Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 02:05 am GMT

PDB ID	:	6TQ7
Title	:	Crystal structure of the Orexin-1 receptor in complex with SB-334867
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	:	2019-12-16
Resolution	:	2.66 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 (i)) were used in the production of this report:

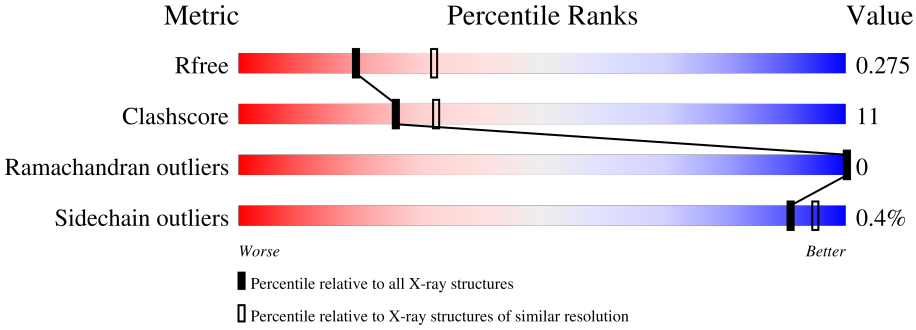
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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	65% 17% 18%
1	B	368	65% 19% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SOG	A	405	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5337 atoms, of which 52 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2386	1581	399	389	17	0	0	0
1	B	311	2492	1654	412	409	17	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

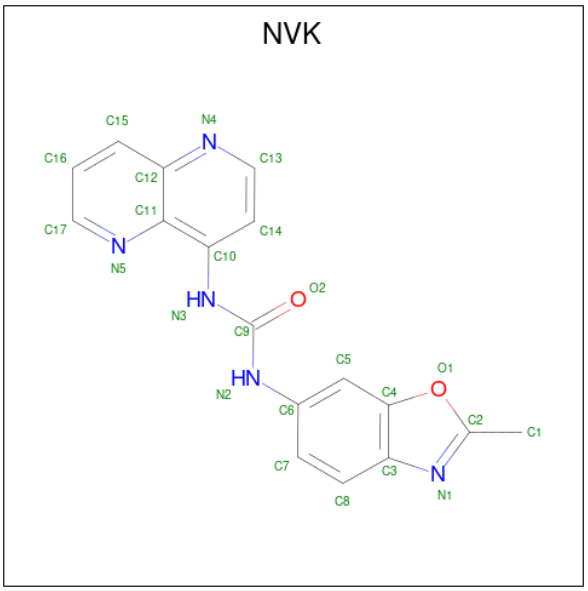
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU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

Continued on next page...

Continued from previous page...

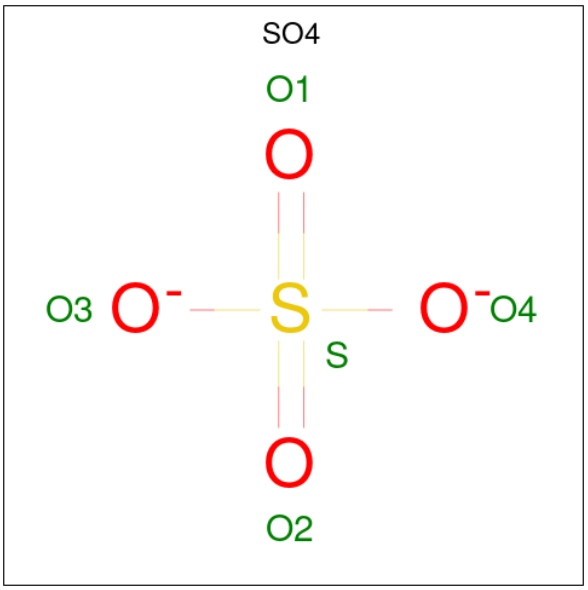
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered 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 1-(2-methyl-1,3-benzoxazol-6-yl)-3-(1,5-naphthyridin-4-yl)urea (three-letter code: NVK) (formula: $C_{17}H_{13}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



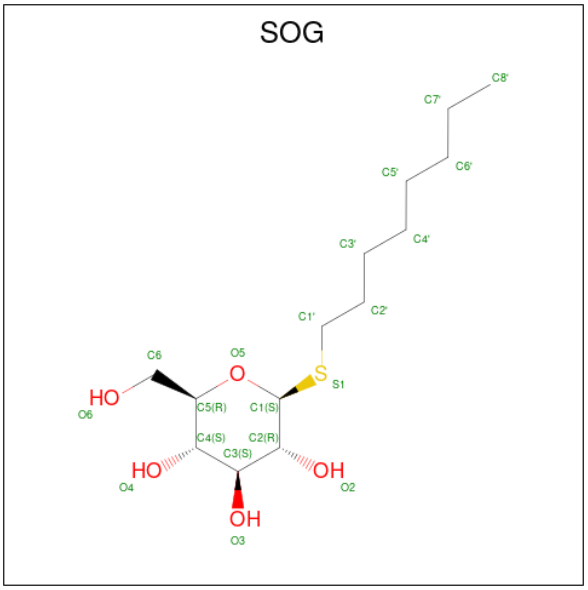
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	37	17	13	5	2	0	0
			Total	C	H	N	O		
2	A	1	37	17	13	5	2	0	0
			Total	C	H	N	O		
2	B	1	37	17	13	5	2	0	0
			Total	C	H	N	O		
2	B	1	37	17	13	5	2	0	0

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



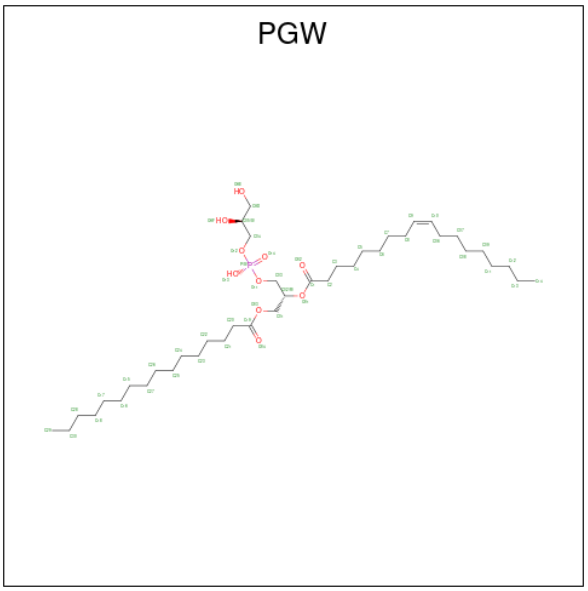
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C O S 20 14 5 1	0	0
4	A	1	Total C S 7 6 1	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 4 4	0	0
4	B	1	Total C O S 20 14 5 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



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

- Molecule 6 is water.

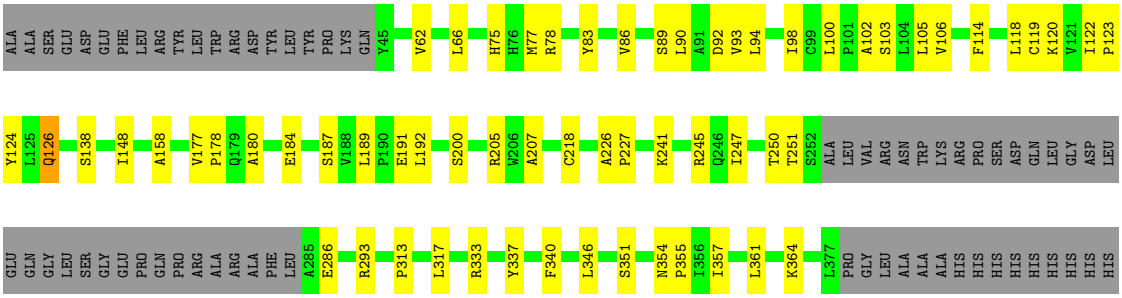
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	11	11	11	0	0
			Total	O		
6	B	8	8	8	0	0

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.

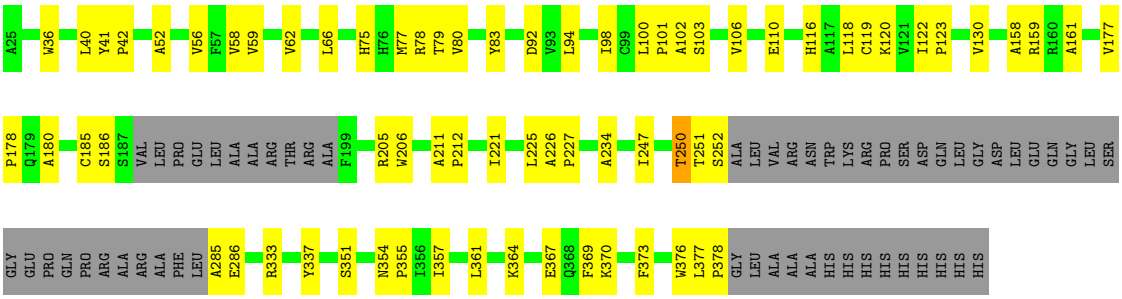
• Molecule 1: Orexin receptor type 1

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	59.77Å 148.24Å 71.67Å 90.00° 112.17° 90.00°	Depositor
Resolution (Å)	33.92 – 2.66 33.92 – 2.51	Depositor EDS
% Data completeness (in resolution range)	58.4 (33.92-2.66) 67.4 (33.92-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.220 , 0.255 0.247 , 0.275	Depositor DCC
R_{free} test set	1696 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SOG, SO4, NVK, PGW

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	0.32	1/2452 (0.0%)	0.45	0/3345
1	B	0.27	0/2564	0.43	0/3496
All	All	0.29	1/5016 (0.0%)	0.44	0/6841

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLN	CG-CD	8.59	1.70	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	0	2453	57	0
1	B	2492	0	2535	52	0
2	A	48	26	0	1	0
2	B	48	26	0	2	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	95	0	128	14	0
4	B	80	0	112	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	51	0	76	3	0
5	B	51	0	76	2	0
6	A	11	0	0	0	0
6	B	8	0	0	0	0
All	All	5285	52	5380	112	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 11.

