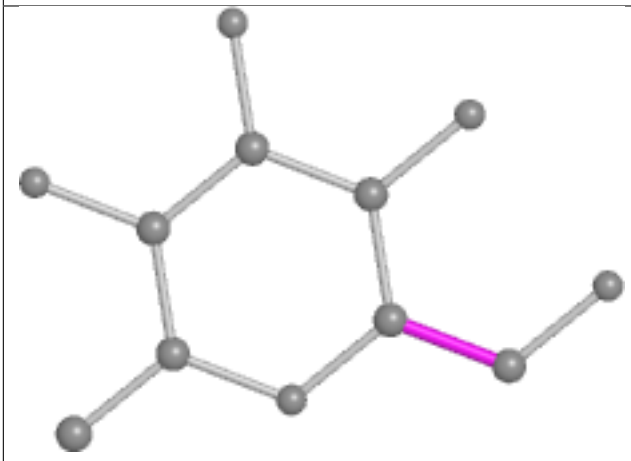

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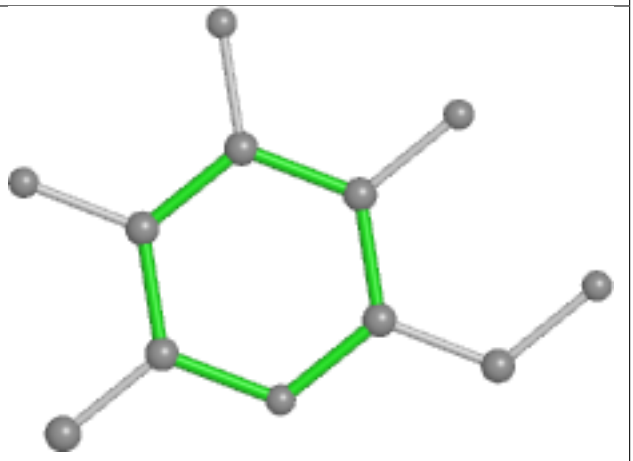
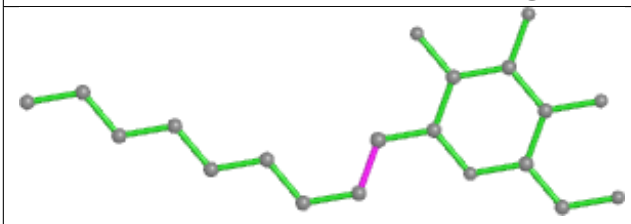


Rings

Ligand SOG A 406



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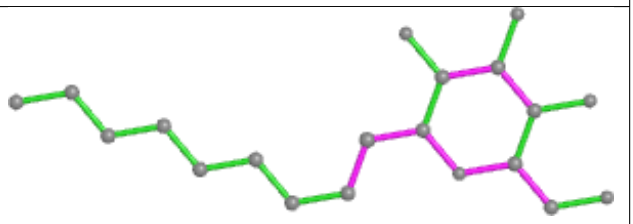
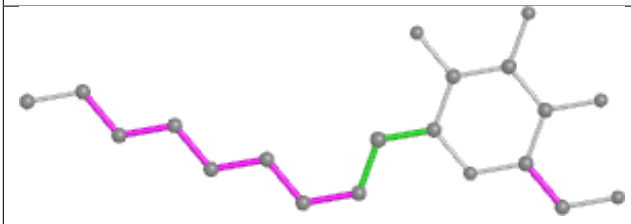


Bond angles



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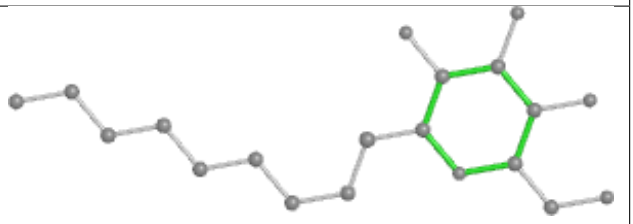
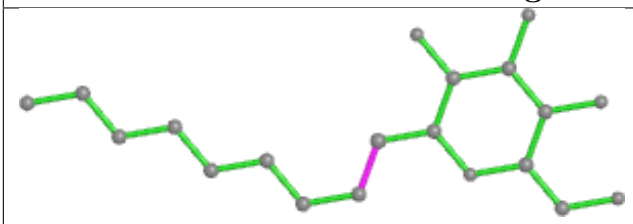


Rings

Ligand SOG B 404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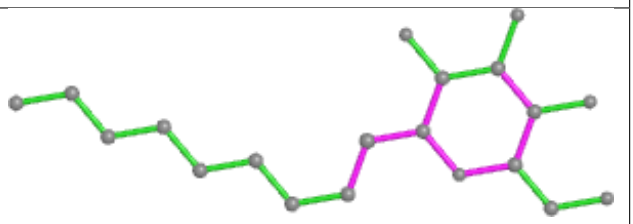
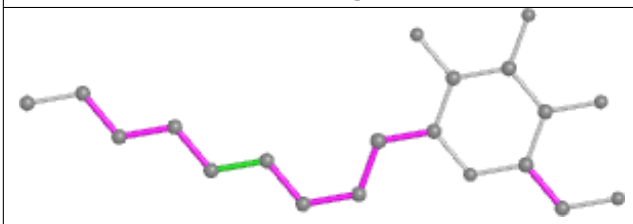
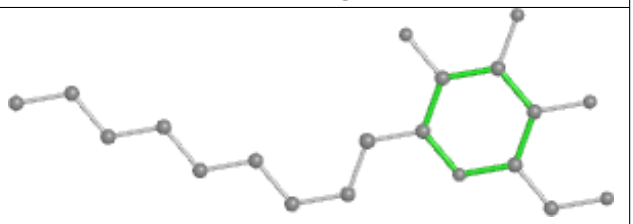
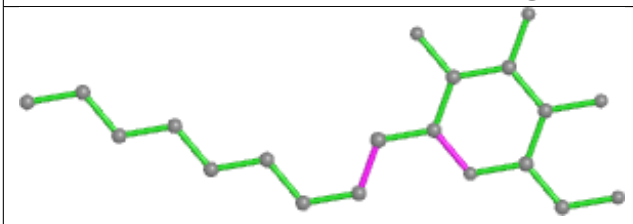
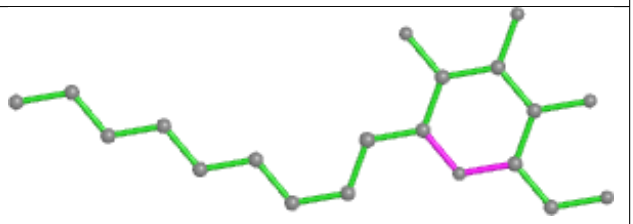

Bond angles

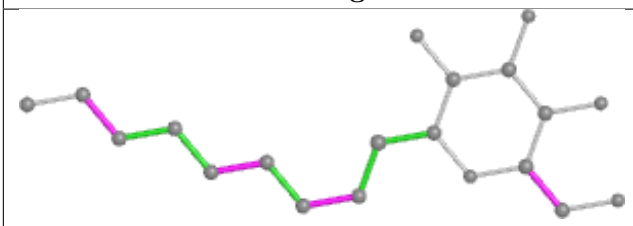

Torsions


Rings

Ligand SOG A 410


Bond lengths


Bond angles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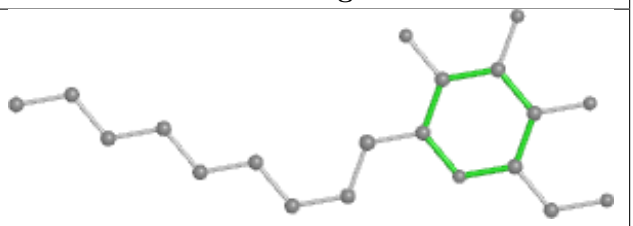
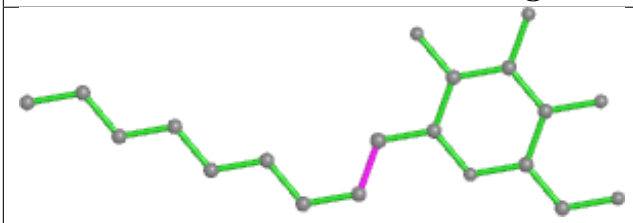

