



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:46 AM UTC

PDB ID : 6TQ4 / pdb_00006tq4
Title : Crystal structure of the Orexin-1 receptor in complex with Compound 16
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 : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

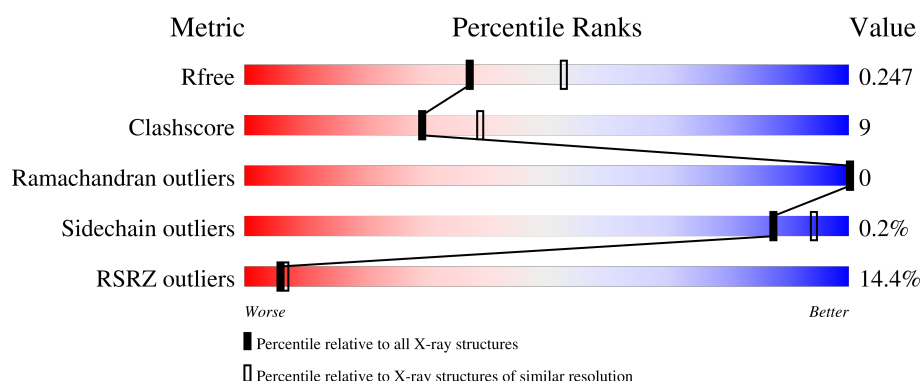
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

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
5	SOG	A	411	-	-	-	X
5	SOG	A	412	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5217 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	297	Total	C	N	O	S	0	0	0
			2388	1589	393	389	17			
1	B	299	Total	C	N	O	S	0	0	0
			2374	1576	397	384	17			

There are 52 discrepancies between the modelled and reference sequences:

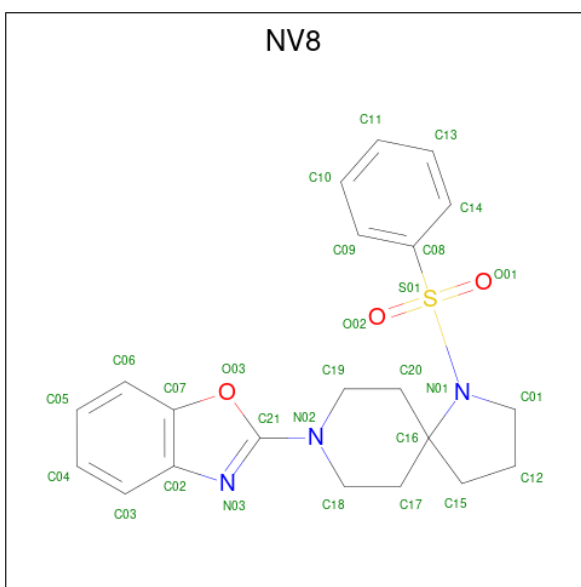
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU	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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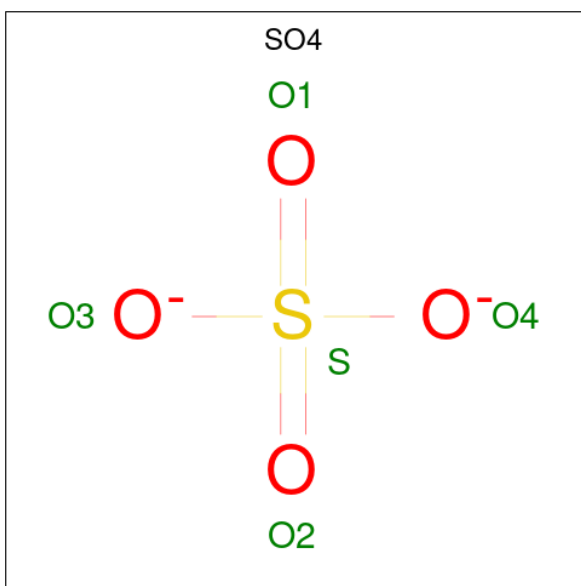
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered 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-[1-(phenylsulfonyl)-1,8-diazaspiro[4.5]decan-8-yl]-1,3-benzoxazole (CCD ID: NV8) (formula: C₂₁H₂₃N₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			51	21	23	3	3	1		
2	B	1	Total	C	H	N	O	S	0	0
			51	21	23	3	3	1		

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



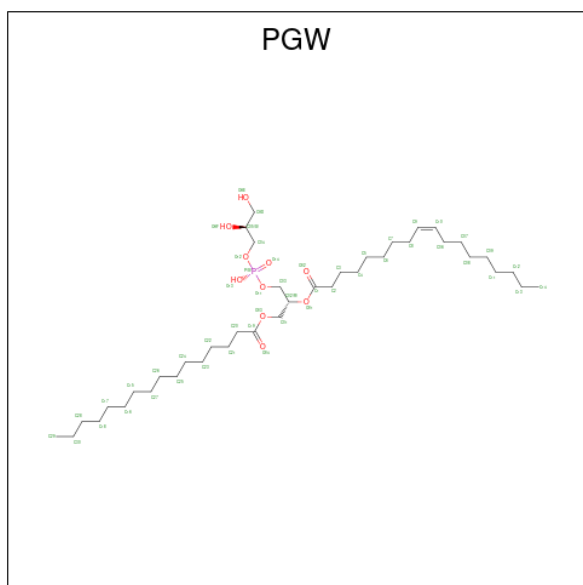
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		

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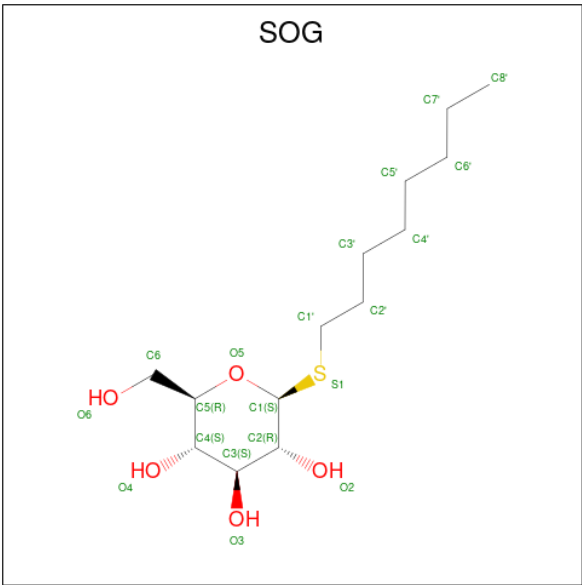
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: $C_{40}H_{77}O_{10}P$).



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

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



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0

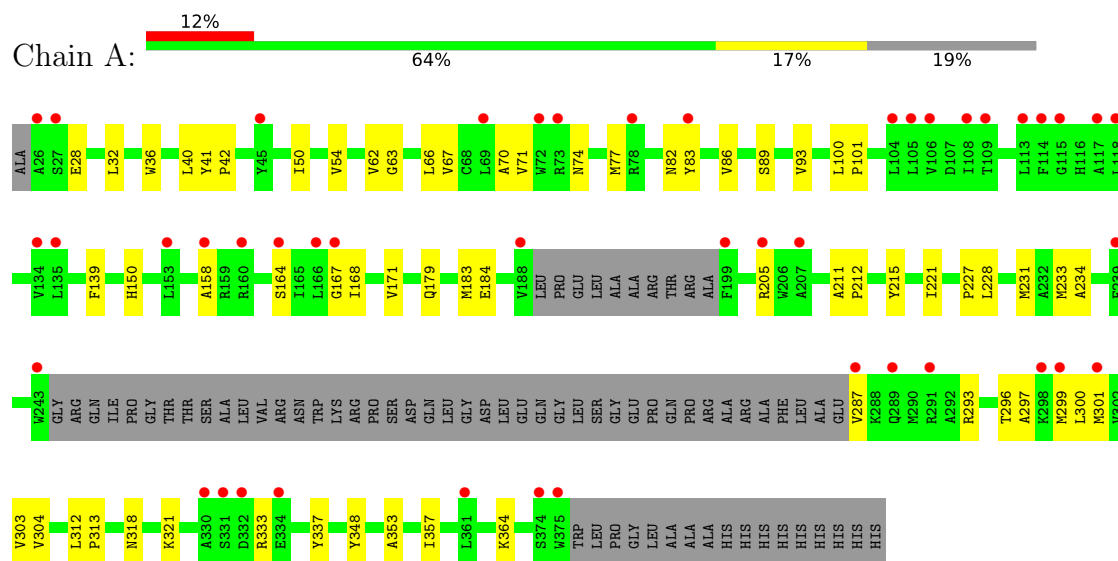
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total 27	O 27	0	0
7	B	15	Total 15	O 15	0	0