All (112) 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:251:THR:HB	1:B:286:GLU:HG2	1.37	1.06
1:A:241:LYS:HD2	1:A:245:ARG:HG3	1.34	1.06
1:B:377:LEU:HB3	1:B:378:PRO:HD2	1.38	1.03
1:A:333:ARG:CG	1:A:337:TYR:CE2	2.51	0.94
1:A:333:ARG:HG3	1:A:337:TYR:CE2	2.09	0.88
1:A:333:ARG:HG2	1:A:337:TYR:CE2	2.16	0.79
1:B:116:HIS:CD2	1:B:185:CYS:HB3	2.19	0.78
1:A:247:ILE:HG13	1:A:250:THR:HG23	1.71	0.71
1:A:333:ARG:CG	1:A:337:TYR:HE2	2.01	0.71
1:A:184:GLU:OE2	4:A:405:SOG:H5'2	1.91	0.71
1:B:377:LEU:HB3	1:B:378:PRO:CD	2.19	0.70
1:A:89:SER:O	1:A:93:VAL:HG22	1.92	0.69
1:A:247:ILE:HG13	1:A:250:THR:CG2	2.22	0.69
1:B:75:HIS:HA	1:B:78:ARG:CD	2.21	0.69
1:A:333:ARG:HE	1:A:337:TYR:HE2	1.39	0.69
1:B:75:HIS:HA	1:B:78:ARG:HD2	1.75	0.69
1:B:376:TRP:CE3	1:B:377:LEU:HG	2.28	0.68
1:A:251:THR:OG1	1:A:286:GLU:HG3	1.95	0.67
1:A:184:GLU:OE2	4:A:405:SOG:C5'	2.42	0.67
1:A:189:LEU:HB2	1:A:192:LEU:HD13	1.78	0.66
1:A:100:LEU:O	1:A:103:SER:HB2	1.96	0.66
1:B:250:THR:HG22	1:B:286:GLU:HB2	1.79	0.65
1:B:247:ILE:HD12	1:B:247:ILE:H	1.61	0.65
1:A:148:ILE:CD1	1:A:293:ARG:HD3	2.26	0.64
1:A:205:ARG:O	4:A:405:SOG:H3'2	1.96	0.64
1:A:187:SER:HA	1:A:200:SER:HA	1.77	0.64
1:B:377:LEU:CB	1:B:378:PRO:HD2	2.23	0.64
1:B:251:THR:HB	1:B:286:GLU:CG	2.22	0.63
1:B:251:THR:HG22	1:B:285:ALA:H	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:406:SOG:S1	4:A:407:SOG:H3	2.41	0.61
1:B:36:TRP:HA	1:B:40:LEU:HB2	1.85	0.58
1:B:118:LEU:HB3	1:B:122:ILE:HD12	1.85	0.57
1:B:226:ALA:HB3	1:B:227:PRO:HD3	1.86	0.57
1:A:178:PRO:HD3	5:B:409:PGW:H20A	1.87	0.56
1:A:333:ARG:NE	1:A:337:TYR:HE2	2.04	0.56
1:A:226:ALA:HB3	1:A:227:PRO:HD3	1.87	0.55
1:A:333:ARG:HG3	1:A:337:TYR:CZ	2.41	0.55
1:B:75:HIS:HA	1:B:78:ARG:HD3	1.88	0.55
1:B:103:SER:HA	2:B:402:NVK:C1	2.35	0.55
1:A:105:LEU:HD12	1:A:114:PHE:HZ	1.71	0.55
1:B:77:MET:CE	1:B:364:LYS:HB3	2.36	0.55
4:A:405:SOG:O2	4:A:405:SOG:H1'2	2.07	0.55
1:A:177:VAL:N	1:A:178:PRO:HD2	2.22	0.53
1:A:83:TYR:HE2	1:A:158:ALA:HB1	1.73	0.53
1:A:94:LEU:HD12	1:A:98:ILE:HD12	1.91	0.53
1:B:177:VAL:N	1:B:178:PRO:HD2	2.23	0.53
1:A:78:ARG:HB3	1:A:83:TYR:CZ	2.43	0.53
1:B:130:VAL:HG11	2:B:402:NVK:C17	2.38	0.52
1:A:118:LEU:HB3	1:A:122:ILE:HD12	1.92	0.52
1:B:94:LEU:HD12	1:B:98:ILE:HD12	1.90	0.52
1:A:103:SER:HA	2:A:402:NVK:C1	2.40	0.52
1:A:184:GLU:OE2	4:A:405:SOG:H5'1	2.10	0.51
1:B:367:GLU:HA	1:B:370:LYS:HB2	1.92	0.51
1:A:77:MET:HE1	1:A:364:LYS:HB3	1.93	0.51
1:B:77:MET:HE1	1:B:364:LYS:HB3	1.93	0.51
4:A:406:SOG:H3'1	4:A:407:SOG:O3	2.11	0.51
1:A:205:ARG:O	4:A:405:SOG:H2'1	2.11	0.51
1:A:75:HIS:HA	1:A:78:ARG:HH11	1.76	0.51
1:A:119:CYS:O	1:A:123:PRO:HG2	2.11	0.50
1:B:92:ASP:HB3	1:B:351:SER:HB3	1.93	0.50
1:A:92:ASP:HB3	1:A:351:SER:HB3	1.94	0.49
1:B:120:LYS:HE2	1:B:180:ALA:O	2.12	0.49
1:A:227:PRO:HG3	5:A:411:PGW:H14	1.93	0.49
1:B:116:HIS:NE2	1:B:185:CYS:O	2.46	0.49
1:A:189:LEU:O	1:A:192:LEU:HB2	2.13	0.49
1:A:120:LYS:HE3	1:A:180:ALA:O	2.13	0.48
1:B:119:CYS:O	1:B:123:PRO:HG2	2.13	0.48
1:B:357:ILE:HG23	1:B:361:LEU:HD12	1.96	0.48
1:A:191:GLU:H	1:A:191:GLU:CD	2.17	0.47
1:A:86:VAL:O	1:A:90:LEU:HD13	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HG23	1:A:361:LEU:HD12	1.95	0.47
4:A:406:SOG:H8'1	1:B:221:ILE:HD11	1.97	0.47
1:A:205:ARG:O	4:A:405:SOG:C2'	2.63	0.46
1:B:52:ALA:O	1:B:56:VAL:HG22	2.16	0.46
1:B:333:ARG:HD3	1:B:337:TYR:CE2	2.49	0.46
1:B:41:TYR:N	1:B:42:PRO:HD2	2.30	0.46
1:A:148:ILE:HD12	1:A:293:ARG:HD3	1.95	0.46
1:B:102:ALA:O	1:B:106:VAL:HG23	2.16	0.46
1:A:102:ALA:O	1:A:106:VAL:HG23	2.16	0.46
1:A:207:ALA:HB2	4:A:405:SOG:H1'1	1.98	0.45
1:B:251:THR:HG22	1:B:252:SER:N	2.31	0.45
1:A:317:LEU:HB3	1:A:340:PHE:CE1	2.52	0.45
1:A:313:PRO:HG2	1:A:346:LEU:HD23	1.99	0.44
1:B:80:VAL:HG23	1:B:161:ALA:HB2	1.99	0.44
1:B:106:VAL:O	1:B:110:GLU:HA	2.17	0.44
1:A:241:LYS:CD	1:A:245:ARG:HG3	2.26	0.44
1:B:354:ASN:HB2	1:B:355:PRO:HD3	1.99	0.44
1:A:251:THR:HG1	1:A:286:GLU:HG3	1.83	0.44
5:A:411:PGW:H23	1:B:206:TRP:HZ3	1.83	0.43
1:A:354:ASN:HB2	1:A:355:PRO:HD3	2.00	0.43
1:B:79:THR:HG22	1:B:80:VAL:N	2.33	0.43
1:A:77:MET:CE	1:A:364:LYS:HB3	2.48	0.43
1:A:138:SER:HB3	5:A:411:PGW:H07	2.01	0.43
4:A:406:SOG:C8'	1:B:221:ILE:HD11	2.49	0.43
1:A:124:TYR:HB2	1:A:180:ALA:HB2	2.02	0.42
1:B:186:SER:HB3	1:B:205:ARG:NH2	2.35	0.41
1:B:211:ALA:N	1:B:212:PRO:HD2	2.35	0.41
1:B:62:VAL:O	1:B:66:LEU:HG	2.20	0.41
1:B:369:PHE:O	1:B:373:PHE:CD2	2.73	0.41
1:B:77:MET:HE2	1:B:364:LYS:HB3	2.02	0.41
1:B:100:LEU:HB3	1:B:101:PRO:HD3	2.01	0.41
1:A:62:VAL:O	1:A:66:LEU:HG	2.20	0.41
1:A:105:LEU:HD12	1:A:114:PHE:CZ	2.54	0.41
1:A:218:CYS:SG	1:B:225:LEU:HD23	2.60	0.41
1:B:159:ARG:HH11	1:B:159:ARG:HD2	1.77	0.41
4:A:405:SOG:O2	4:A:405:SOG:C1'	2.69	0.41
1:B:234:ALA:HB2	5:B:409:PGW:H24	2.02	0.41
1:A:205:ARG:O	4:A:405:SOG:C3'	2.65	0.41
1:A:333:ARG:HG2	1:A:337:TYR:CD2	2.55	0.41
1:B:120:LYS:NZ	4:B:406:SOG:H6'1	2.37	0.40
1:B:58:VAL:HG23	1:B:59:VAL:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TYR:HE2	1:B:158:ALA:HB1	1.87	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	299/368 (81%)	291 (97%)	8 (3%)	0	100	100
1	B	307/368 (83%)	298 (97%)	9 (3%)	0	100	100
All	All	606/736 (82%)	589 (97%)	17 (3%)	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	250/305 (82%)	249 (100%)	1 (0%)	91	95
1	B	261/305 (86%)	260 (100%)	1 (0%)	91	95
All	All	511/610 (84%)	509 (100%)	2 (0%)	91	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	250	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	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)

20 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	$\#\|Z\| > 2$
4	SOG	A	408	-	6,6,20	0.22	0	5,5,25	0.17	0
5	PGW	A	411	-	50,50,50	0.29	0	53,56,56	0.43	0
4	SOG	A	410	-	3,3,20	0.23	0	2,2,25	0.52	0
2	NVK	A	401	-	24,27,27	0.74	0	31,38,38	1.06	3 (9%)
5	PGW	B	409	-	50,50,50	0.28	0	53,56,56	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NVK	A	402	-	24,27,27	0.74	0	31,38,38	1.09	3 (9%)
4	SOG	A	407	-	20,20,20	0.32	0	24,25,25	0.44	0
4	SOG	B	406	-	20,20,20	0.26	0	24,25,25	0.50	0
4	SOG	A	405	-	20,20,20	0.19	0	24,25,25	0.81	2 (8%)
4	SOG	A	409	-	3,3,20	0.24	0	2,2,25	0.52	0
4	SOG	B	405	-	20,20,20	0.45	0	24,25,25	1.21	3 (12%)
4	SOG	B	408	-	20,20,20	0.38	0	24,25,25	0.52	0
4	SOG	A	404	-	20,20,20	0.32	0	24,25,25	0.72	0
3	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SOG	A	406	-	20,20,20	0.36	0	24,25,25	0.61	0
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.06	0
2	NVK	B	401	-	24,27,27	0.73	0	31,38,38	1.05	3 (9%)
4	SOG	B	407	-	20,20,20	0.21	0	24,25,25	0.32	0
3	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.06	0
2	NVK	B	402	-	24,27,27	0.73	0	31,38,38	1.08	3 (9%)