Rings

Ligand SOG B 405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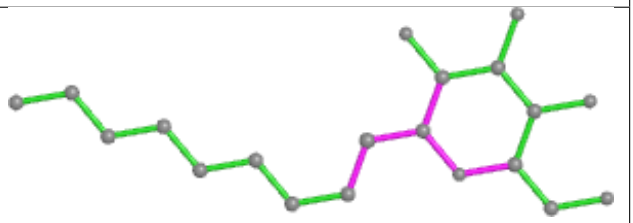
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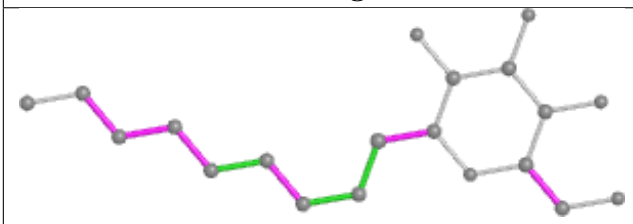
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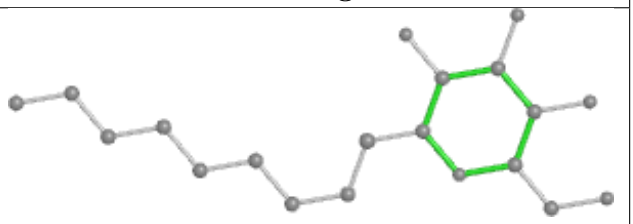
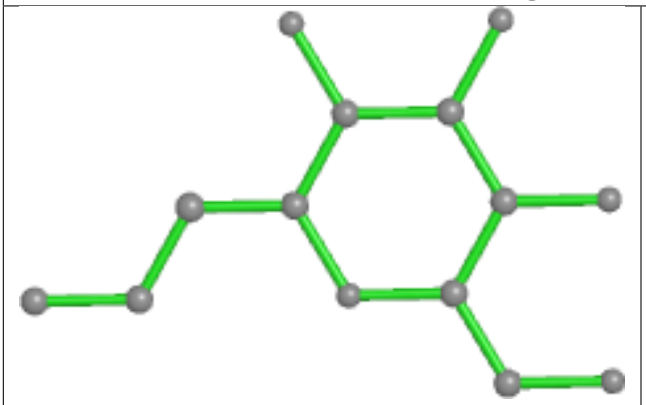
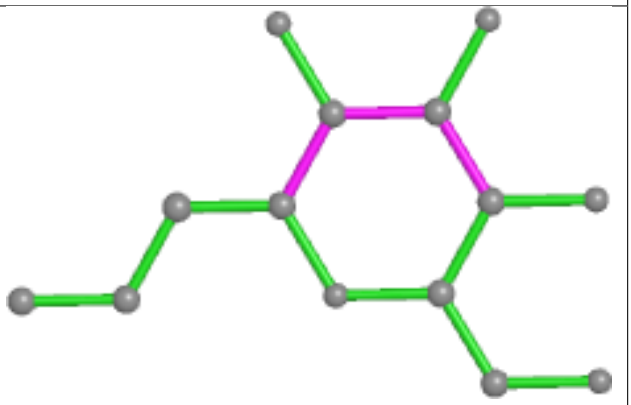

Rings

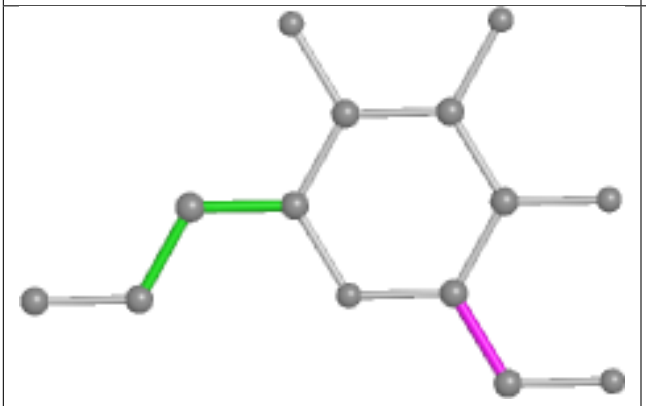
Ligand SOG A 408



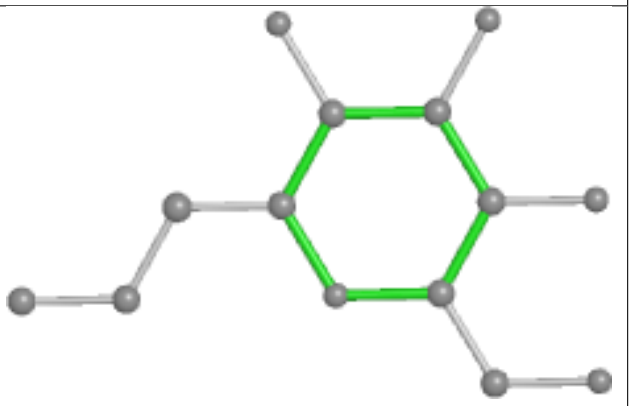
Bond lengths



Bond angles

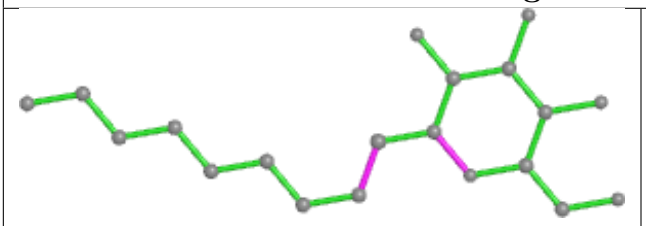


Torsions

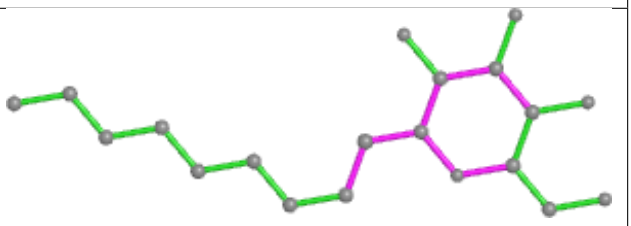


Rings

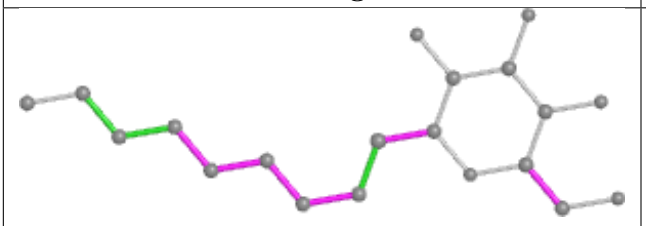
Ligand SOG A 407



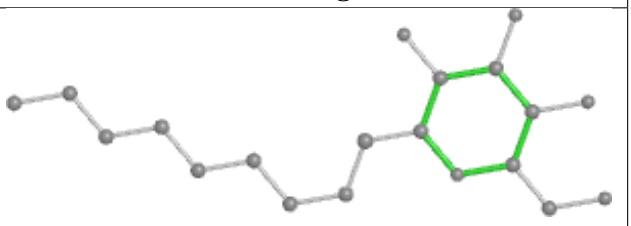
Bond lengths



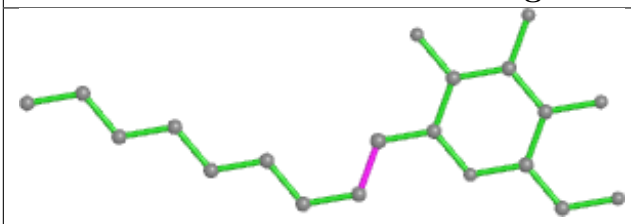
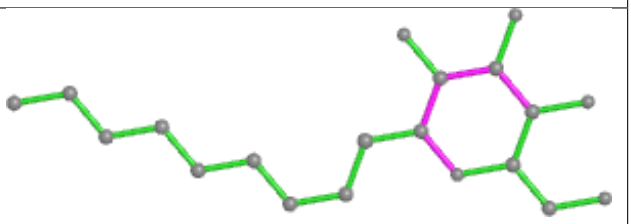
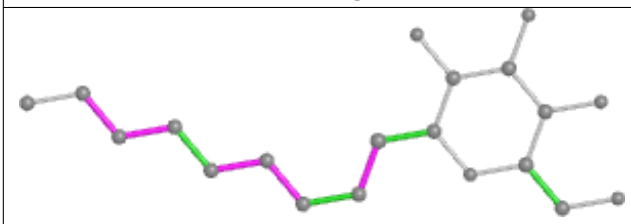
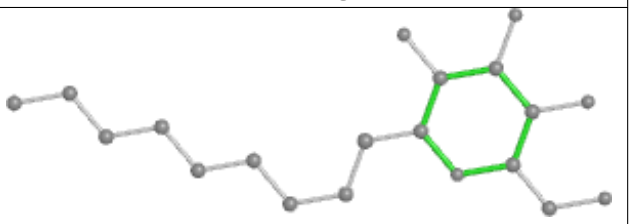
Bond angles