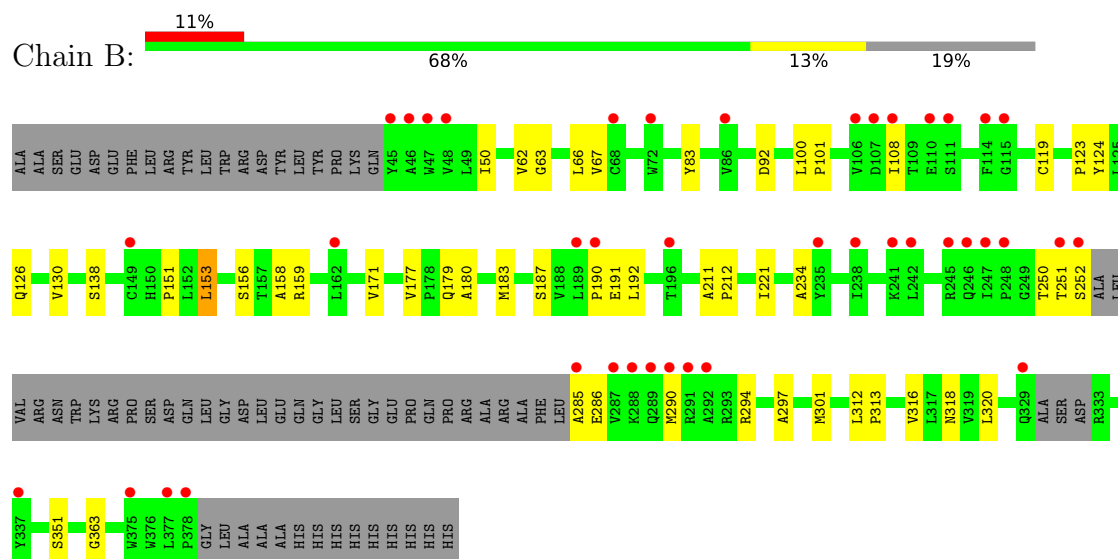
3 Residue-property plots

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

• Molecule 1: Orexin receptor type 1



• Molecule 1: Orexin receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.34Å 145.89Å 71.34Å 90.00° 112.33° 90.00°	Depositor
Resolution (Å)	34.69 – 2.30 34.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.1 (34.69-2.30) 87.0 (34.69-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.209 , 0.236 0.222 , 0.247	Depositor DCC
R_{free} test set	2465 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5217	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SOG, NA, NV8, 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	0.18	0/2455	0.39	0/3344
1	B	0.21	0/2440	0.46	1/3328 (0.0%)
All	All	0.20	0/4895	0.43	1/6672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PRO	N-CA-C	9.11	126.19	113.53

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	2388	0	2434	53	0
1	B	2374	0	2445	35	0
2	A	28	23	0	1	0
2	B	28	23	0	1	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
4	A	51	0	76	11	0
4	B	51	0	76	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	116	0	149	4	0
5	B	72	0	86	3	0
6	A	1	0	0	0	0
7	A	27	0	0	1	0
7	B	15	0	0	1	0
All	All	5171	46	5266	89	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 9.

All (89) 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:233:MET:HB3	4:A:404:PGW:H2A	1.38	1.05
1:A:71:VAL:HG21	1:A:86:VAL:HG21	1.51	0.93
1:B:234:ALA:HB2	4:B:404:PGW:H7A	1.54	0.90
1:A:233:MET:HE1	4:A:404:PGW:H23A	1.55	0.89
1:A:228:LEU:HD23	1:A:231:MET:HE3	1.54	0.86
1:A:150:HIS:HE1	5:B:409:SOG:H2'1	1.44	0.83
1:A:318:ASN:ND2	2:A:401:NV8:O01	2.16	0.78
1:A:83:TYR:HE2	1:A:158:ALA:HB1	1.52	0.74
1:A:150:HIS:CE1	5:B:409:SOG:H2'1	2.24	0.72
1:A:71:VAL:HG21	1:A:86:VAL:CG2	2.20	0.72
1:A:233:MET:HE1	4:A:404:PGW:H21A	1.72	0.71
1:B:83:TYR:HE2	1:B:158:ALA:HB1	1.57	0.69
1:A:83:TYR:CE2	1:A:158:ALA:HB1	2.26	0.69
1:B:138:SER:HB3	4:B:404:PGW:H07	1.76	0.68
1:B:190:PRO:HG2	1:B:191:GLU:OE1	1.94	0.68
1:B:83:TYR:CE2	1:B:158:ALA:HB1	2.31	0.65
1:A:233:MET:CB	4:A:404:PGW:H2A	2.23	0.65
1:B:318:ASN:ND2	2:B:401:NV8:O01	2.30	0.64
1:A:228:LEU:HD23	1:A:231:MET:CE	2.28	0.61
1:B:363:GLY:N	3:B:403:SO4:O2	2.34	0.61
1:B:156:SER:HB3	5:B:405:SOG:S1	2.41	0.60
1:A:233:MET:CE	4:A:404:PGW:H23A	2.29	0.59
1:B:153:LEU:HD23	1:B:153:LEU:N	2.18	0.58
1:A:36:TRP:HA	1:A:40:LEU:HB2	1.85	0.58
1:A:234:ALA:HB2	4:A:404:PGW:H7A	1.87	0.57
1:B:250:THR:CG2	1:B:286:GLU:HG3	2.35	0.57
1:A:233:MET:HE1	4:A:404:PGW:C23	2.33	0.55
1:A:74:ASN:HB3	1:A:77:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:O	1:A:171:VAL:HG23	2.07	0.54
1:B:290:MET:O	1:B:294:ARG:HG3	2.07	0.53
1:A:82:ASN:O	1:A:86:VAL:HG23	2.07	0.53
1:A:70:ALA:HB1	1:A:77:MET:HE1	1.91	0.53
1:A:139:PHE:HZ	5:A:406:SOG:H5'2	1.74	0.53
4:B:404:PGW:H02	4:B:404:PGW:H04A	1.92	0.52
1:B:191:GLU:OE1	1:B:191:GLU:N	2.43	0.52
1:A:293:ARG:HA	1:A:296:THR:HG22	1.92	0.52
1:B:92:ASP:HB3	1:B:351:SER:HB3	1.92	0.51
1:B:251:THR:HG22	1:B:285:ALA:H	1.77	0.50
1:A:333:ARG:HD3	1:A:337:TYR:OH	2.12	0.50
1:A:77:MET:SD	1:A:364:LYS:HB3	2.52	0.50
1:B:100:LEU:C	1:B:100:LEU:HD23	2.36	0.50
1:B:50:ILE:HG12	1:B:108:ILE:HD11	1.95	0.49
1:A:179:GLN:O	1:A:183:MET:HG2	2.13	0.49
1:B:297:ALA:O	1:B:301:MET:HG3	2.13	0.49
1:B:250:THR:HG23	1:B:286:GLU:HG3	1.95	0.49
5:A:412:SOG:H8'1	7:A:525:HOH:O	2.13	0.48
1:A:184:GLU:HG3	1:A:205:ARG:HE	1.78	0.48
1:A:333:ARG:HG2	1:A:337:TYR:CE2	2.50	0.47
1:A:353:ALA:O	1:A:357:ILE:HG13	2.14	0.47
1:A:233:MET:HE1	4:A:404:PGW:C21	2.45	0.46
1:A:50:ILE:O	1:A:54:VAL:HG23	2.15	0.46
1:A:321:LYS:NZ	5:A:412:SOG:H8'2	2.30	0.46
1:A:63:GLY:O	1:A:67:VAL:HG23	2.16	0.46
1:A:100:LEU:HB3	1:A:101:PRO:HD3	1.97	0.46
1:B:126:GLN:O	1:B:130:VAL:HG23	2.16	0.45
1:A:28:GLU:O	1:A:32:LEU:HD12	2.16	0.45
1:B:62:VAL:O	1:B:66:LEU:HG	2.16	0.45
1:A:164:SER:O	1:A:168:ILE:HG13	2.16	0.45
1:A:312:LEU:HB3	1:A:313:PRO:HD3	1.98	0.45
1:A:211:ALA:N	1:A:212:PRO:HD2	2.31	0.45
1:A:62:VAL:O	1:A:66:LEU:HG	2.16	0.45
1:B:316:VAL:O	1:B:320:LEU:HG	2.17	0.45
5:A:406:SOG:H4'1	1:B:171:VAL:HG21	1.98	0.44
1:A:299:MET:O	1:A:303:VAL:HG23	2.17	0.44
1:A:215:TYR:HB2	4:B:404:PGW:H24	1.99	0.44
1:B:63:GLY:O	1:B:67:VAL:HG23	2.17	0.44
1:B:312:LEU:HB3	1:B:313:PRO:HD3	1.99	0.44
1:B:159:ARG:NH2	7:B:501:HOH:O	2.45	0.44
1:B:251:THR:HG22	1:B:252:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HD3	4:A:404:PGW:H14B	2.01	0.43
1:A:100:LEU:C	1:A:100:LEU:HD23	2.43	0.43
1:A:100:LEU:HD12	1:A:348:TYR:HB3	1.99	0.43
1:B:124:TYR:HB2	1:B:180:ALA:HB2	2.00	0.43
1:A:221:ILE:HD12	1:B:221:ILE:HG13	2.01	0.42
1:A:287:VAL:HG22	1:A:287:VAL:O	2.19	0.42
1:B:250:THR:HG22	1:B:286:GLU:HG3	2.01	0.42
1:A:300:LEU:O	1:A:304:VAL:HG23	2.19	0.42
1:B:179:GLN:O	1:B:183:MET:HG2	2.19	0.42
1:B:211:ALA:N	1:B:212:PRO:HD2	2.35	0.42
1:A:297:ALA:O	1:A:301:MET:HG3	2.20	0.41
4:A:404:PGW:O02	1:B:177:VAL:HG12	2.20	0.41
1:A:89:SER:O	1:A:93:VAL:HG23	2.21	0.41
1:A:41:TYR:HB3	1:A:42:PRO:HD3	2.03	0.41
1:A:227:PRO:O	1:A:231:MET:HG3	2.21	0.41
1:B:100:LEU:HB3	1:B:101:PRO:HD3	2.02	0.41
1:B:187:SER:OG	1:B:192:LEU:HB3	2.21	0.41
1:A:233:MET:CE	4:A:404:PGW:H21A	2.45	0.40
1:A:28:GLU:HG2	1:A:32:LEU:HD11	2.02	0.40
1:B:119:CYS:O	1:B:123:PRO:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/368 (79%)	288 (99%)	3 (1%)	0	100	100
1	B	295/368 (80%)	292 (99%)	3 (1%)	0	100	100
All	All	586/736 (80%)	580 (99%)	6 (1%)	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	251/305 (82%)	251 (100%)	0	100	100
1	B	249/305 (82%)	248 (100%)	1 (0%)	84	92
All	All	500/610 (82%)	499 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	LEU