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	SOG	A	408	-	-	1/4/4/31	-
4	SOG	A	407	-	-	1/11/31/31	0/1/1/1
4	SOG	B	408	-	-	2/11/31/31	0/1/1/1
4	SOG	A	405	-	-	5/11/31/31	0/1/1/1
4	SOG	A	409	-	-	0/1/1/31	-
4	SOG	A	406	-	-	0/11/31/31	0/1/1/1
4	SOG	A	410	-	-	0/1/1/31	-
2	NVK	A	401	-	-	0/8/8/8	0/4/4/4
5	PGW	A	411	-	-	14/55/55/55	-
5	PGW	B	409	-	-	32/55/55/55	-
2	NVK	A	402	-	-	0/8/8/8	0/4/4/4
4	SOG	B	406	-	-	0/11/31/31	0/1/1/1
2	NVK	B	401	-	-	0/8/8/8	0/4/4/4
4	SOG	B	407	-	-	2/11/31/31	0/1/1/1
4	SOG	A	404	-	-	1/11/31/31	0/1/1/1
4	SOG	B	405	-	-	0/11/31/31	0/1/1/1
2	NVK	B	402	-	-	0/8/8/8	0/4/4/4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	NVK	C10-C11-N5	3.56	120.51	117.48
4	B	405	SOG	C4-C3-C2	3.38	116.72	110.82
2	A	401	NVK	C10-C11-N5	3.34	120.32	117.48
2	A	402	NVK	C10-C11-N5	3.34	120.32	117.48
2	B	401	NVK	C10-C11-N5	3.31	120.29	117.48
4	B	405	SOG	C1-C2-C3	2.98	116.47	110.59
4	B	405	SOG	O5-C1-C2	2.89	113.95	110.31
4	A	405	SOG	C2'-C1'-S1	-2.88	103.10	112.40
4	A	405	SOG	C1'-S1-C1	2.57	104.89	100.09
2	A	402	NVK	C6-C5-C4	-2.55	117.03	119.46
2	B	402	NVK	C13-C14-C10	-2.38	118.41	119.60
2	A	401	NVK	C13-C14-C10	-2.28	118.46	119.60
2	B	401	NVK	C13-C14-C10	-2.24	118.48	119.60
2	B	402	NVK	C6-C5-C4	-2.19	117.38	119.46
2	A	402	NVK	C13-C14-C10	-2.11	118.55	119.60
2	A	401	NVK	C6-C5-C4	-2.09	117.47	119.46
2	B	401	NVK	C6-C5-C4	-2.04	117.52	119.46

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	SOG	C2-C1-S1-C1'
4	A	405	SOG	C2-C1-S1-C1'
4	A	405	SOG	O5-C1-S1-C1'
4	A	407	SOG	O5-C1-S1-C1'
4	B	407	SOG	O5-C1-S1-C1'
4	B	408	SOG	C2'-C1'-S1-C1
5	A	411	PGW	C04-O12-P-O14
5	B	409	PGW	C04-O12-P-O14
5	B	409	PGW	O12-C04-C05-OAF
5	A	411	PGW	C1-C2-C3-C4
4	B	408	SOG	C1'-C2'-C3'-C4'
5	B	409	PGW	OAF-C05-CAD-OAE
5	A	411	PGW	C19-C20-C21-C22
4	A	405	SOG	S1-C1'-C2'-C3'
5	B	409	PGW	C1-C2-C3-C4
5	B	409	PGW	C19-C20-C21-C22
5	B	409	PGW	C03-O11-P-O12
5	A	411	PGW	C06-C07-C08-C09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	409	PGW	C5-C6-C7-C8
5	B	409	PGW	C15-C16-C17-C18
5	B	409	PGW	C04-C05-CAD-OAE
5	B	409	PGW	C2-C1-O01-C02
5	B	409	PGW	C07-C08-C09-C11
5	B	409	PGW	C25-C26-C27-C15
5	B	409	PGW	C16-C15-C27-C26
5	B	409	PGW	O02-C1-O01-C02
5	B	409	PGW	C06-C07-C08-C09
5	A	411	PGW	C20-C21-C22-C23
5	A	411	PGW	C20-C19-O03-C01
4	B	407	SOG	C2'-C3'-C4'-C5'
4	A	405	SOG	C3'-C4'-C5'-C6'
5	A	411	PGW	C2-C3-C4-C5
5	A	411	PGW	C21-C22-C23-C24
5	A	411	PGW	C02-C03-O11-P
5	B	409	PGW	C02-C03-O11-P
5	B	409	PGW	C01-C02-C03-O11
5	B	409	PGW	O03-C01-C02-C03
5	B	409	PGW	C20-C19-O03-C01
5	A	411	PGW	C16-C15-C27-C26
5	A	411	PGW	O04-C19-O03-C01
5	A	411	PGW	C04-O12-P-O11
5	B	409	PGW	O01-C02-C03-O11
5	B	409	PGW	O04-C19-O03-C01
5	B	409	PGW	C04-O12-P-O11
5	B	409	PGW	C03-O11-P-O13
5	B	409	PGW	C03-O11-P-O14
5	B	409	PGW	C04-O12-P-O13
5	B	409	PGW	O03-C01-C02-O01
5	A	411	PGW	C22-C23-C24-C25
5	B	409	PGW	O01-C1-C2-C3
5	A	411	PGW	C7-C8-C9-C10
4	A	405	SOG	C4'-C5'-C6'-C7'
5	B	409	PGW	C24-C25-C26-C27
5	B	409	PGW	C08-C09-C11-C12
4	A	408	SOG	C2'-C3'-C4'-C5'
5	B	409	PGW	C7-C8-C9-C10
5	B	409	PGW	O12-C04-C05-CAD
5	B	409	PGW	C4-C5-C6-C7

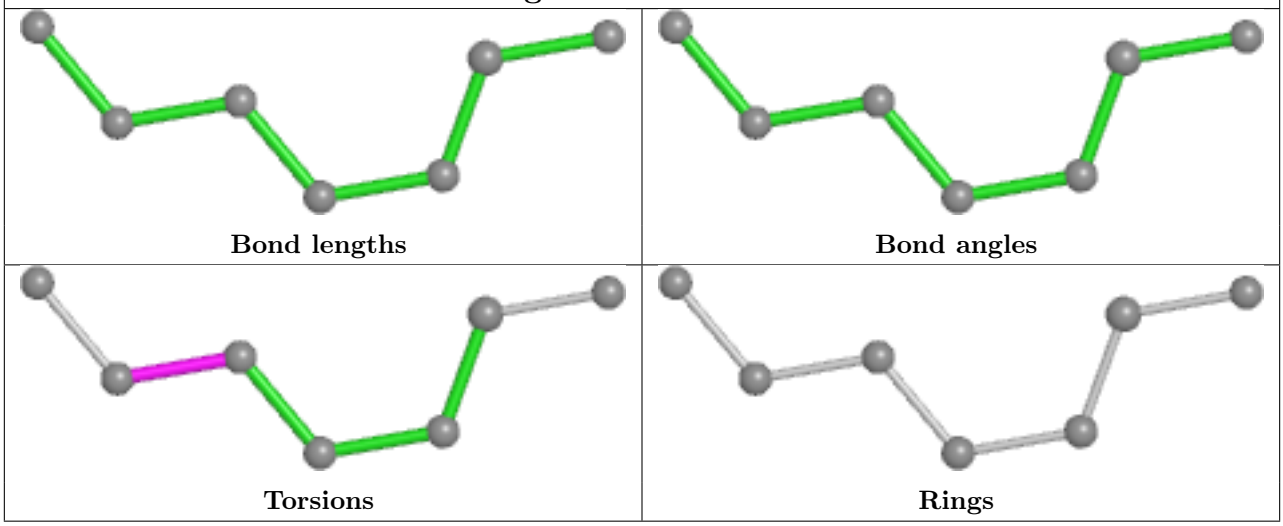
There are no ring outliers.

8 monomers are involved in 23 short contacts:

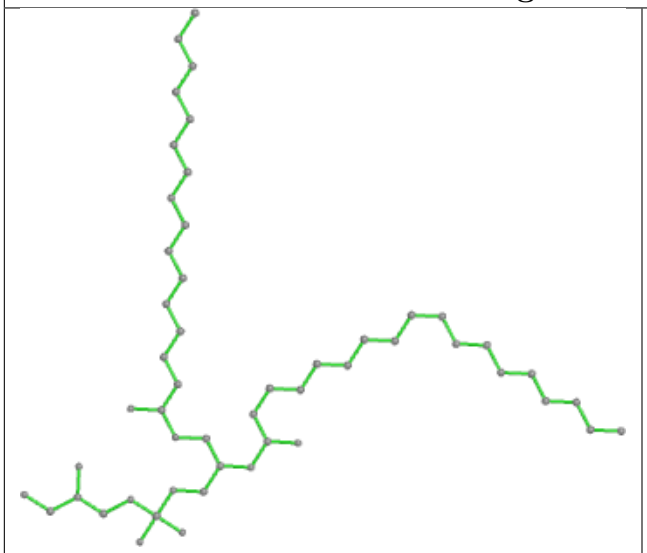
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	411	PGW	3	0
5	B	409	PGW	2	0
2	A	402	NVK	1	0
4	A	407	SOG	2	0
4	B	406	SOG	1	0
4	A	405	SOG	10	0
4	A	406	SOG	4	0
2	B	402	NVK	2	0