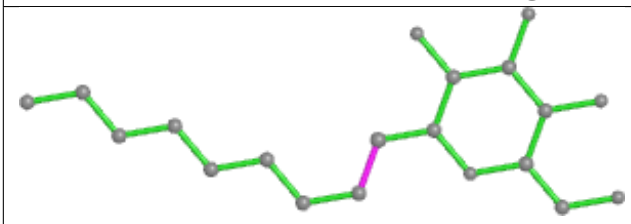
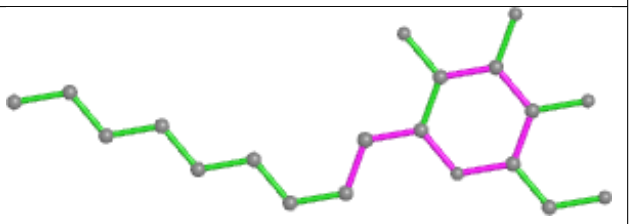
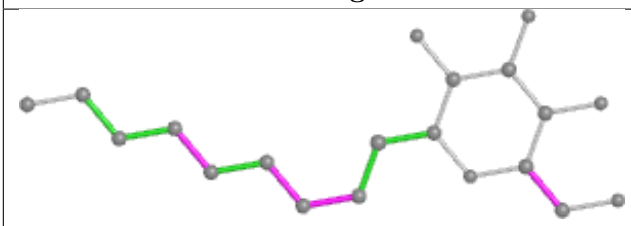
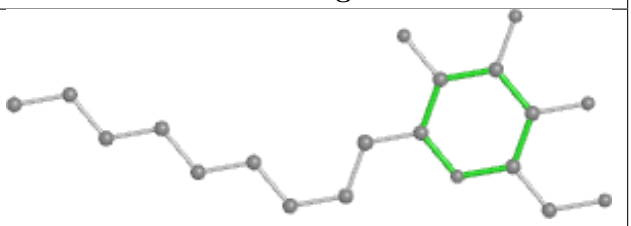


Torsions

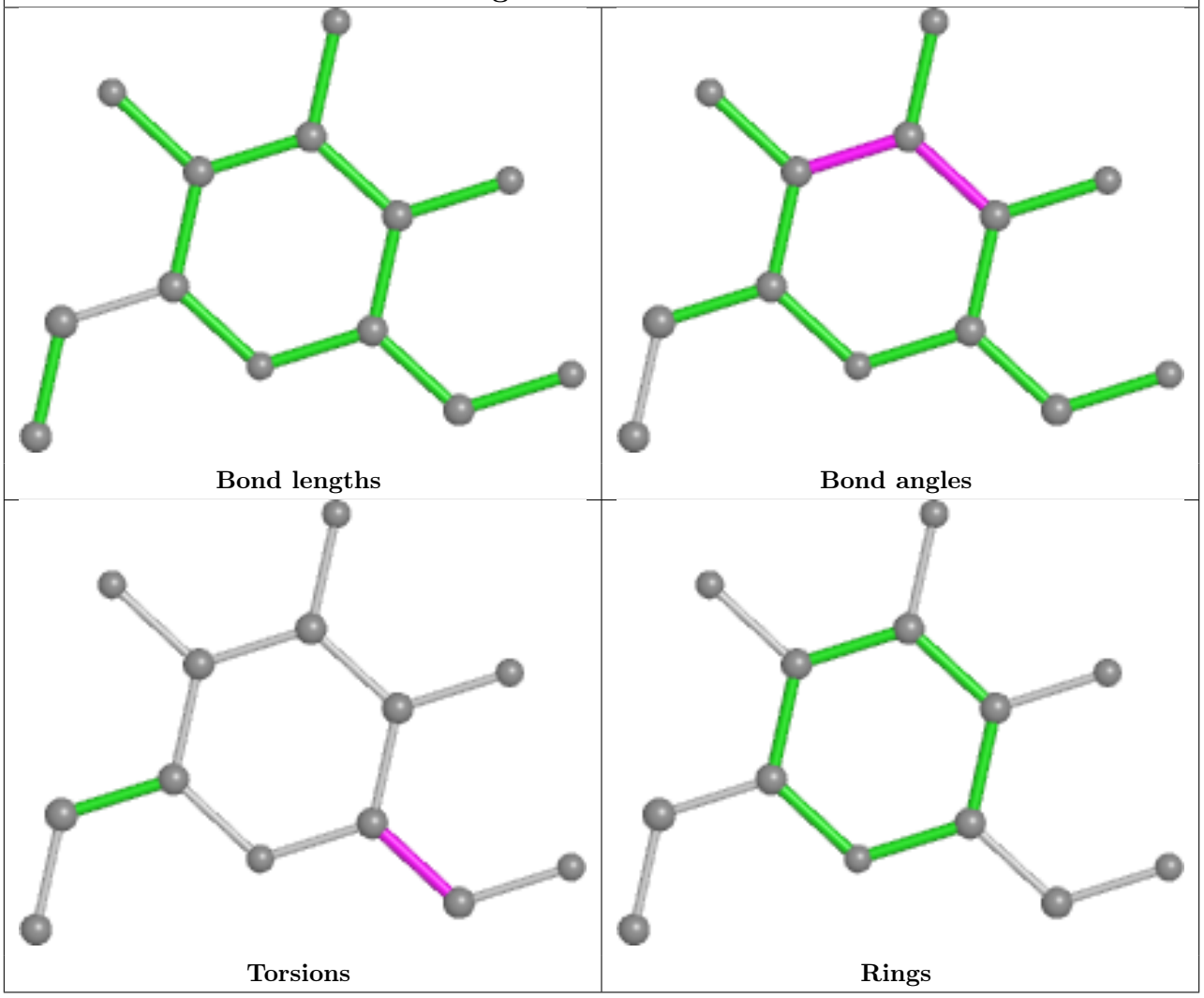


Rings

Ligand SOG B 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SOG A 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SOG B 406



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.

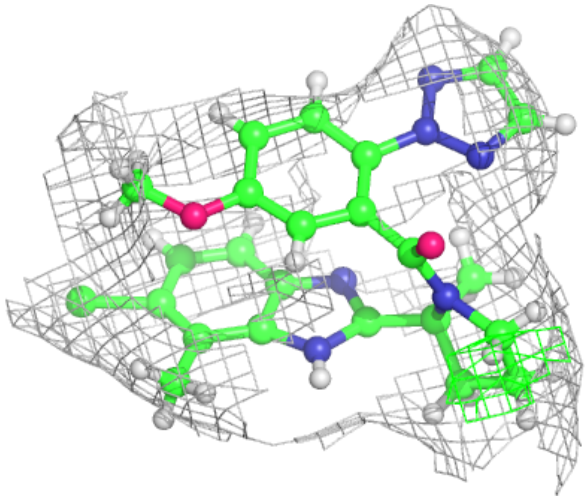
6.4 Ligands

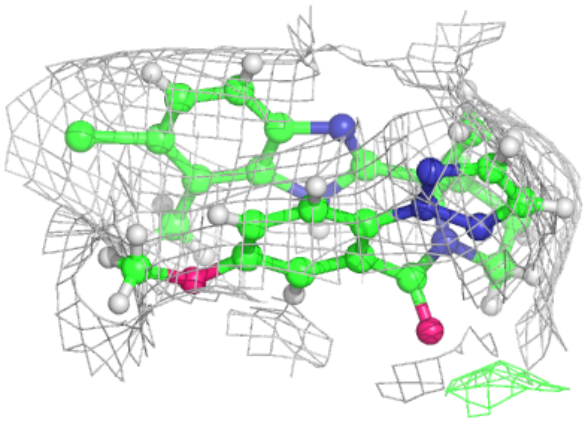
Unable to reproduce the depositors R factor - this section is therefore empty.