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	A	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SOG	A	405	-	20,20,20	0.98	2 (10%)	24,25,25	0.82	1 (4%)
5	SOG	B	407	-	4,4,20	0.54	0	3,3,25	0.84	0
5	SOG	A	407	-	20,20,20	0.90	1 (5%)	24,25,25	1.08	2 (8%)
5	SOG	A	409	-	14,14,20	0.73	1 (7%)	18,19,25	0.56	0
5	SOG	A	411	-	4,4,20	0.56	0	3,3,25	0.91	0
3	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SOG	B	408	-	20,20,20	0.82	1 (5%)	24,25,25	0.65	0
5	SOG	B	406	-	12,13,20	0.53	0	17,18,25	0.66	0
5	SOG	B	405	-	14,14,20	0.70	1 (7%)	18,19,25	0.76	0
5	SOG	A	410	-	20,20,20	0.92	2 (10%)	24,25,25	0.73	0
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SOG	B	409	-	20,20,20	0.94	2 (10%)	24,25,25	0.65	0
5	SOG	A	412	-	3,3,20	0.34	0	2,2,25	0.65	0
4	PGW	B	404	-	50,50,50	0.92	2 (4%)	53,56,56	1.09	4 (7%)
3	SO4	B	403	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	A	403	-	4,4,4	0.24	0	6,6,6	0.06	0
4	PGW	A	404	-	50,50,50	0.93	2 (4%)	53,56,56	1.12	4 (7%)
5	SOG	A	408	-	12,13,20	0.56	0	17,18,25	0.72	0
5	SOG	A	406	-	20,20,20	0.94	2 (10%)	24,25,25	0.45	0
2	NV8	A	401	-	31,32,32	1.69	3 (9%)	37,48,48	1.35	6 (16%)
2	NV8	B	401	-	31,32,32	1.64	4 (12%)	37,48,48	1.35	6 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	A	405	-	-	4/11/31/31	0/1/1/1
4	PGW	A	404	-	-	12/55/55/55	-
5	SOG	B	409	-	-	1/11/31/31	0/1/1/1
5	SOG	B	407	-	-	0/2/2/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	A	407	-	-	4/11/31/31	0/1/1/1
5	SOG	A	408	-	-	2/4/24/31	0/1/1/1
5	SOG	A	409	-	-	1/5/25/31	0/1/1/1
5	SOG	B	408	-	-	1/11/31/31	0/1/1/1
5	SOG	A	406	-	-	2/11/31/31	0/1/1/1
5	SOG	A	412	-	-	0/1/1/31	-
5	SOG	B	406	-	-	0/4/24/31	0/1/1/1
2	NV8	A	401	-	-	1/16/41/41	0/5/5/5
2	NV8	B	401	-	-	0/16/41/41	0/5/5/5
4	PGW	B	404	-	-	17/55/55/55	-
5	SOG	A	410	-	-	5/11/31/31	0/1/1/1
5	SOG	B	405	-	-	1/5/25/31	0/1/1/1
5	SOG	A	411	-	-	0/2/2/31	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NV8	S01-N01	8.10	1.77	1.63
2	B	401	NV8	S01-N01	7.53	1.76	1.63
4	A	404	PGW	O03-C19	4.41	1.46	1.33
4	B	404	PGW	O03-C19	4.22	1.45	1.33
4	B	404	PGW	O01-C1	4.10	1.45	1.34
4	A	404	PGW	O01-C1	4.05	1.45	1.34
5	A	405	SOG	C1'-S1	-3.48	1.76	1.81
5	B	409	SOG	C1'-S1	-3.38	1.76	1.81
5	A	406	SOG	C1'-S1	-3.33	1.76	1.81
5	A	410	SOG	C1'-S1	-3.26	1.76	1.81
5	A	407	SOG	C1'-S1	-3.22	1.76	1.81
5	B	408	SOG	C1'-S1	-2.94	1.77	1.81
2	B	401	NV8	O03-C07	-2.41	1.34	1.38
5	A	405	SOG	C1-S1	-2.33	1.76	1.80
5	B	409	SOG	C1-S1	-2.28	1.76	1.80
5	A	409	SOG	C1-S1	-2.27	1.76	1.80
2	A	401	NV8	C02-N03	-2.26	1.35	1.39
5	A	406	SOG	C1-S1	-2.23	1.77	1.80
2	A	401	NV8	O03-C07	-2.21	1.35	1.38
5	A	410	SOG	C1-S1	-2.19	1.77	1.80
2	B	401	NV8	C08-S01	2.15	1.79	1.76
5	B	405	SOG	C1-S1	-2.14	1.77	1.80
2	B	401	NV8	C02-N03	-2.05	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	PGW	O01-C1-C2	4.66	121.55	111.48
4	B	404	PGW	O01-C1-C2	4.40	121.00	111.48
2	B	401	NV8	C20-C19-N02	4.10	118.50	110.82
2	A	401	NV8	O01-S01-C08	-3.33	103.96	108.10
4	A	404	PGW	C02-O01-C1	-3.16	110.23	117.80
2	A	401	NV8	C12-C15-C16	3.07	108.64	104.62
2	A	401	NV8	C20-C19-N02	3.04	116.50	110.82
5	A	407	SOG	C1-C2-C3	2.95	116.31	110.55
2	A	401	NV8	C17-C18-N02	2.94	116.33	110.82
2	B	401	NV8	C12-C15-C16	2.78	108.26	104.62
2	A	401	NV8	O02-S01-N01	2.74	112.86	107.64
4	B	404	PGW	C02-O01-C1	-2.73	111.26	117.80
4	A	404	PGW	O03-C19-C20	2.64	119.87	111.83
4	B	404	PGW	O03-C19-C20	2.61	119.80	111.83
4	B	404	PGW	O01-C1-O02	-2.29	118.34	123.70
2	B	401	NV8	C17-C18-N02	2.24	115.01	110.82
2	B	401	NV8	C05-C06-C07	-2.17	115.65	119.60
5	A	407	SOG	O5-C1-C2	2.17	113.31	110.32
5	A	405	SOG	C1'-S1-C1	-2.11	95.89	100.45
4	A	404	PGW	O01-C1-O02	-2.11	118.78	123.70
2	B	401	NV8	C08-S01-N01	-2.04	100.84	106.50
2	B	401	NV8	O01-S01-C08	-2.01	105.60	108.10
2	A	401	NV8	C05-C06-C07	-2.00	115.96	119.60

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	PGW	C03-O11-P-O14
4	B	404	PGW	C03-O11-P-O12
4	B	404	PGW	C03-O11-P-O14
5	A	405	SOG	C2-C1-S1-C1'
5	A	407	SOG	O5-C1-S1-C1'
5	A	410	SOG	O5-C1-S1-C1'
4	A	404	PGW	C1-C2-C3-C4
5	A	408	SOG	C4-C5-C6-O6
5	A	406	SOG	S1-C1'-C2'-C3'
5	A	408	SOG	O5-C5-C6-O6
5	A	409	SOG	O5-C5-C6-O6
4	B	404	PGW	C5-C6-C7-C8
5	A	405	SOG	C4'-C5'-C6'-C7'