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

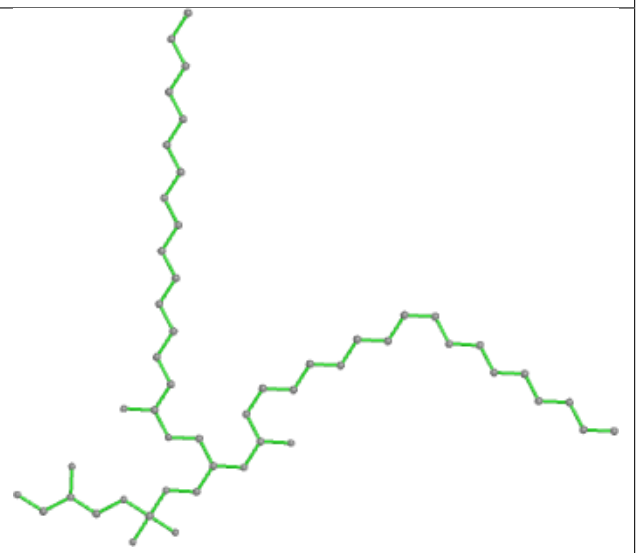
Ligand SOG A 408



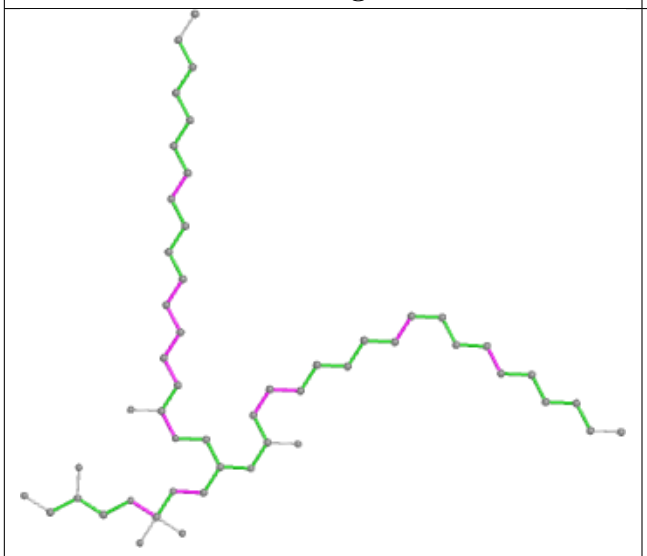
Ligand PGW A 411



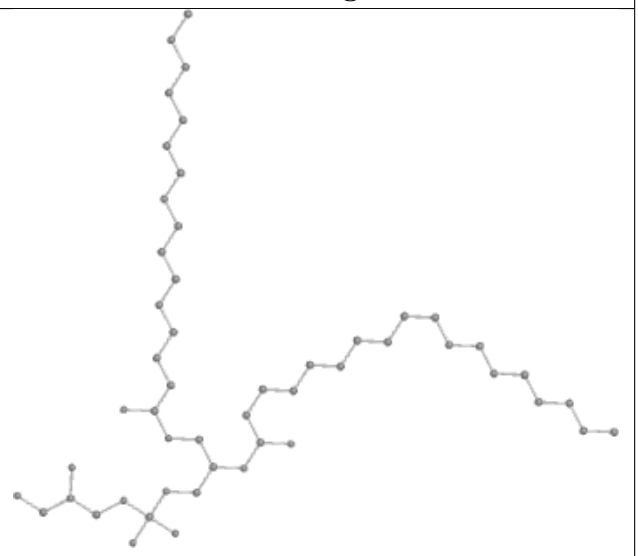
Bond lengths



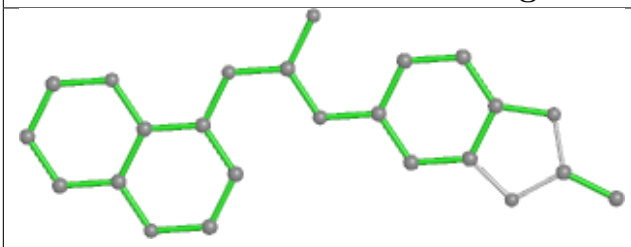
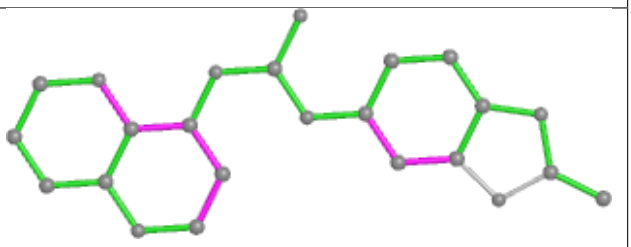
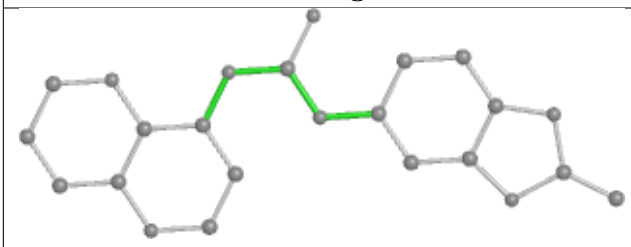
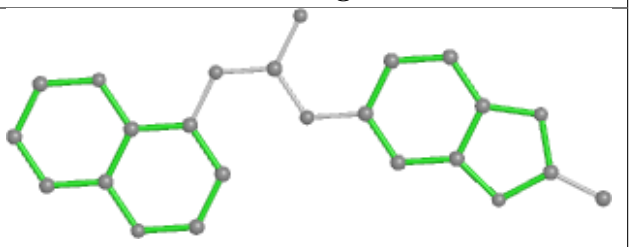
Bond angles