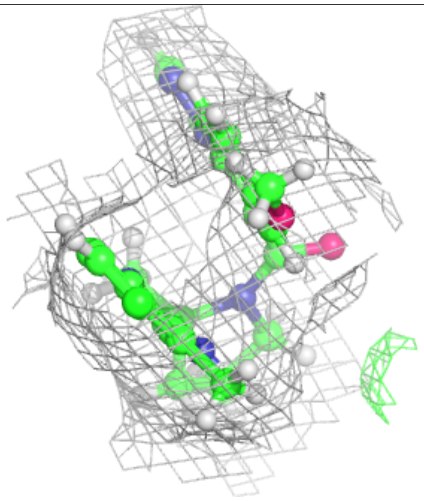
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS2 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)

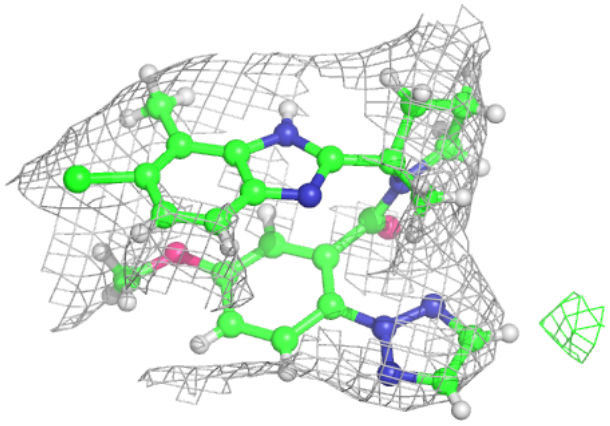


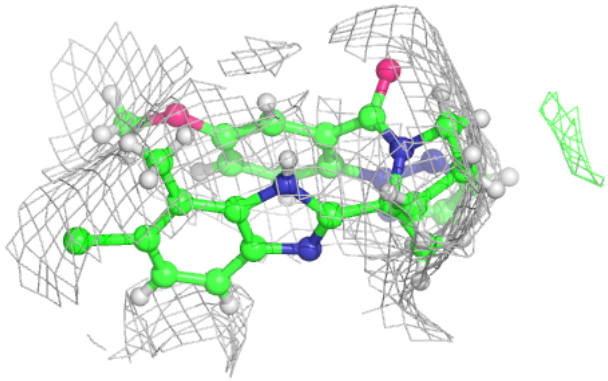


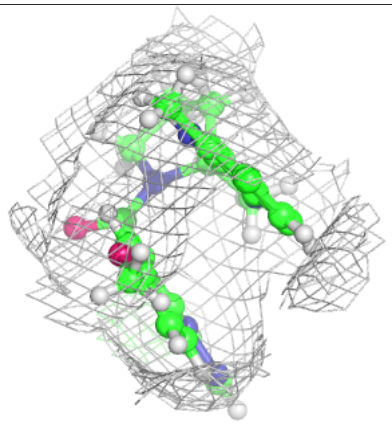


Electron density around NS2 B 401:

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

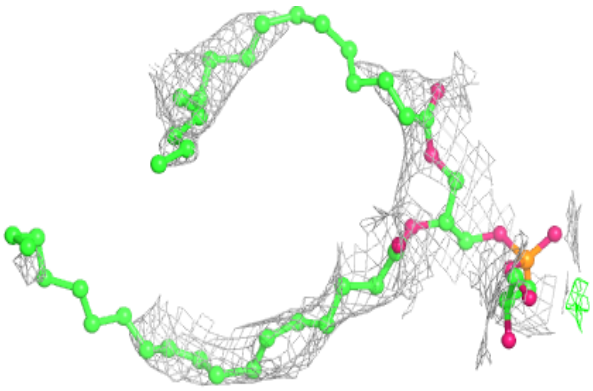


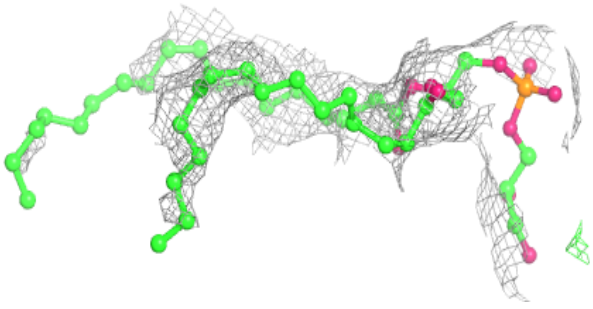




Electron density around PGW A 404:

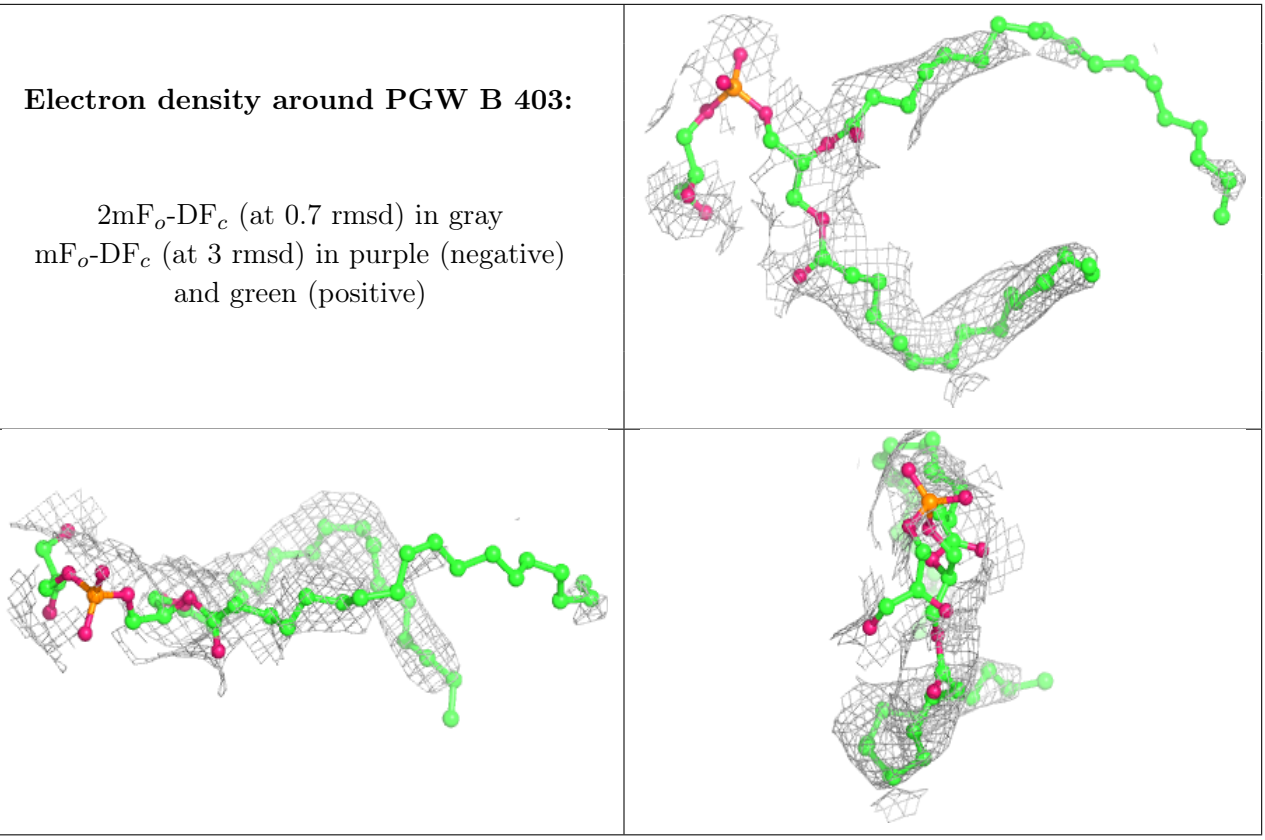
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