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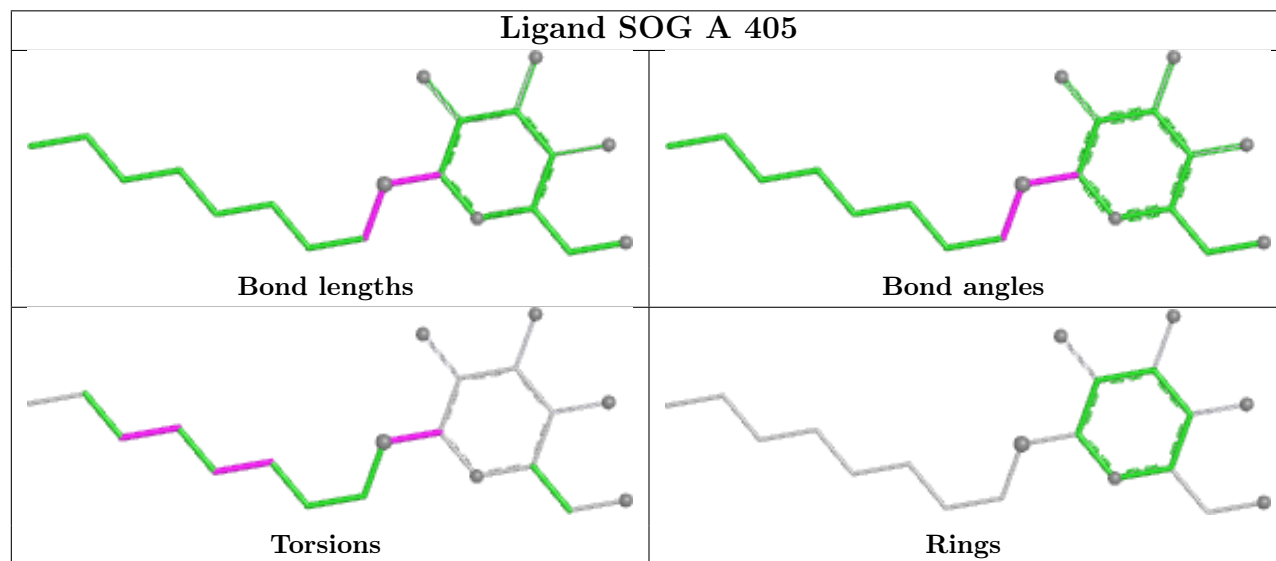
Mol	Chain	Res	Type	Atoms
5	A	410	SOG	C1'-C2'-C3'-C4'
4	A	404	PGW	C19-C20-C21-C22
4	A	404	PGW	C16-C15-C27-C26
5	B	409	SOG	O5-C5-C6-O6
4	B	404	PGW	C2-C3-C4-C5
5	A	405	SOG	C2'-C3'-C4'-C5'
4	B	404	PGW	C24-C25-C26-C27
5	A	406	SOG	O5-C5-C6-O6
5	A	407	SOG	O5-C5-C6-O6
4	A	404	PGW	C3-C4-C5-C6
4	A	404	PGW	C4-C5-C6-C7
5	B	405	SOG	O5-C5-C6-O6
4	B	404	PGW	C2-C1-O01-C02
4	B	404	PGW	C08-C09-C11-C12
4	A	404	PGW	C08-C09-C11-C12
5	B	408	SOG	O5-C5-C6-O6
4	B	404	PGW	C20-C19-O03-C01
5	A	407	SOG	S1-C1'-C2'-C3'
5	A	405	SOG	O5-C1-S1-C1'
4	B	404	PGW	O02-C1-O01-C02
4	B	404	PGW	O04-C19-O03-C01
4	A	404	PGW	O03-C01-C02-C03
5	A	407	SOG	C2-C1-S1-C1'
4	B	404	PGW	C11-C12-C13-C14
4	B	404	PGW	C23-C24-C25-C26
4	B	404	PGW	C03-O11-P-O13
4	A	404	PGW	C7-C8-C9-C10
5	A	410	SOG	C4-C5-C6-O6
4	A	404	PGW	O03-C01-C02-O01
4	B	404	PGW	C7-C8-C9-C10
4	B	404	PGW	C25-C26-C27-C15
5	A	410	SOG	C2-C1-S1-C1'
5	A	410	SOG	C2'-C1'-S1-C1
4	A	404	PGW	C2-C3-C4-C5
4	A	404	PGW	C25-C26-C27-C15
4	B	404	PGW	C01-C02-C03-O11
2	A	401	NV8	O03-C21-N02-C18
4	B	404	PGW	O01-C1-C2-C3

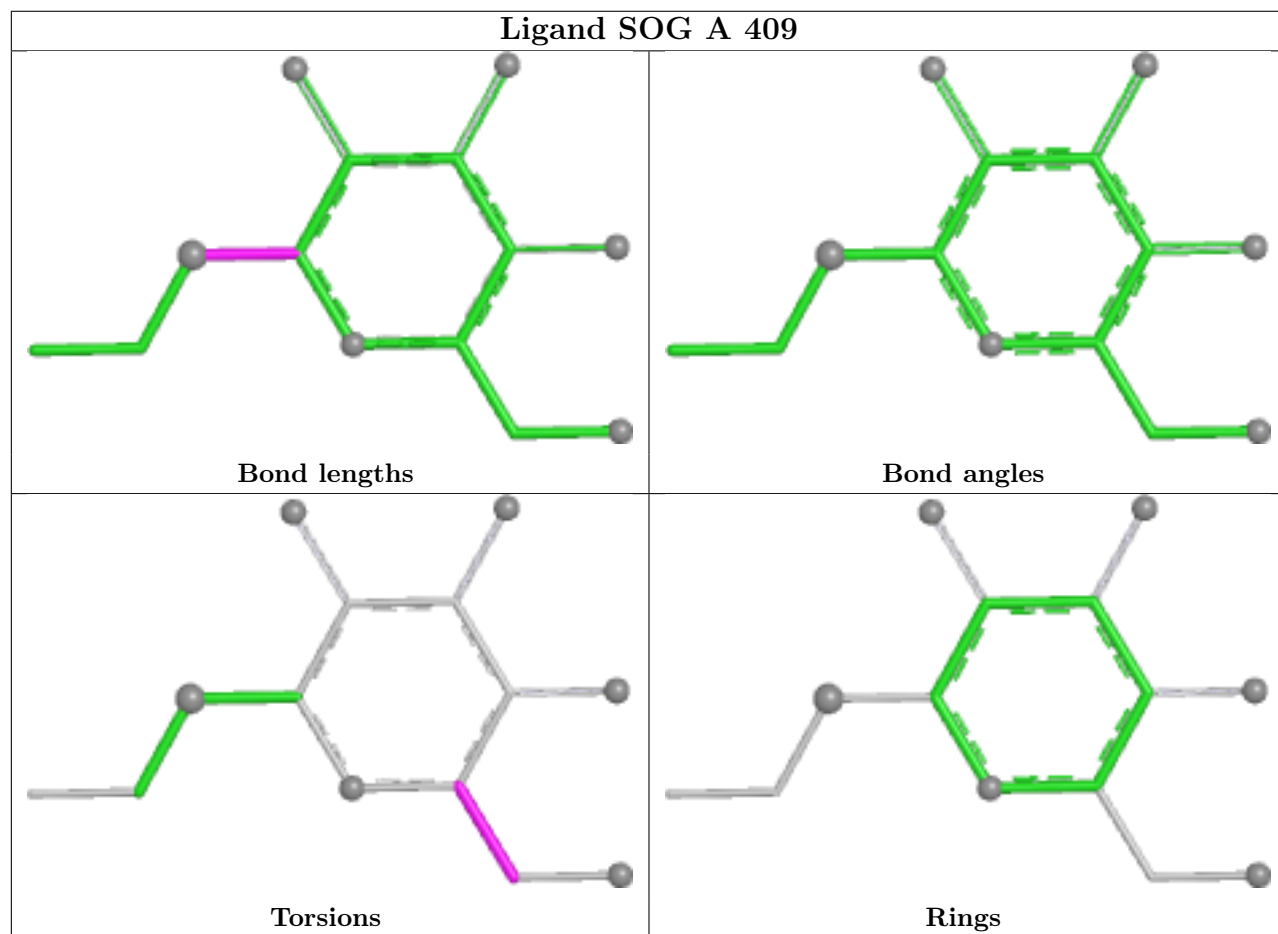
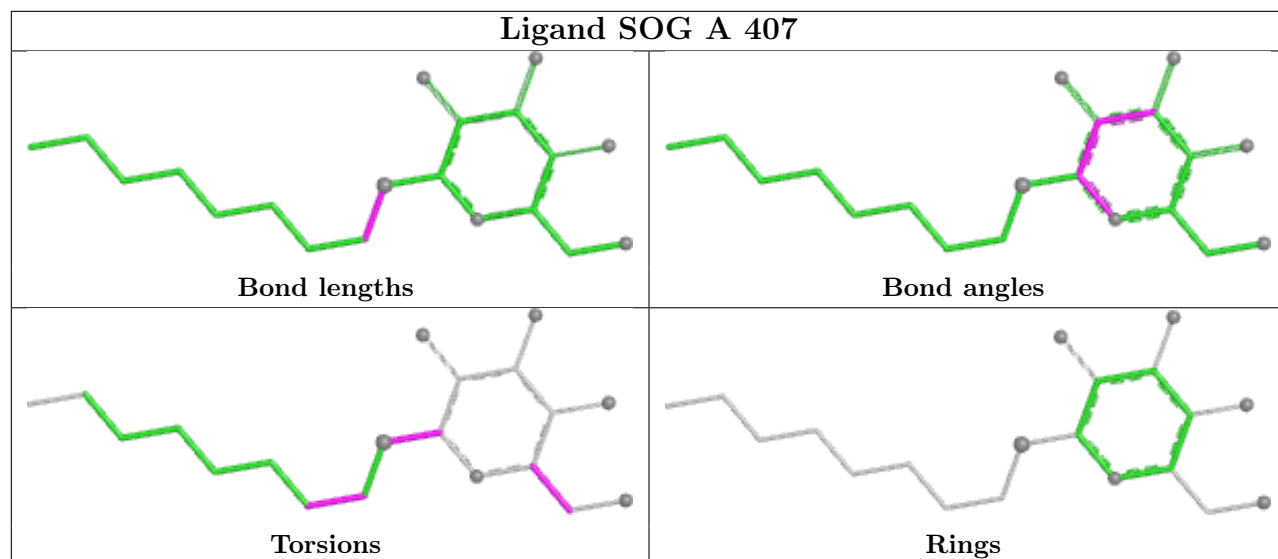
There are no ring outliers.