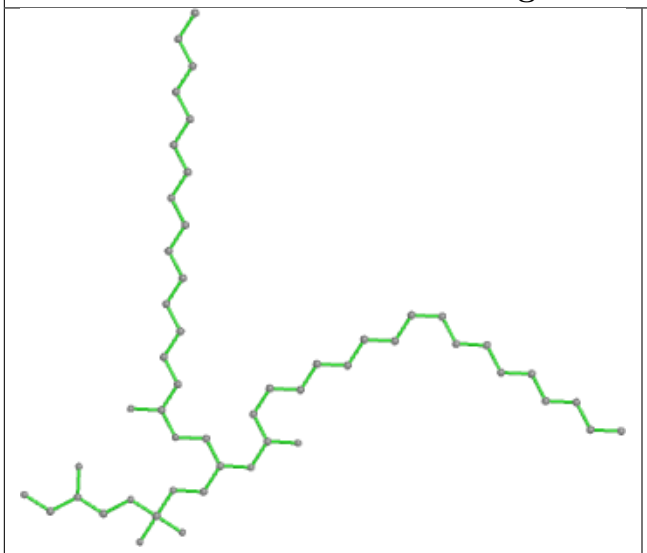
Torsions



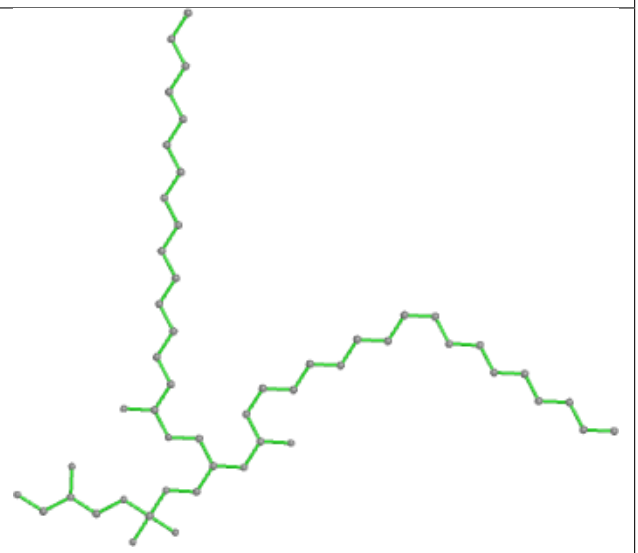
Rings

Ligand NVK A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

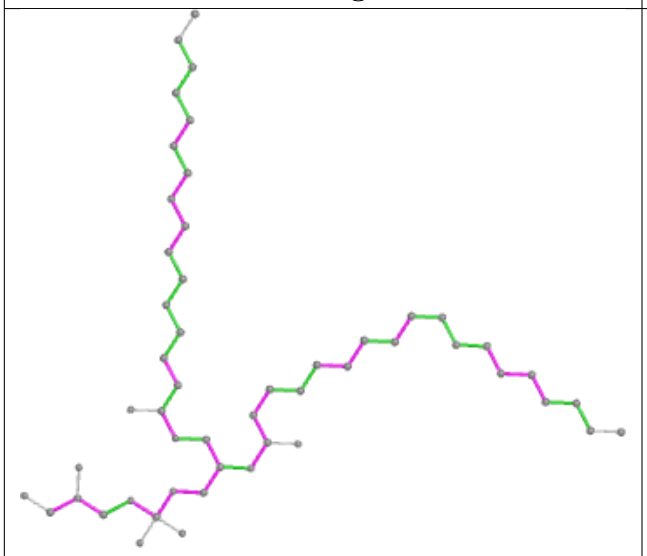
Ligand PGW B 409



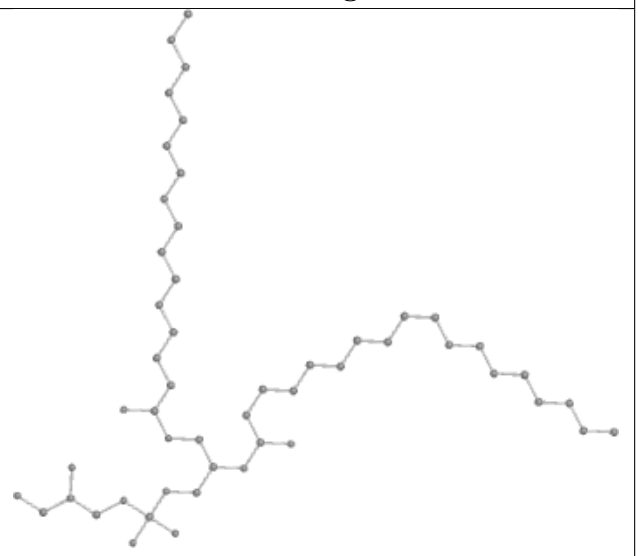
Bond lengths



Bond angles

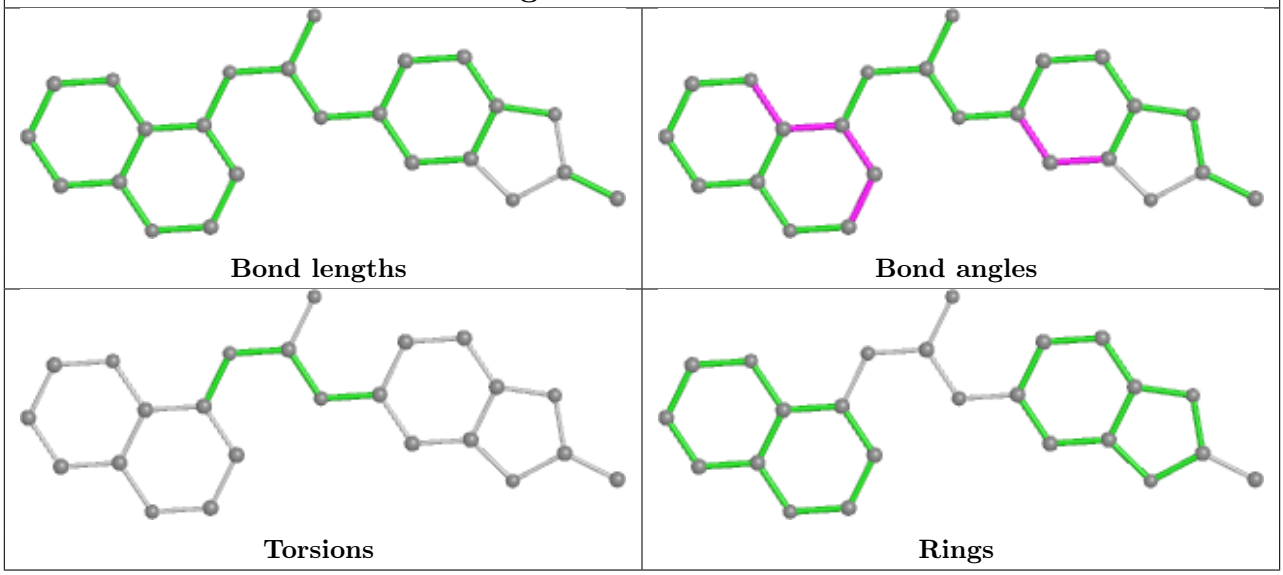


Torsions

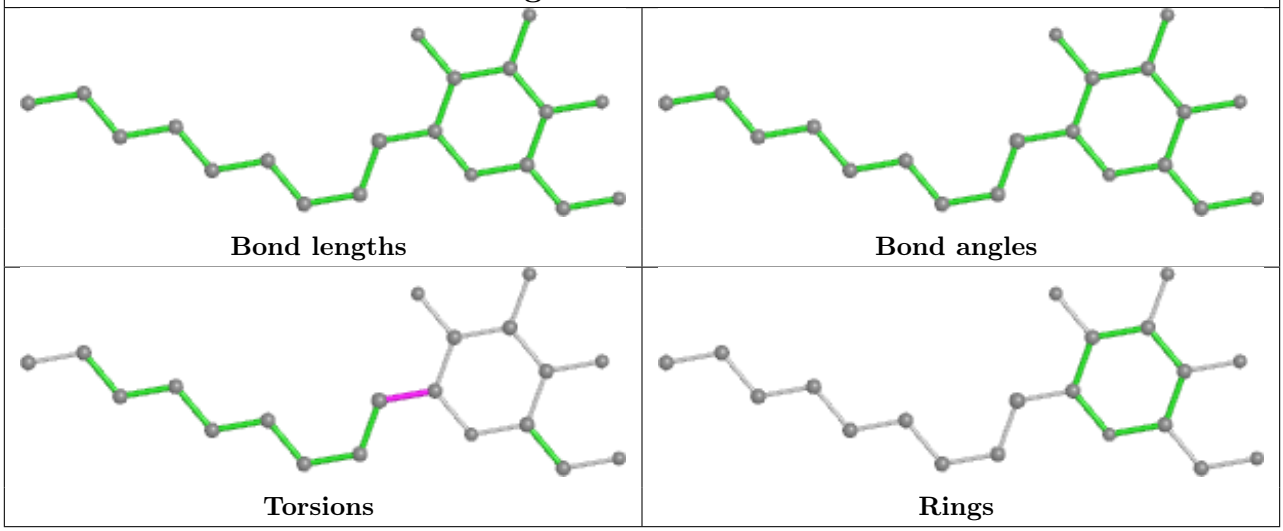


Rings

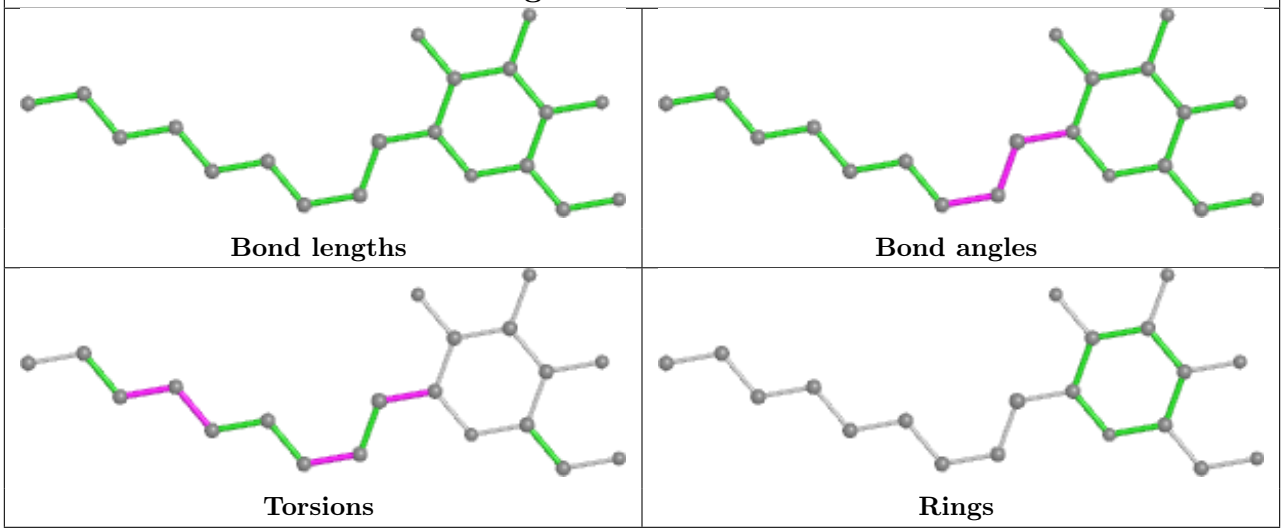
Ligand NVK A 402



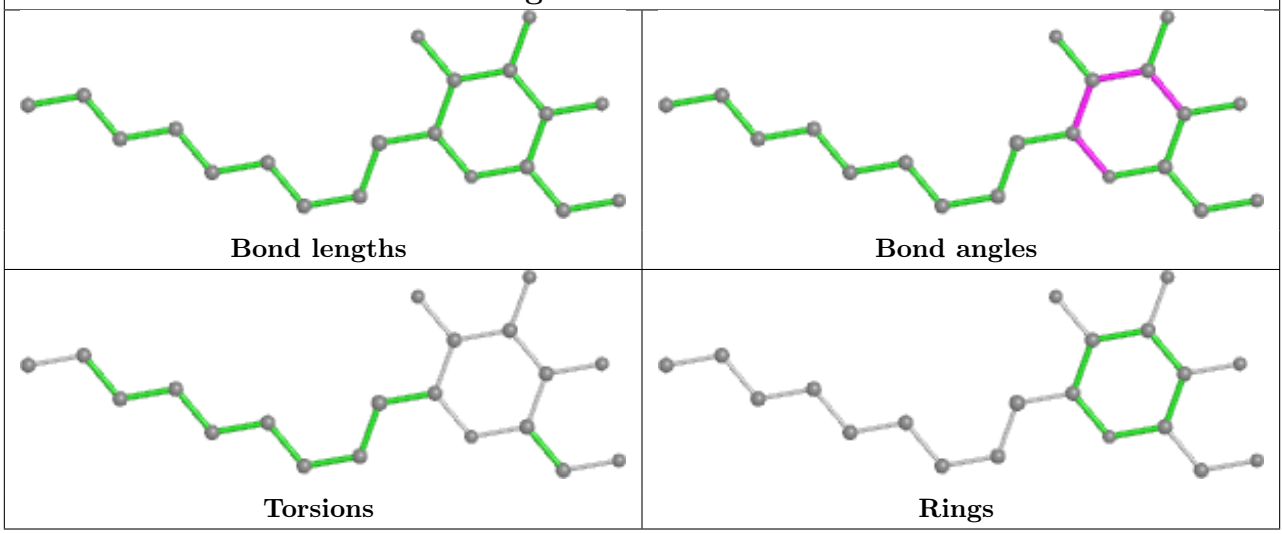
Ligand SOG A 407



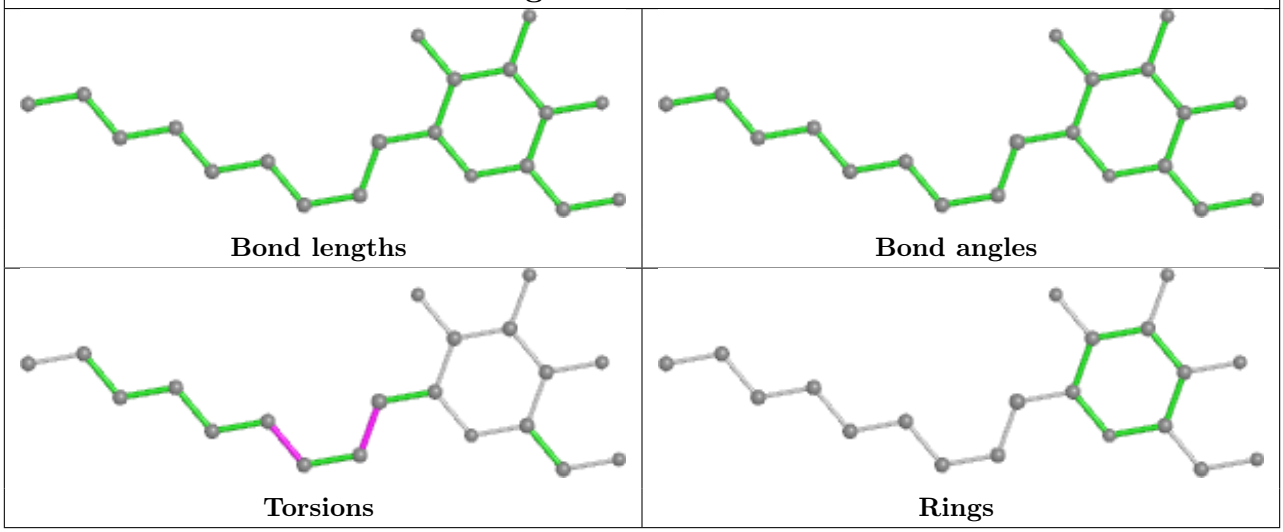
Ligand SOG A 405