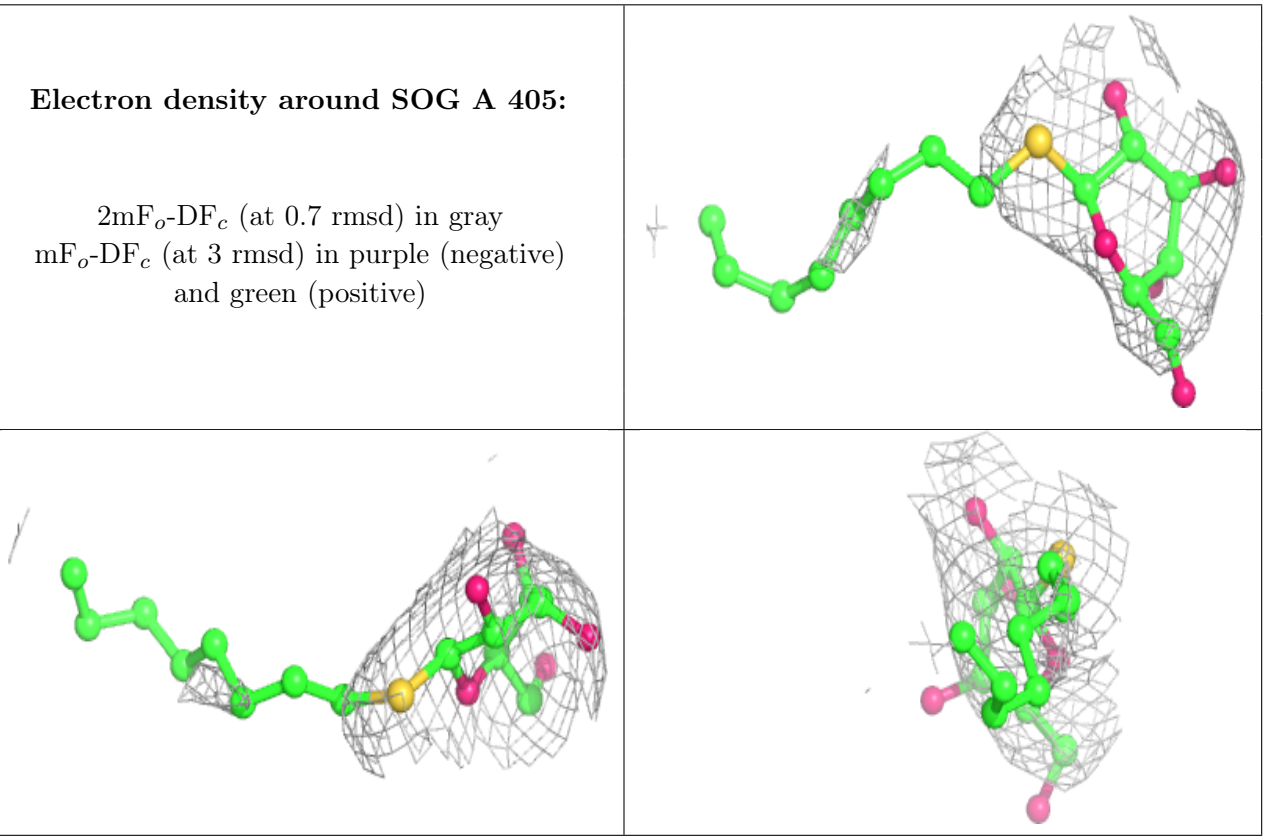
Electron density around PGW B 403:

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



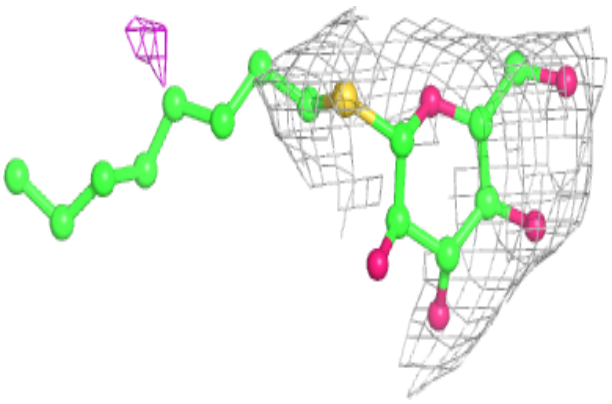
Electron density around SOG A 405:

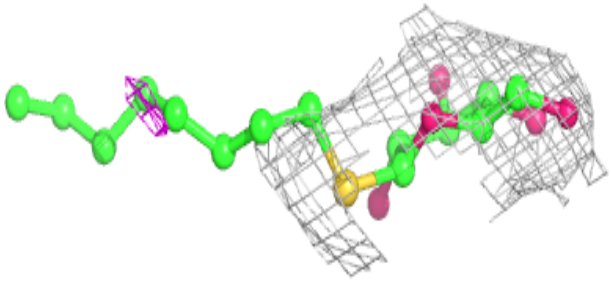
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

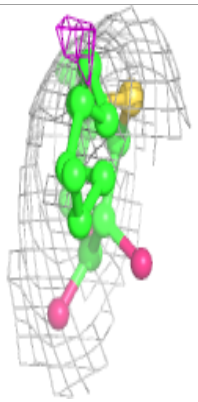


Electron density around SOG A 406:

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

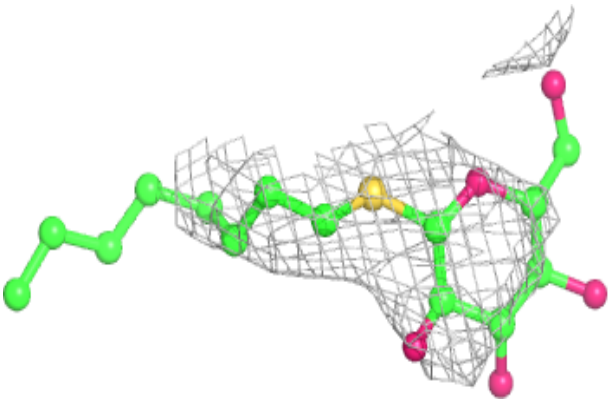


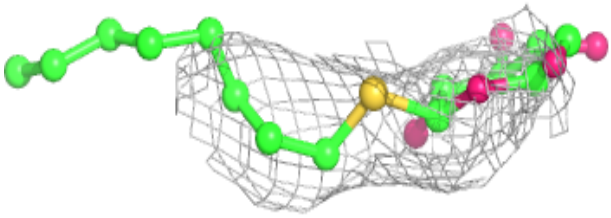


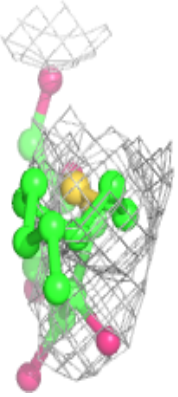


Electron density around SOG A 407:

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

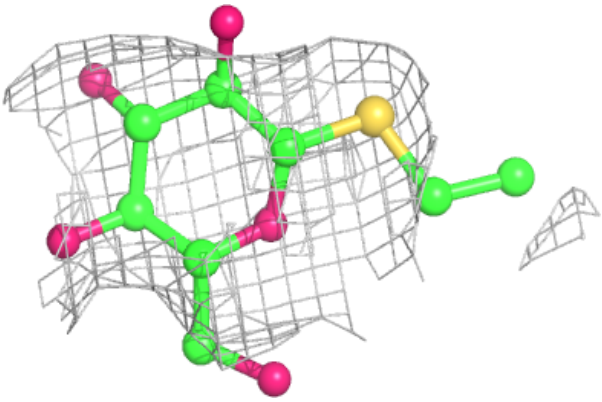


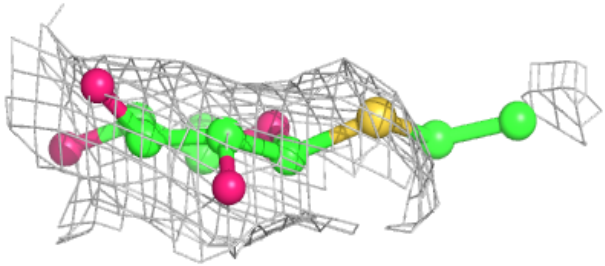


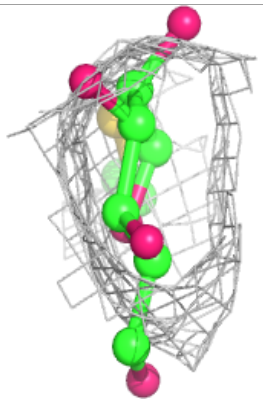


Electron density around SOG A 408:

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

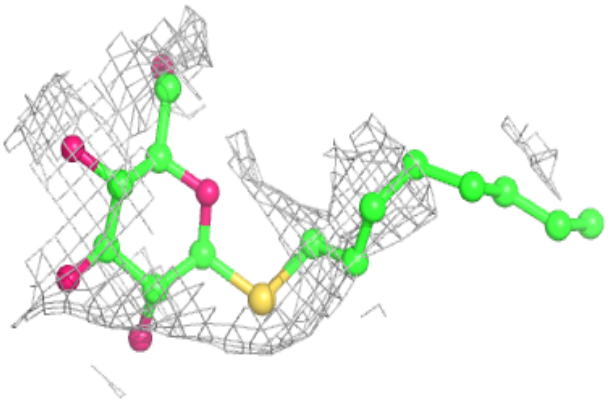


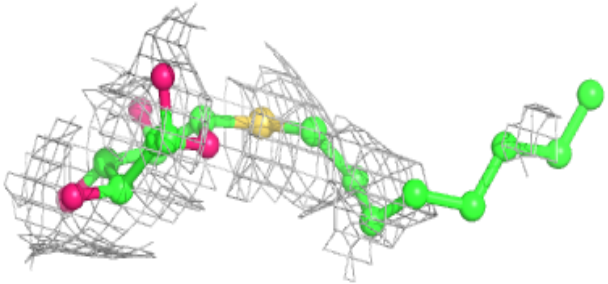


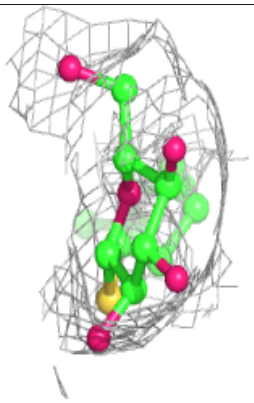


Electron density around SOG A 409:

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

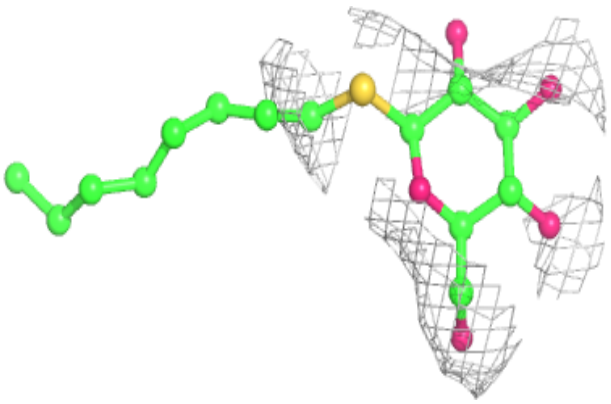


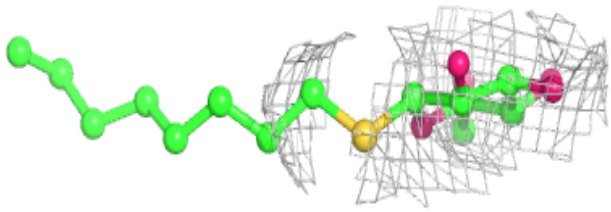


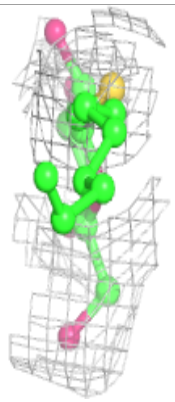


Electron density around SOG A 410:

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

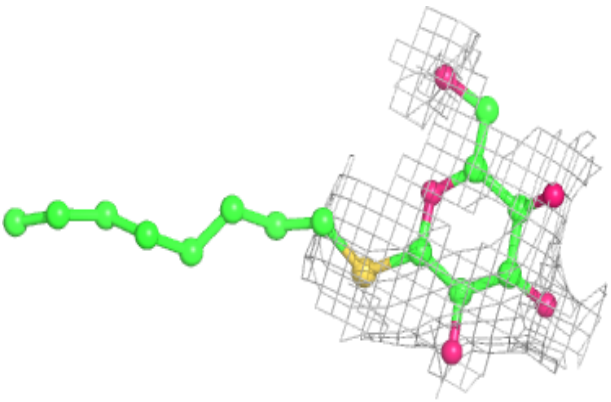


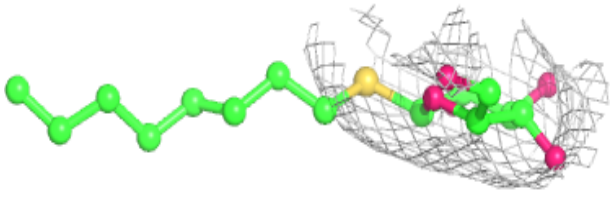


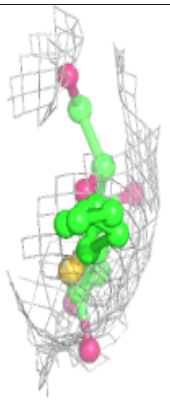


Electron density around SOG A 411:

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

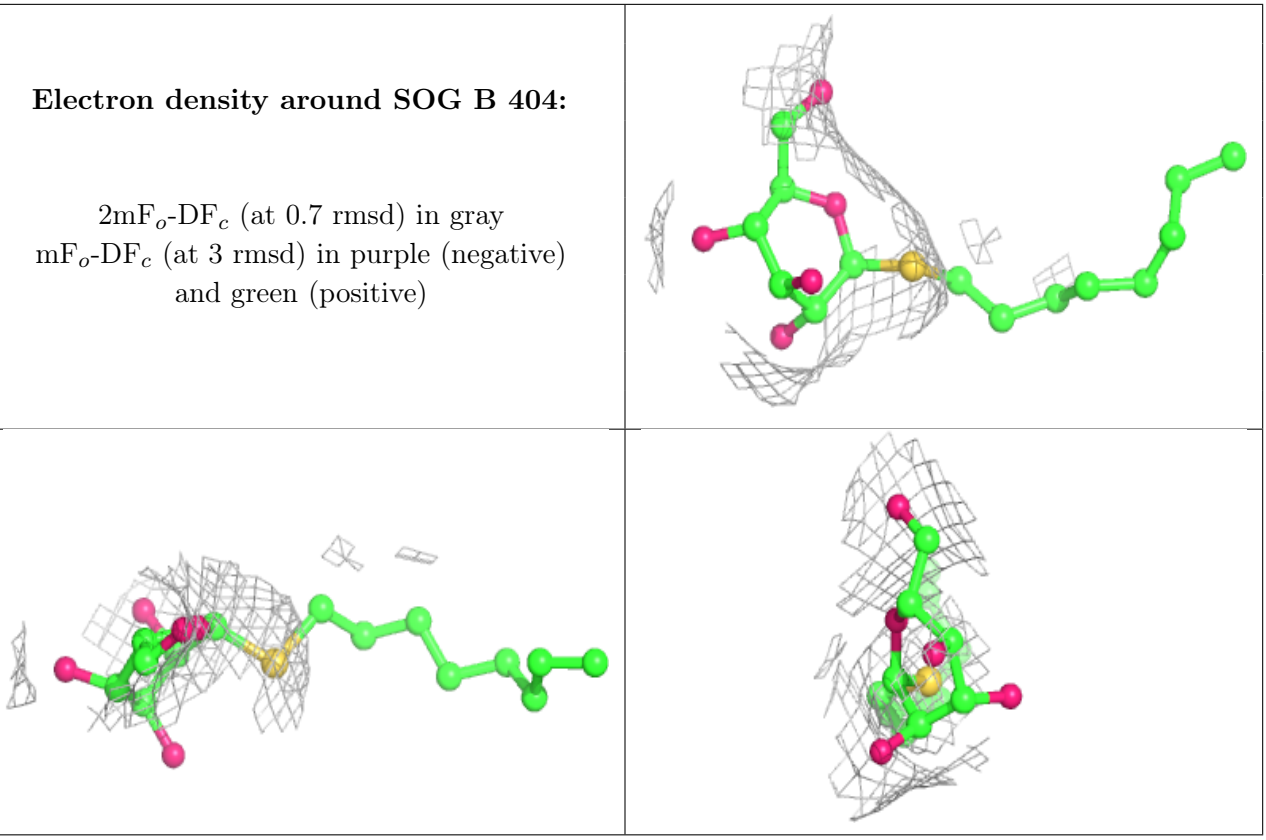






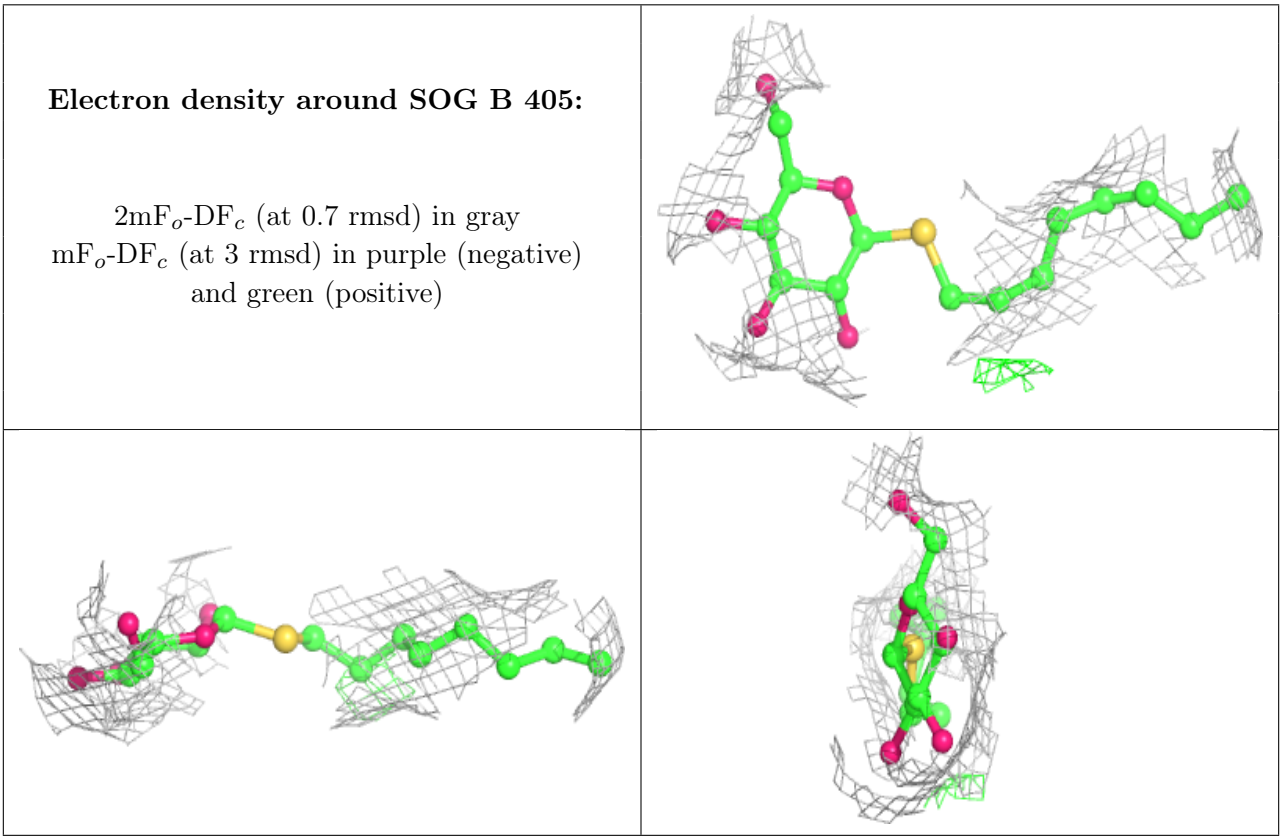
Electron density around SOG B 404:

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



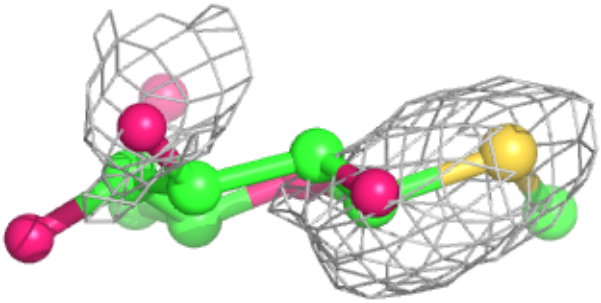
Electron density around SOG B 405:

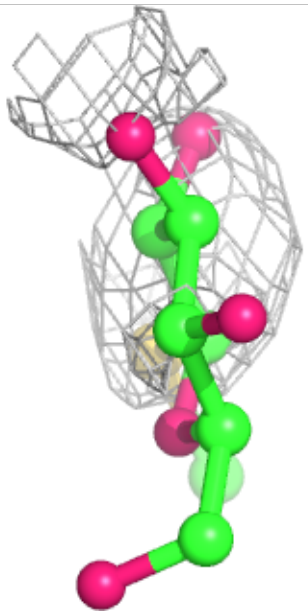
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SOG B 406:

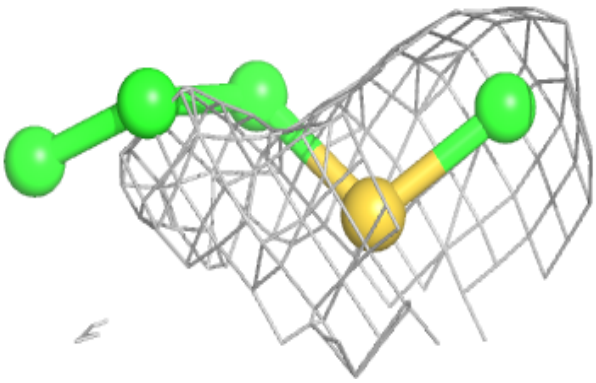
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

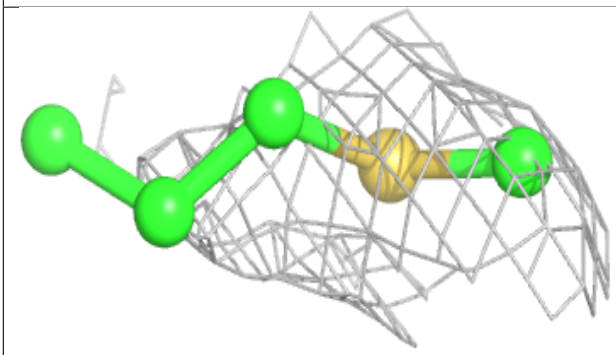


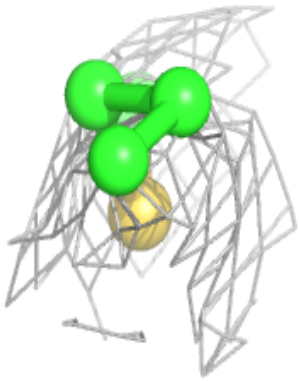


Electron density around SOG B 407:

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

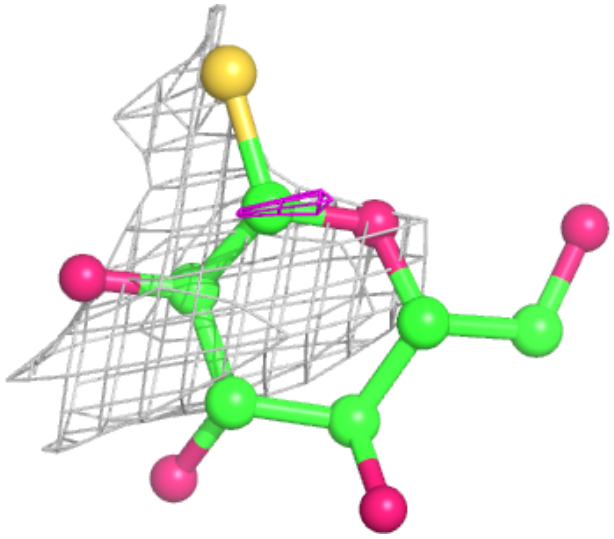


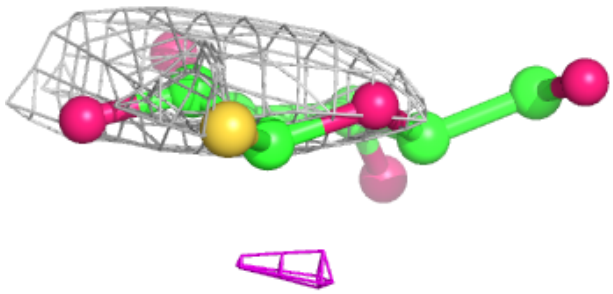


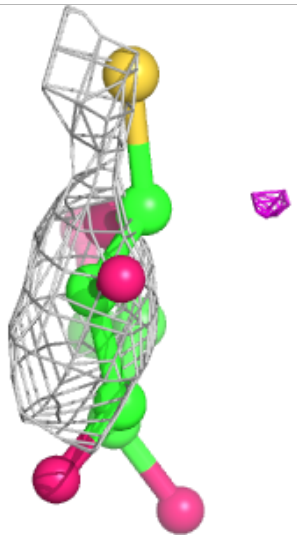


Electron density around SOG B 408:

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

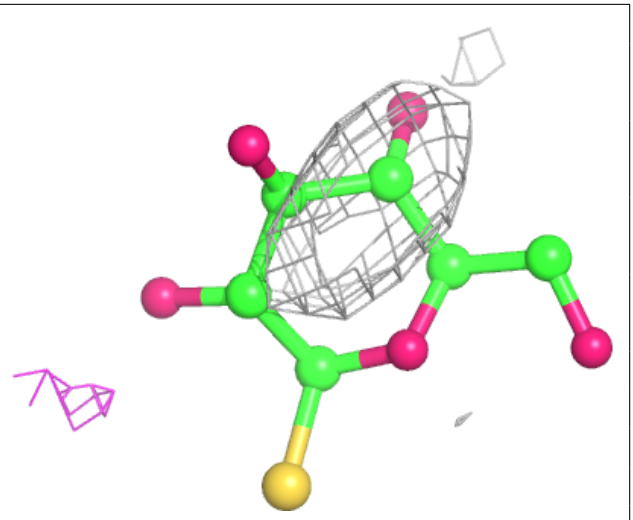


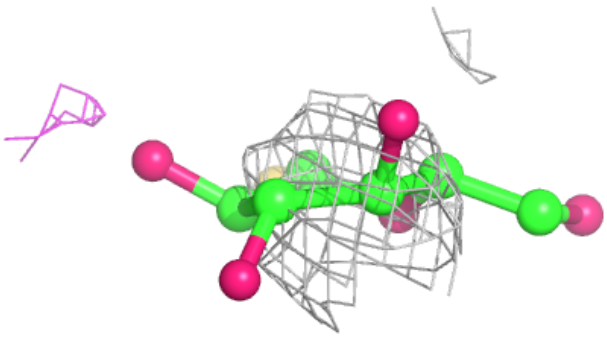


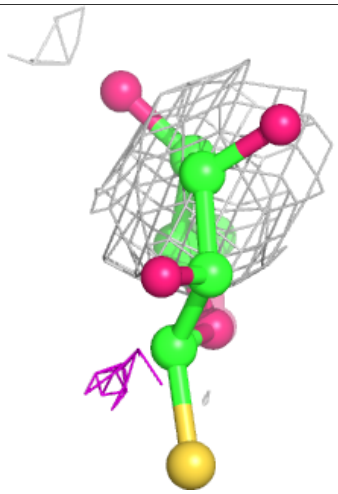


Electron density around SOG B 409:

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

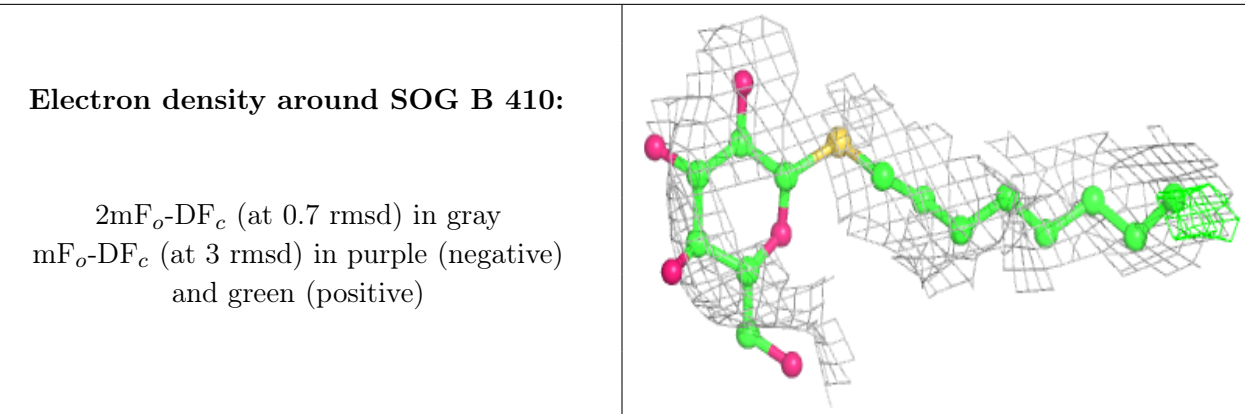


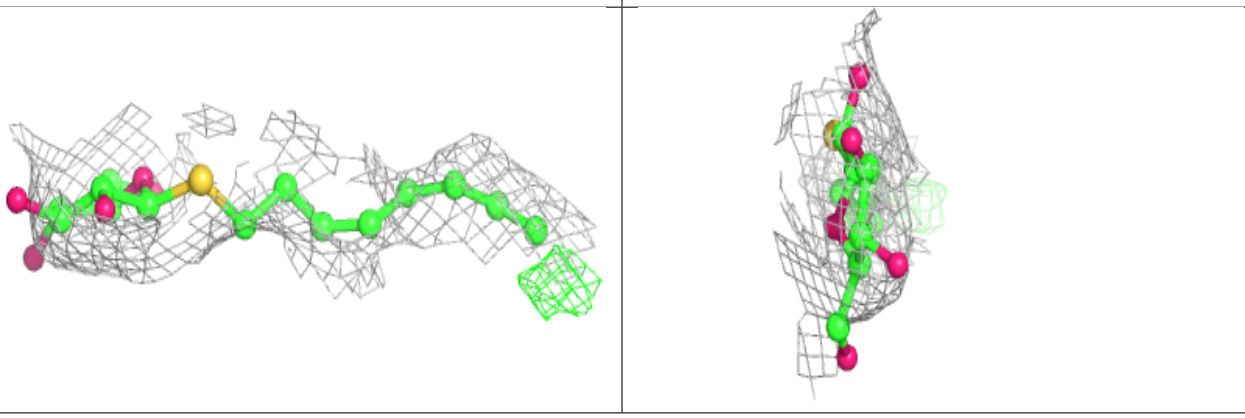




Electron density around SOG B 410:

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





6.5 Other polymers (i)

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