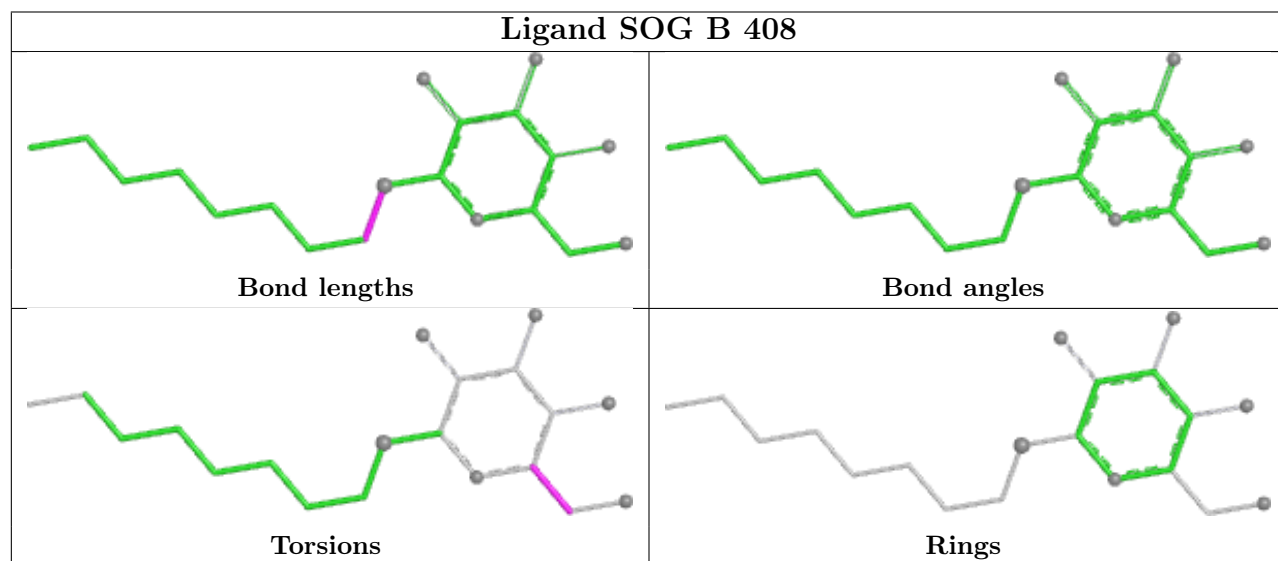
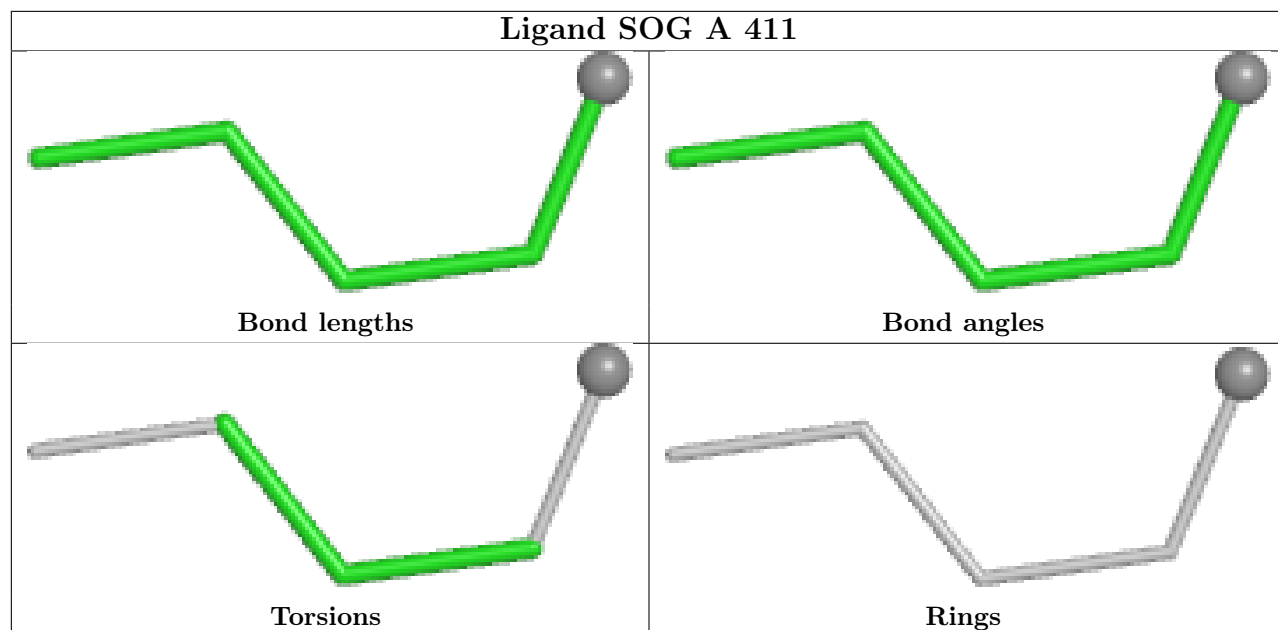
9 monomers are involved in 25 short contacts:

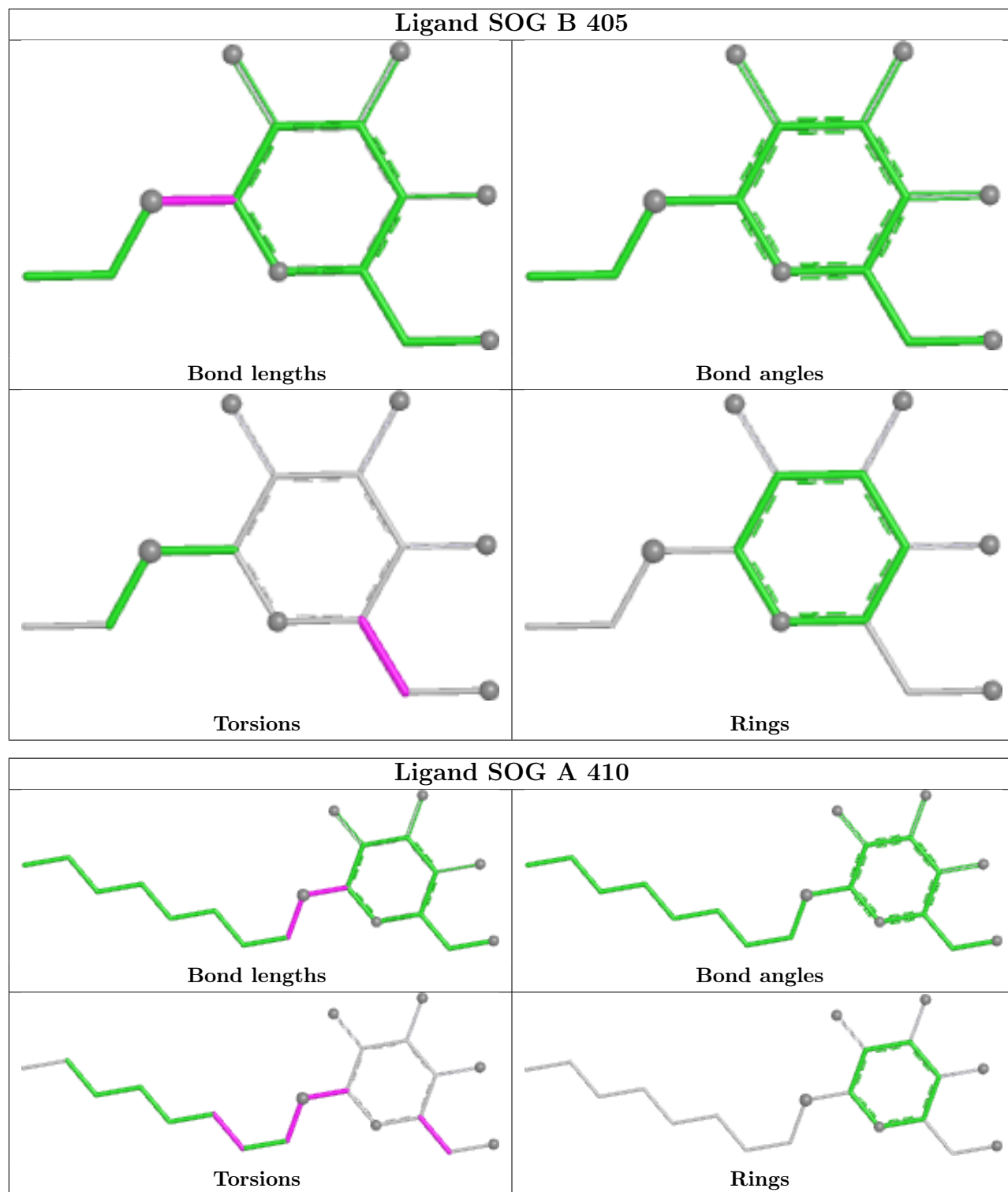
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	SOG	1	0
5	B	409	SOG	2	0
5	A	412	SOG	2	0
4	B	404	PGW	4	0
3	B	403	SO4	1	0
4	A	404	PGW	11	0
5	A	406	SOG	2	0
2	A	401	NV8	1	0
2	B	401	NV8	1	0