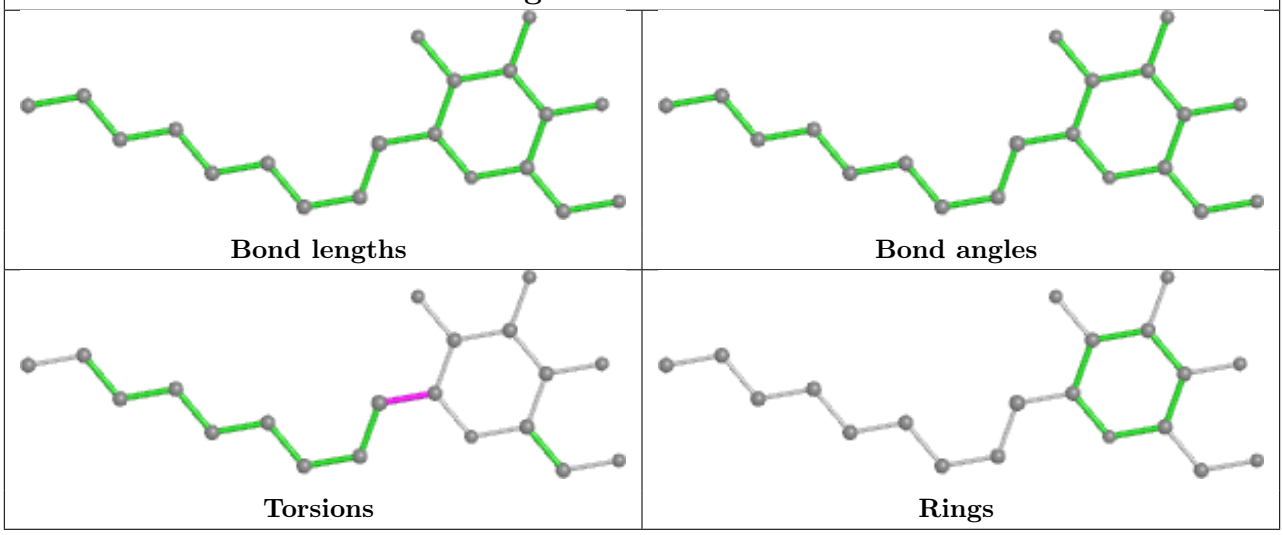
Ligand SOG B 405



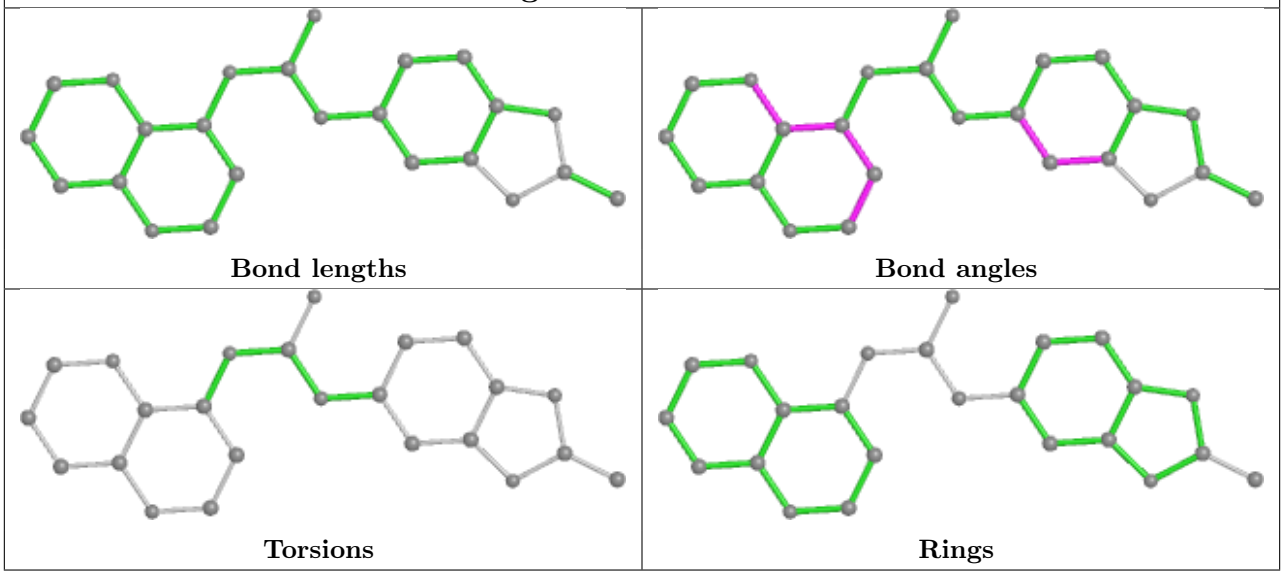
Ligand SOG B 408



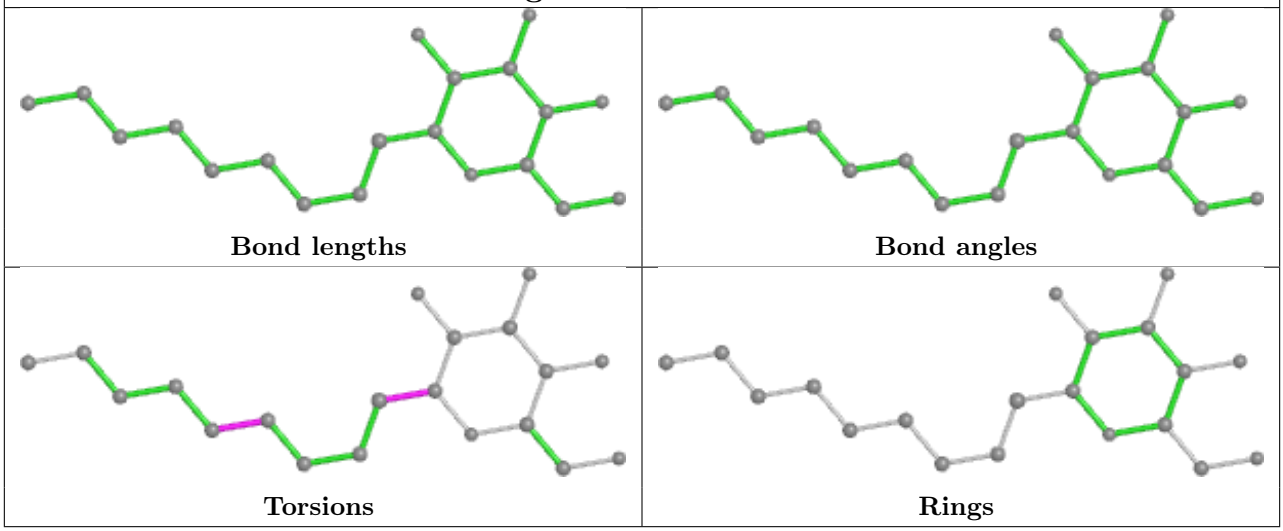
Ligand SOG A 404



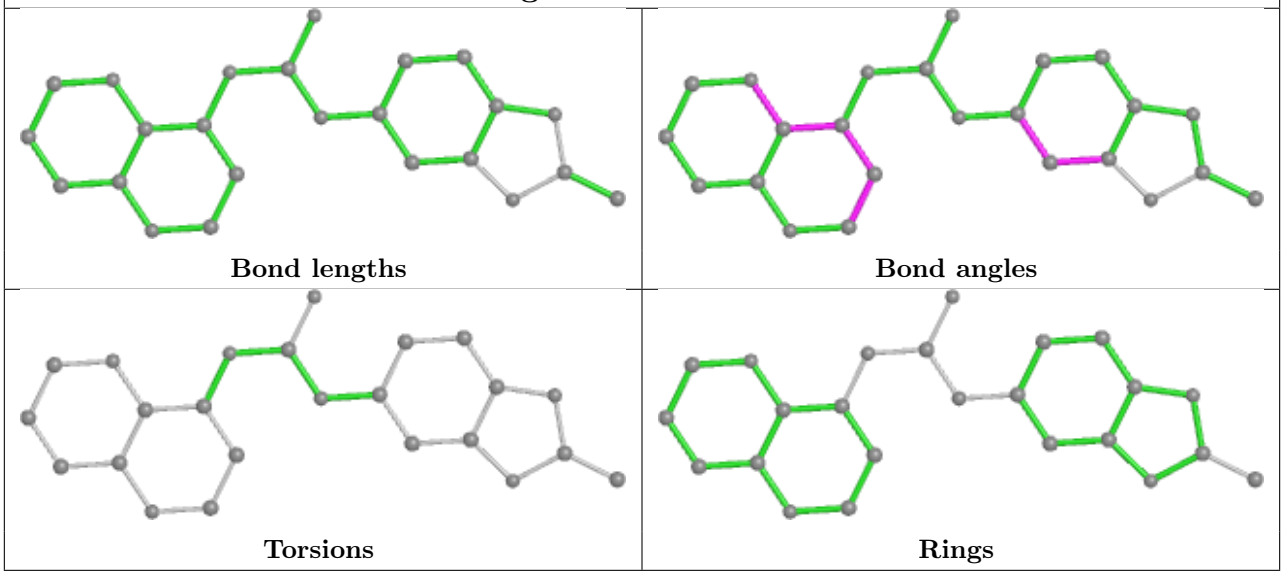
Ligand NVK B 401



Ligand SOG B 407



Ligand NVK B 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

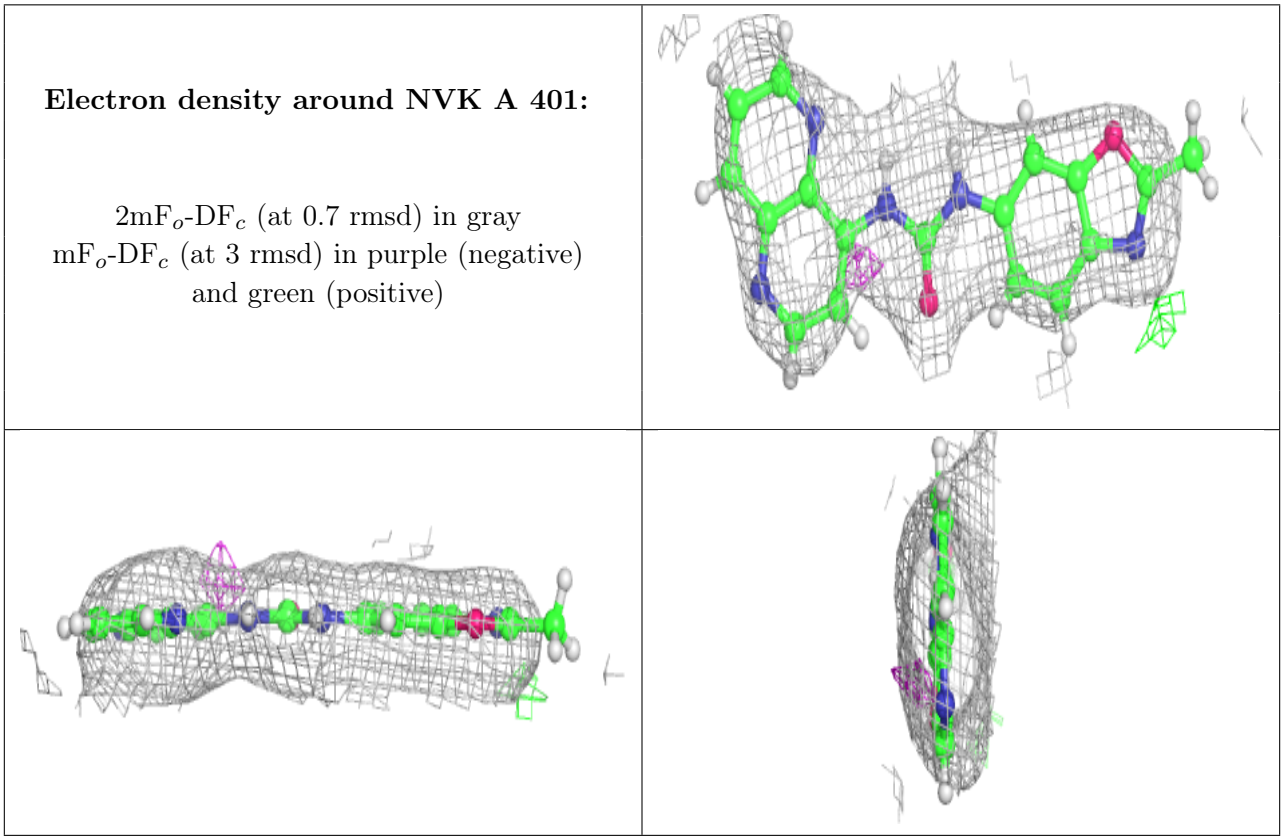
6.3 Carbohydrates (i)

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

6.4 Ligands (i)

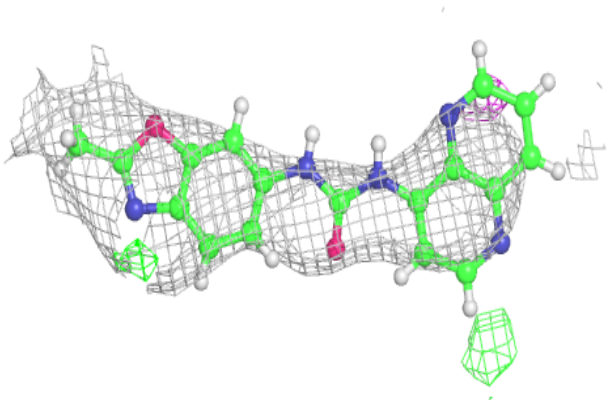
Unable to reproduce the depositors R factor - this section is therefore empty.