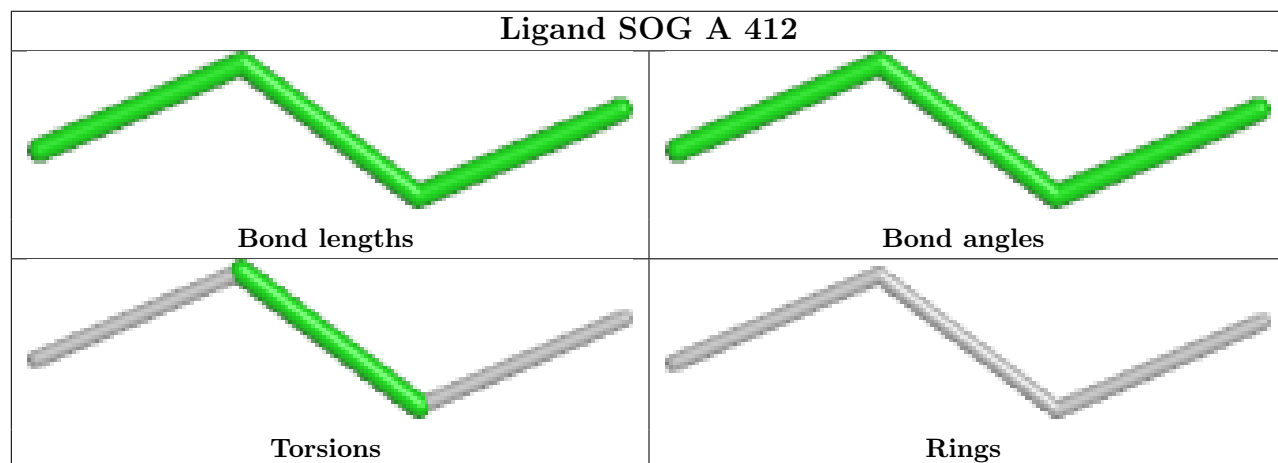
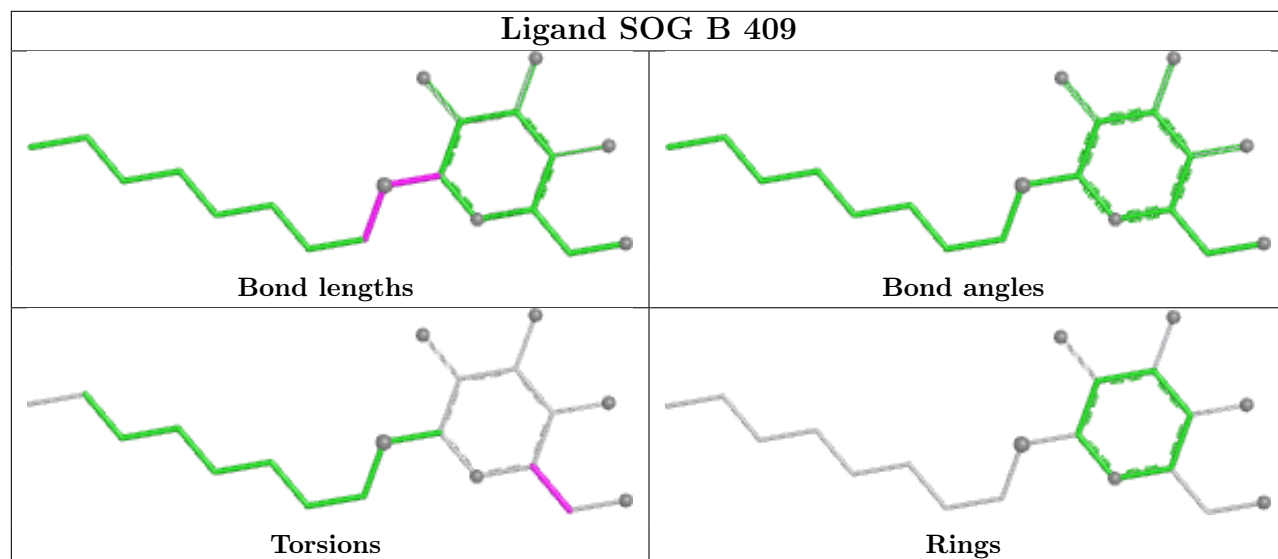
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

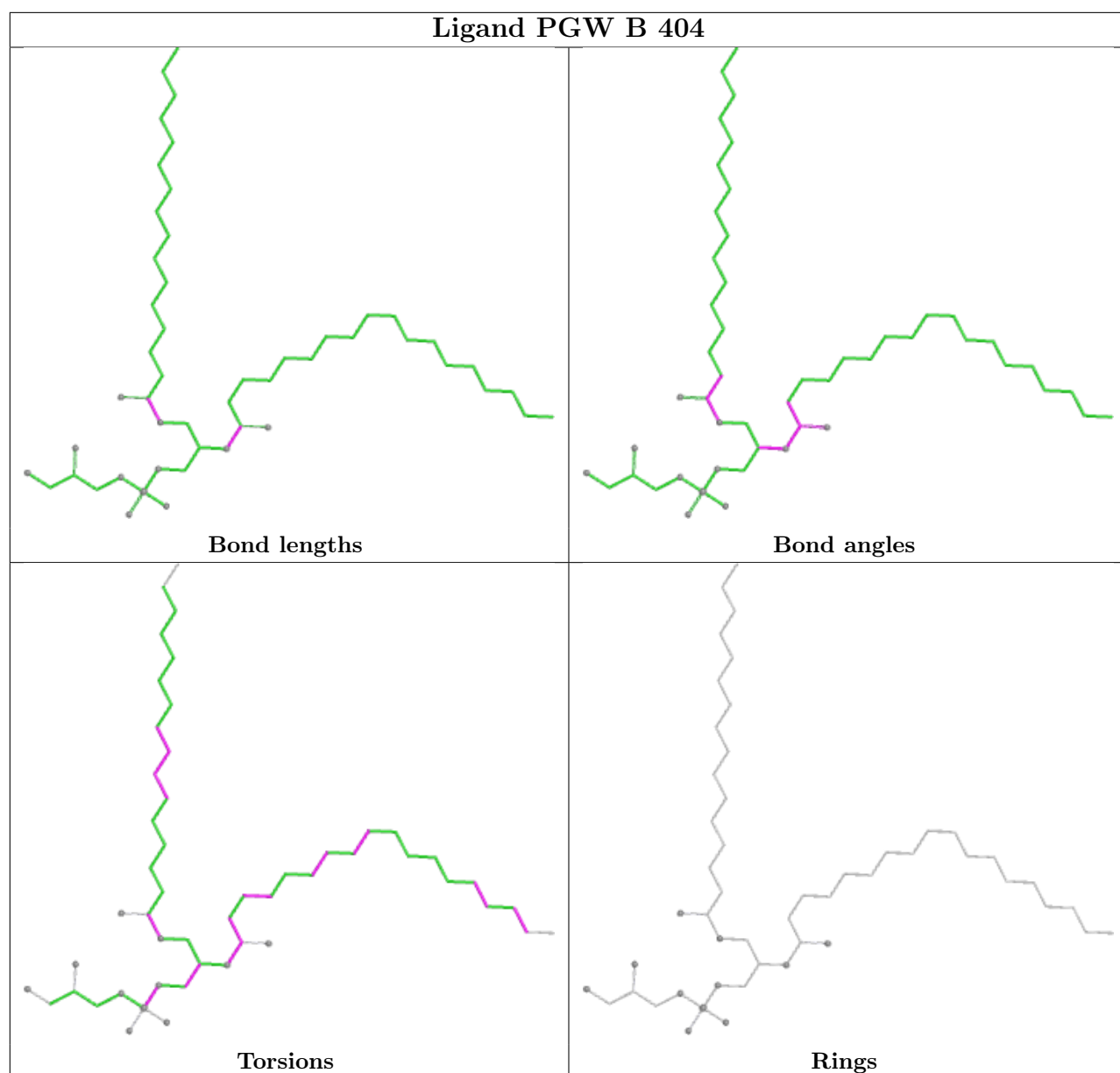


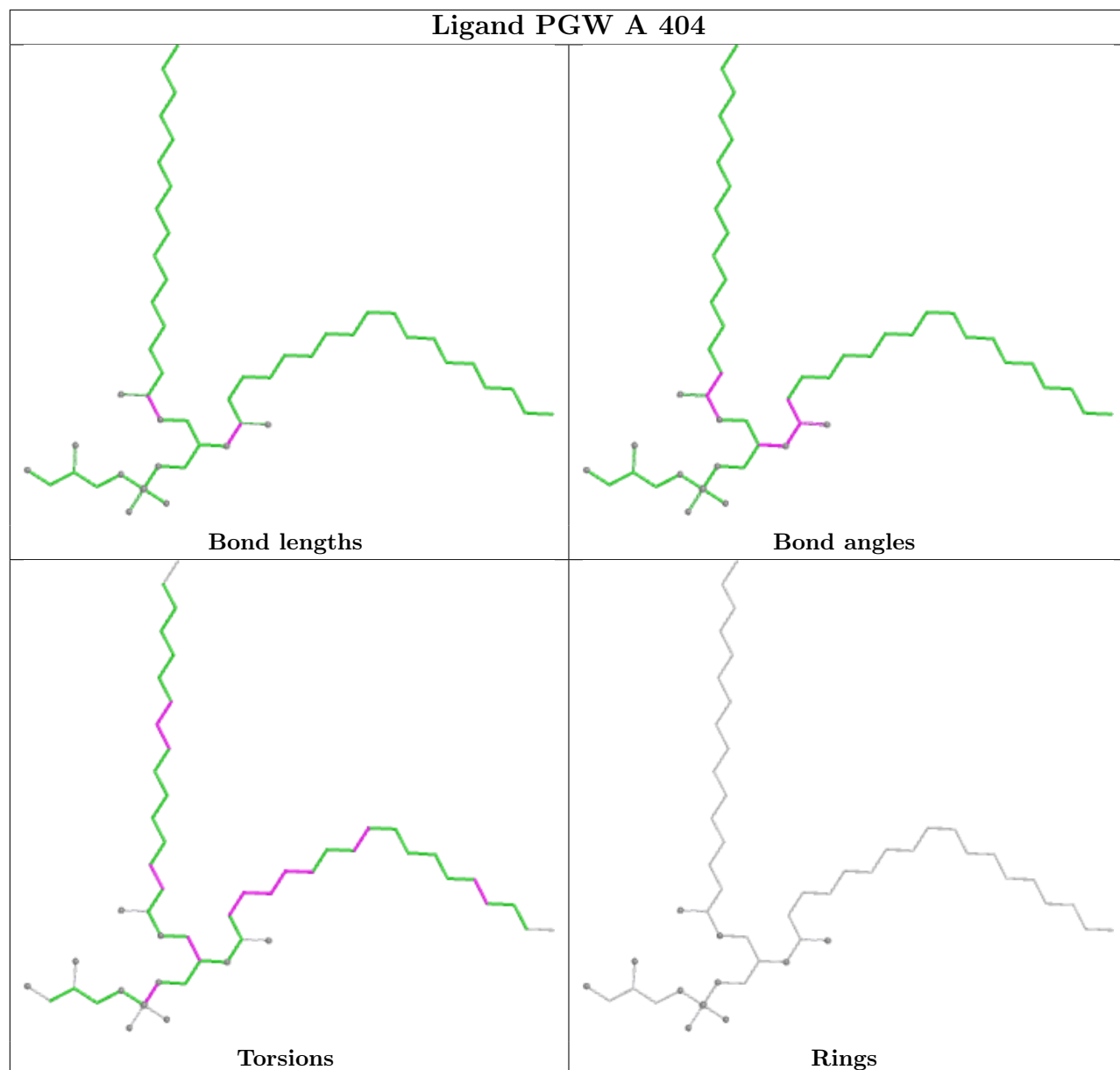




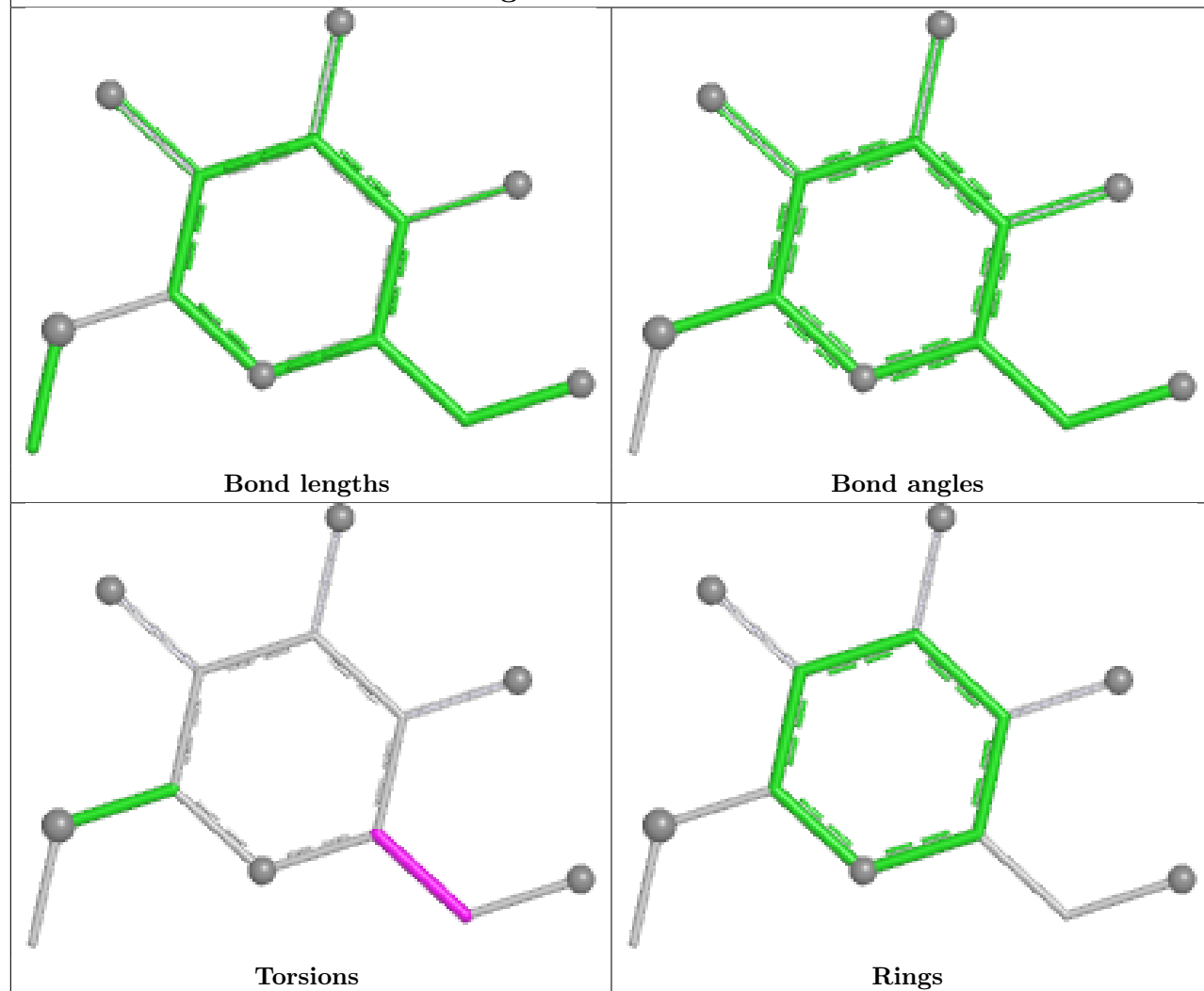




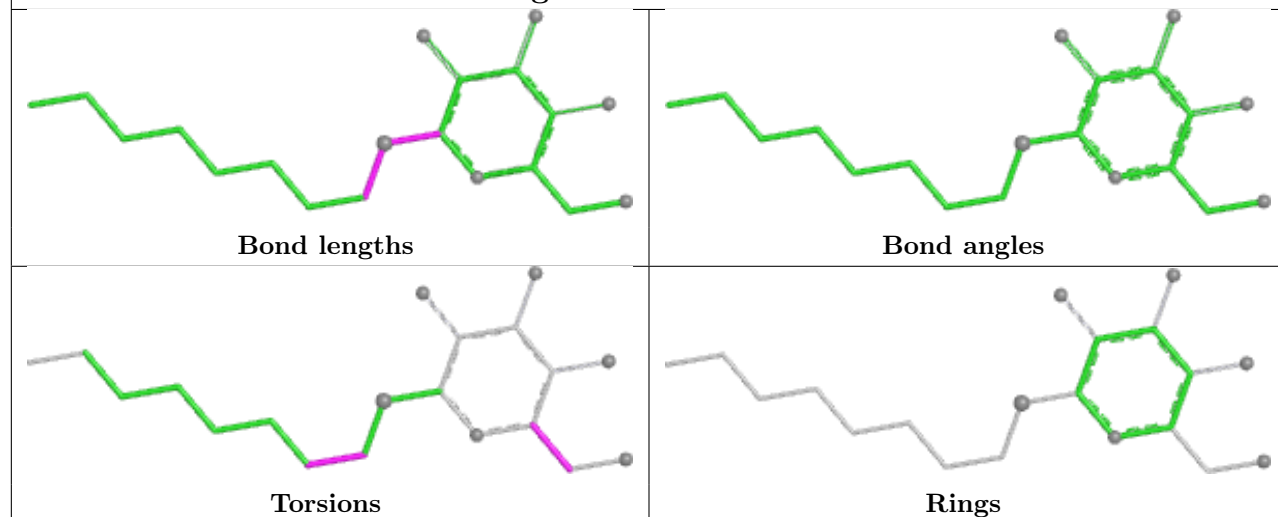


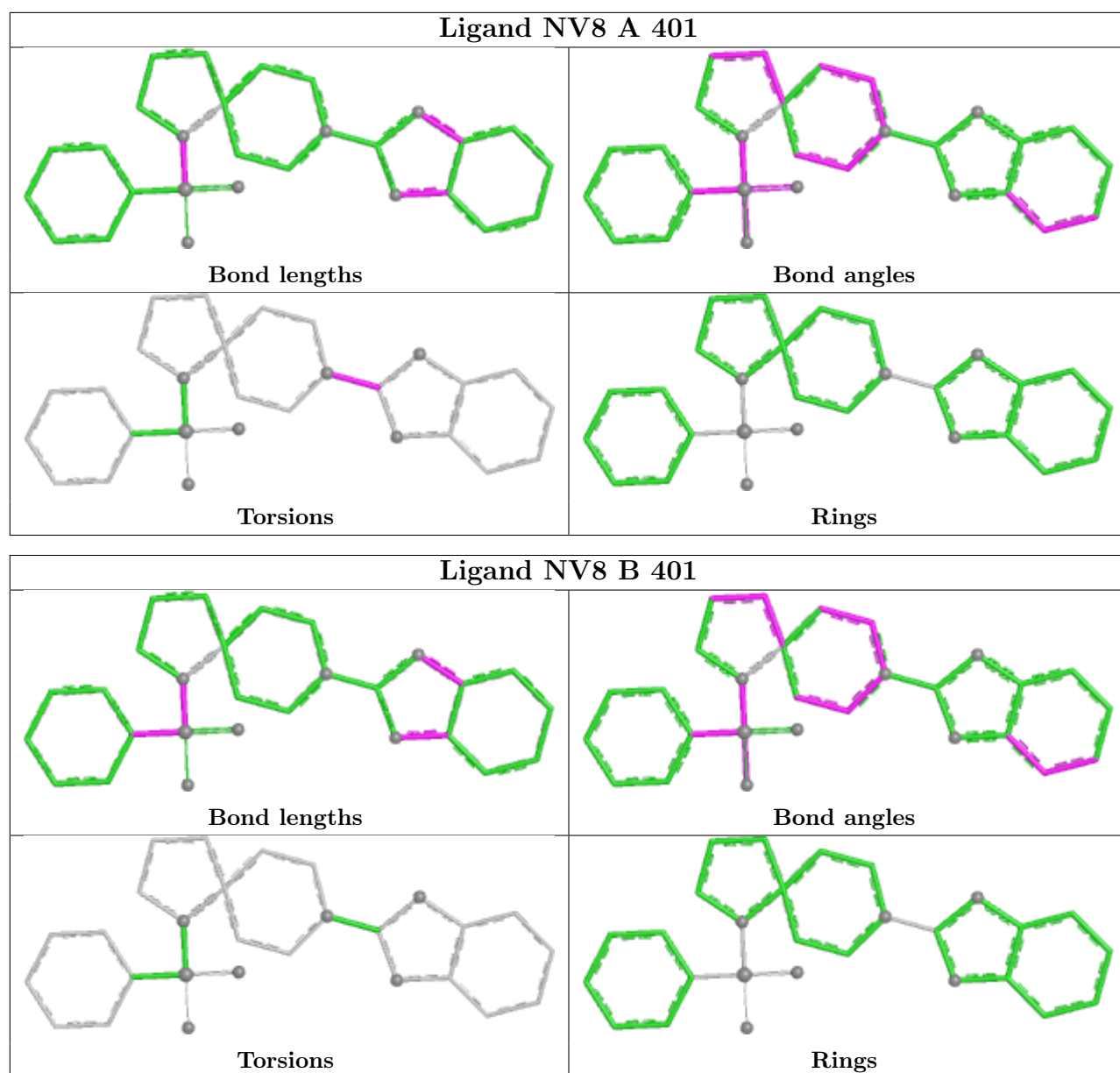


Ligand SOG A 408



Ligand SOG A 406





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/368 (80%)	0.87	45 (15%) 5 6	44, 74, 125, 178	0
1	B	299/368 (81%)	0.82	41 (13%) 6 7	47, 73, 133, 171	0
All	All	596/736 (80%)	0.85	86 (14%) 6 7	44, 73, 130, 178	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ALA	8.1
1	A	331	SER	8.1
1	B	288	LYS	7.8
1	B	108	ILE	7.5
1	B	287	VAL	6.9
1	B	107	ASP	6.1
1	B	242	LEU	6.0
1	B	46	ALA	5.9
1	B	337	TYR	5.9
1	A	108	ILE	5.8
1	A	78	ARG	5.6
1	B	47	TRP	5.4
1	B	329	GLN	5.3
1	A	287	VAL	5.2
1	B	45	TYR	5.2
1	B	291	ARG	5.1
1	A	114	PHE	5.0
1	B	110	GLU	5.0
1	A	298	LYS	4.7
1	B	72	TRP	4.6
1	A	330	ALA	4.5
1	A	83	TYR	4.5
1	A	135	LEU	4.1
1	A	105	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	241	LYS	4.0
1	A	27	SER	4.0
1	A	332	ASP	3.9
1	A	109	THR	3.9
1	B	377	LEU	3.7
1	A	104	LEU	3.5
1	A	361	LEU	3.5
1	A	334	GLU	3.4
1	A	69	LEU	3.4
1	A	113	LEU	3.4
1	A	160	ARG	3.4
1	B	375	TRP	3.3
1	B	245	ARG	3.3
1	B	189	LEU	3.3
1	B	86	VAL	3.3
1	B	247	ILE	3.2
1	B	252	SER	3.2
1	B	246	GLN	3.1
1	A	243	TRP	3.1
1	A	375	TRP	3.1
1	A	106	VAL	3.1
1	B	235	TYR	3.0
1	A	301	MET	3.0
1	B	48	VAL	2.9
1	A	117	ALA	2.8
1	B	106	VAL	2.7
1	A	239	PHE	2.7
1	A	166	LEU	2.6
1	B	285	ALA	2.6
1	B	251	THR	2.6
1	B	378	PRO	2.6
1	A	153	LEU	2.5
1	B	248	PRO	2.5