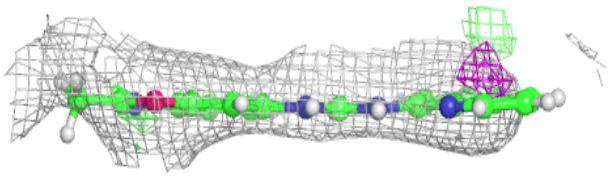
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

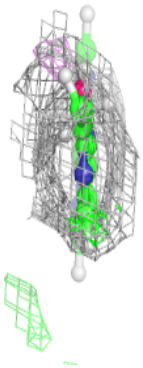


Electron density around NVK A 402:

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

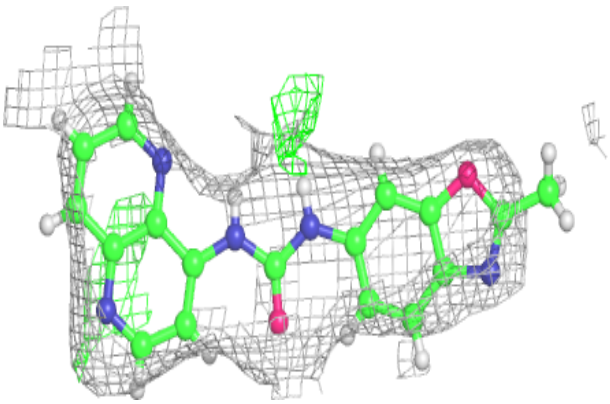


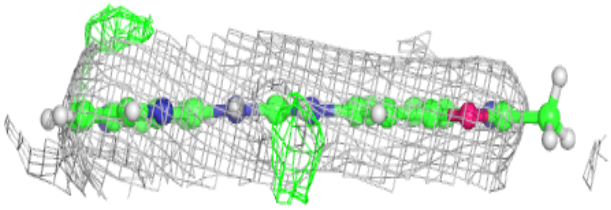


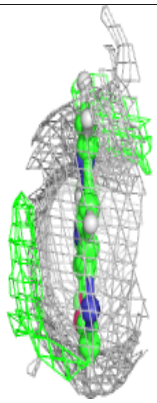


Electron density around NVK B 401:

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

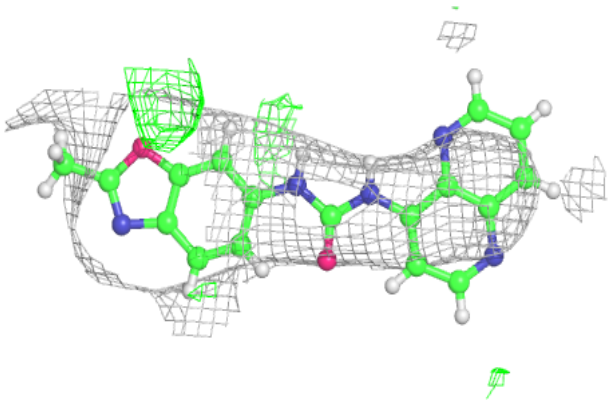


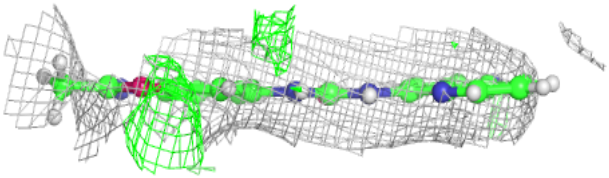


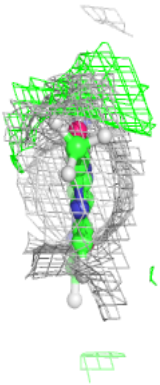


Electron density around NVK B 402:

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

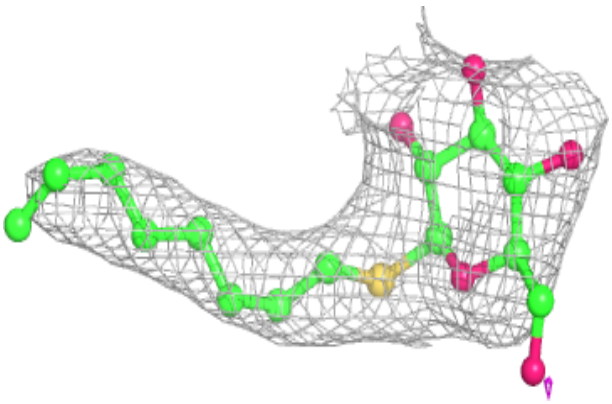


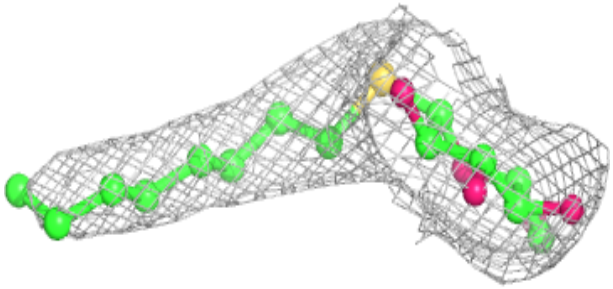


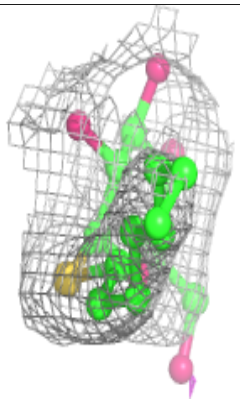


Electron density around SOG A 404:

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

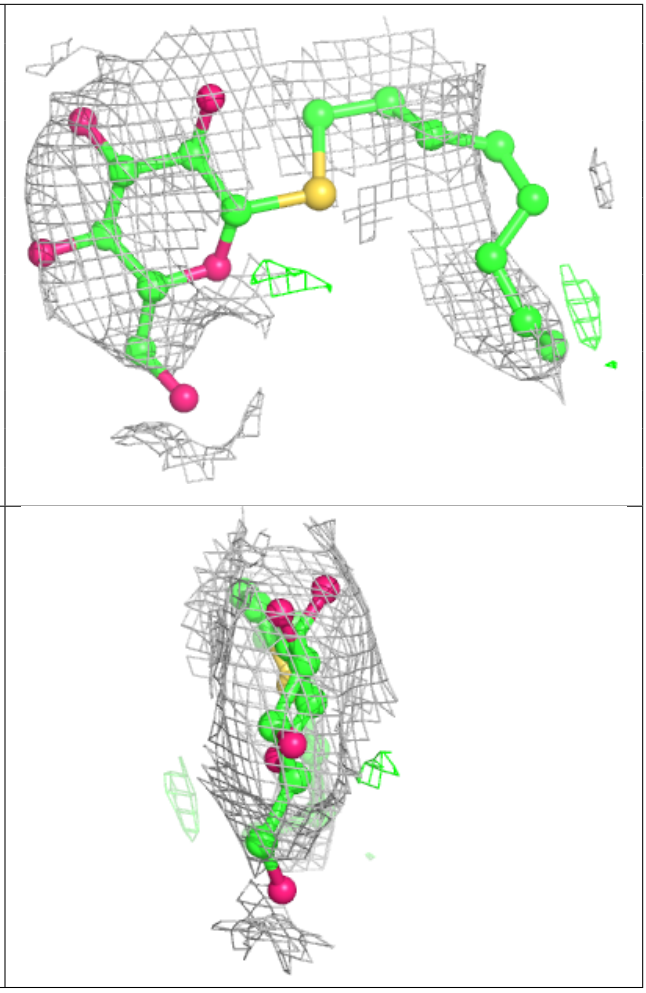






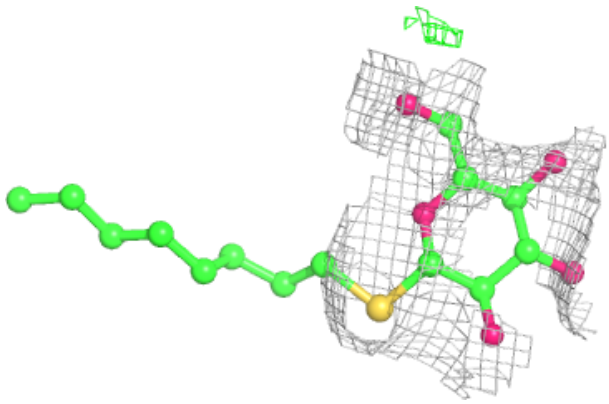
Electron density around SOG A 405:

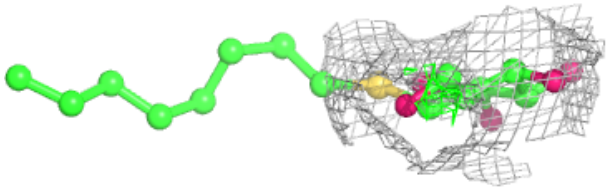
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SOG A 407:

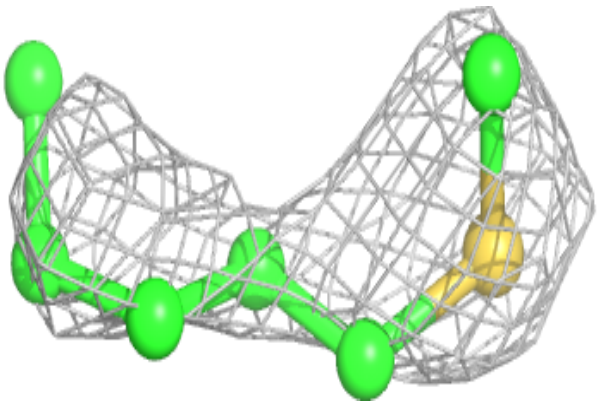
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

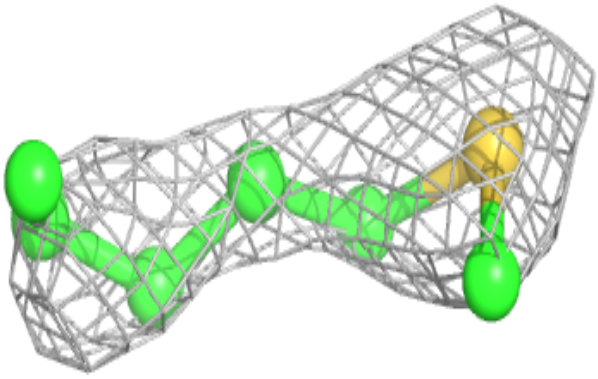


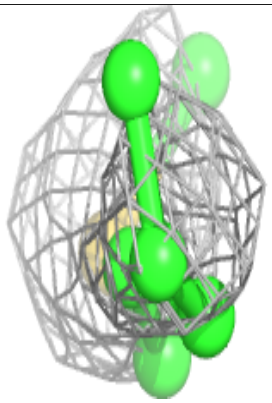


Electron density around SOG A 408:

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

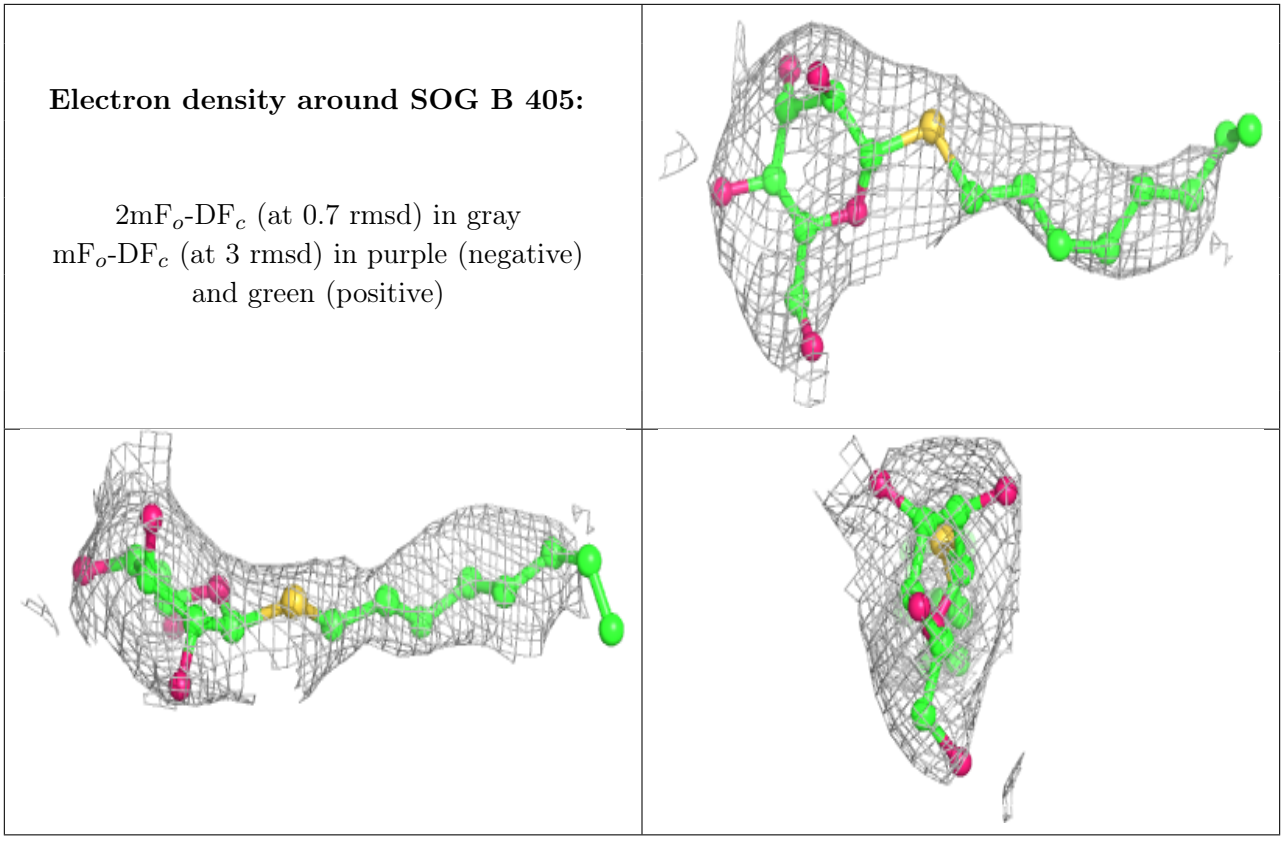






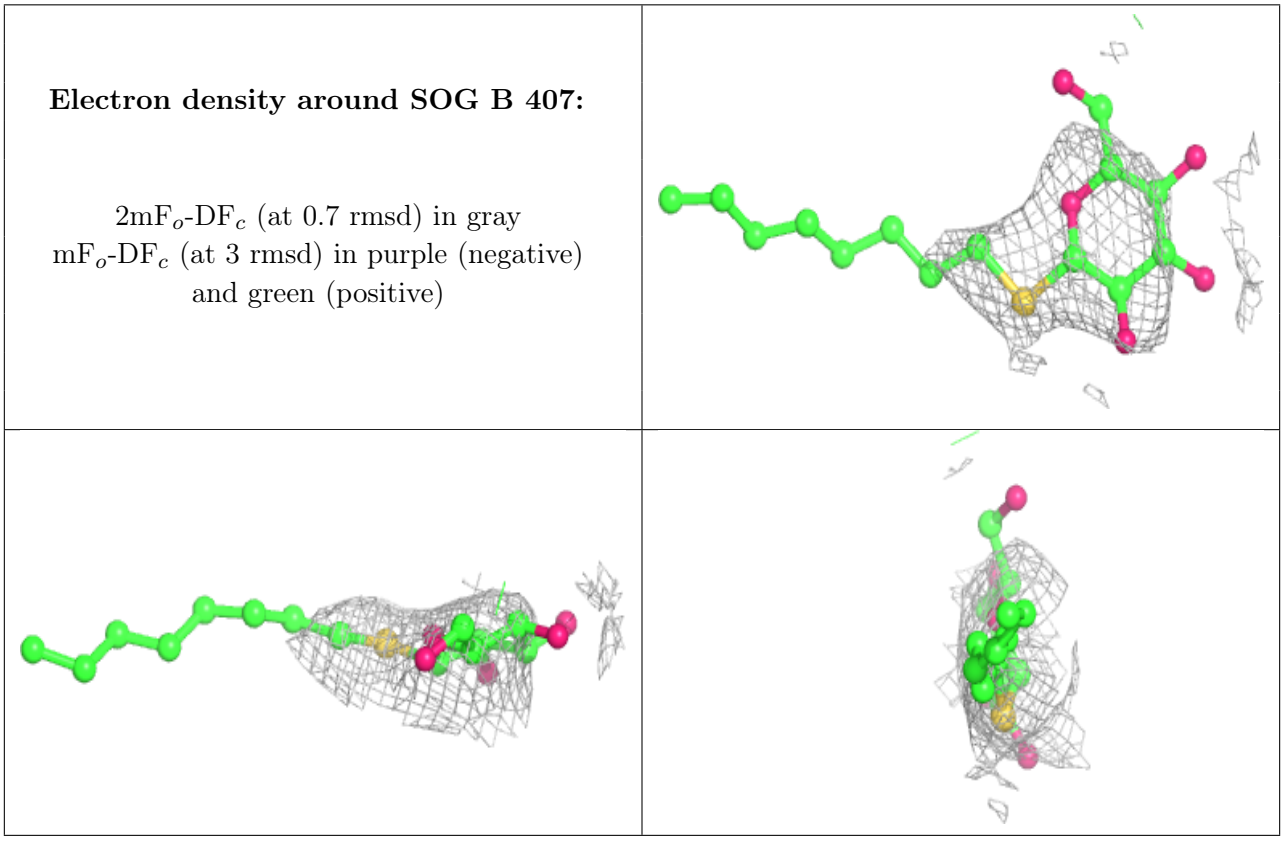
Electron density around SOG B 405:

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



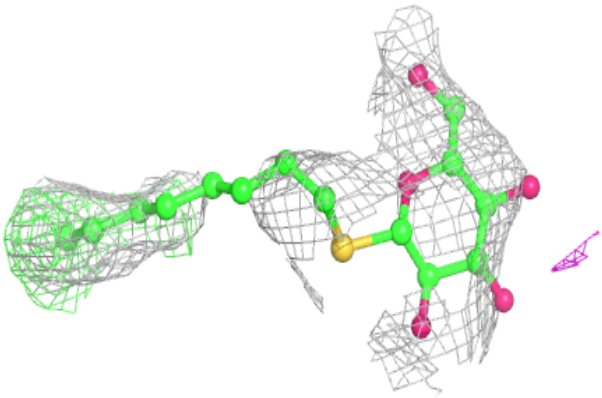
Electron density around SOG B 407:

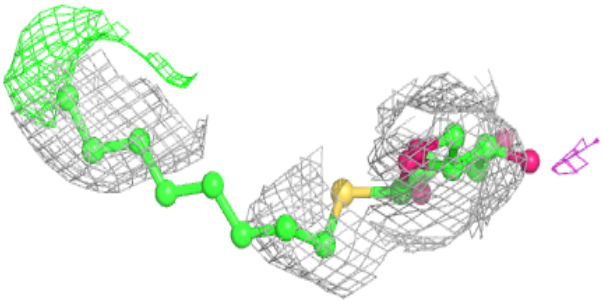
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

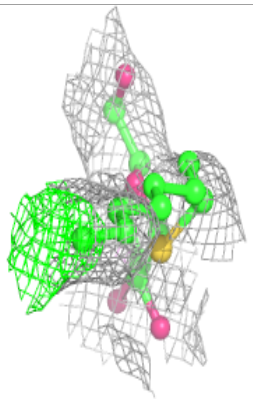


Electron density around SOG B 408:

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

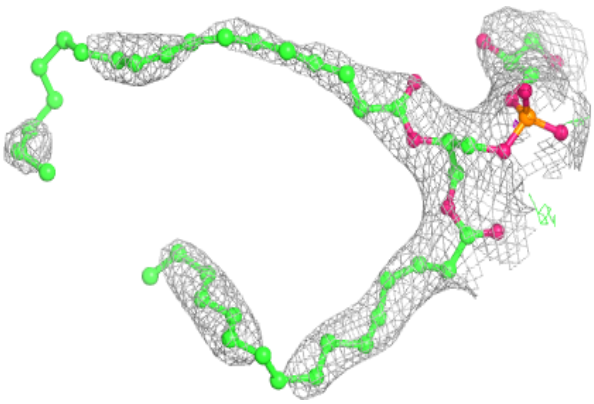


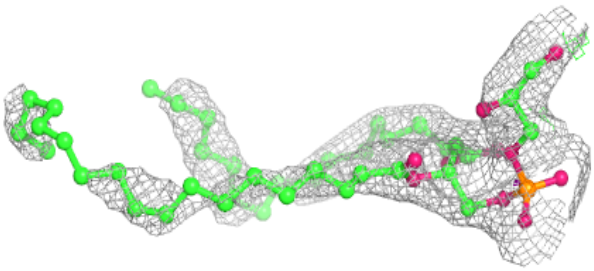


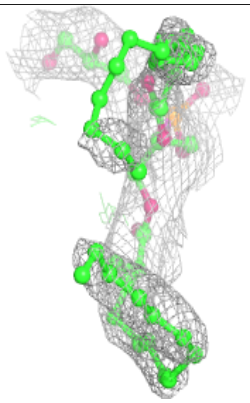


Electron density around PGW A 411:

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

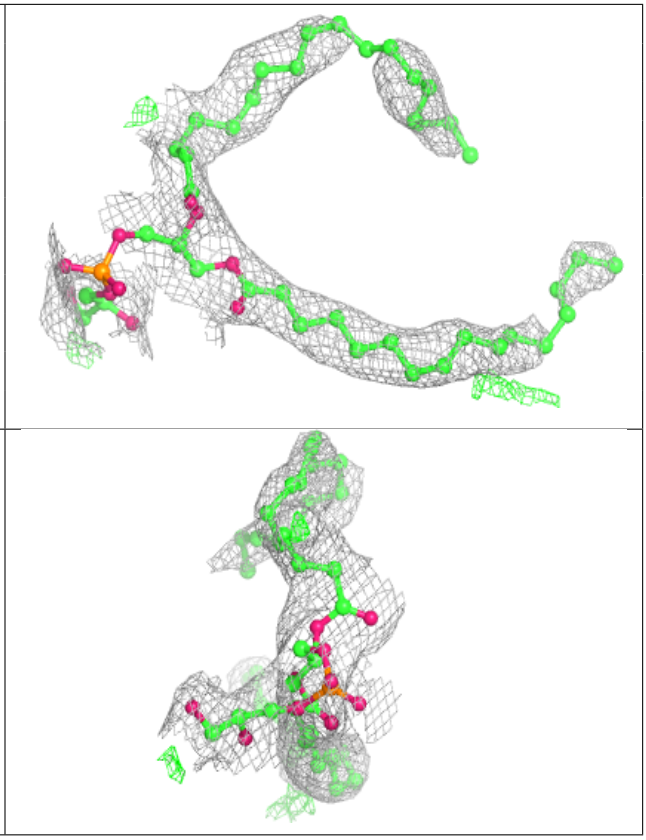






Electron density around PGW B 409:

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



6.5 Other polymers (i)

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