1	B	114	PHE	2.5
1	B	292	ALA	2.5
1	A	167	GLY	2.5
1	B	290	MET	2.4
1	A	291	ARG	2.4
1	B	68	CYS	2.4
1	A	374	SER	2.4
1	A	299	MET	2.4
1	B	162	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	289	GLN	2.3
1	A	134	VAL	2.3
1	A	199	PHE	2.3
1	B	238	ILE	2.3
1	A	289	GLN	2.3
1	B	149	CYS	2.2
1	A	207	ALA	2.2
1	B	115	GLY	2.2
1	A	73	ARG	2.2
1	A	45	TYR	2.2
1	A	72	TRP	2.2
1	A	158	ALA	2.2
1	A	188	VAL	2.1
1	B	111	SER	2.1
1	B	190	PRO	2.1
1	A	115	GLY	2.1
1	A	164	SER	2.0
1	B	196	THR	2.0
1	A	118	LEU	2.0
1	A	205	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SOG	A	409	14/20	0.42	0.24	136,148,152,155	0
5	SOG	A	408	13/20	0.59	0.20	135,145,149,149	0
3	SO4	A	403	5/5	0.61	0.13	124,126,127,133	0

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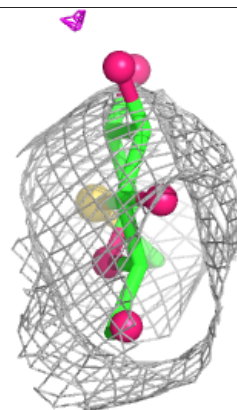
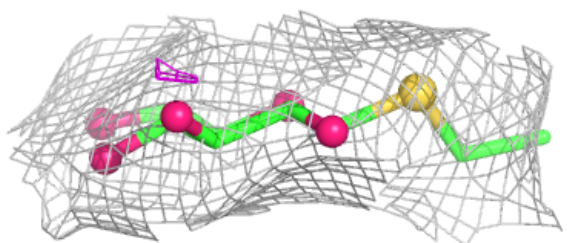
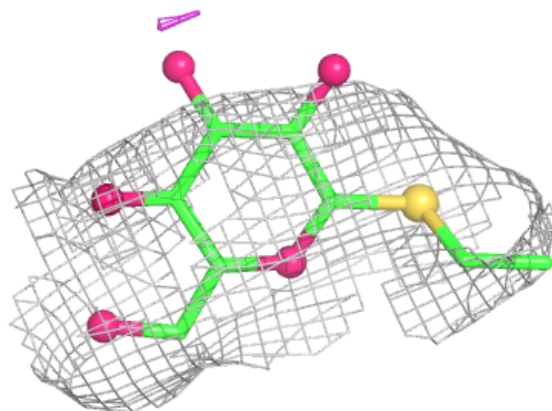
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SOG	A	411	5/20	0.65	0.58	107,112,139,157	0
5	SOG	B	405	14/20	0.68	0.31	160,165,167,168	0
5	SOG	B	409	20/20	0.70	0.22	122,127,138,140	0
5	SOG	A	407	20/20	0.71	0.19	71,126,140,141	0
5	SOG	B	408	20/20	0.71	0.20	102,141,151,156	0
3	SO4	B	403	5/5	0.71	0.12	106,112,120,124	0
5	SOG	B	406	13/20	0.72	0.13	104,124,127,129	0
2	NV8	B	401	28/28	0.73	0.25	80,132,160,162	0
5	SOG	A	412	4/20	0.75	0.41	69,72,74,82	0
5	SOG	A	406	20/20	0.83	0.20	69,125,133,137	0
2	NV8	A	401	28/28	0.87	0.16	81,115,143,145	0
5	SOG	B	407	5/20	0.87	0.19	90,95,99,105	0
4	PGW	B	404	51/51	0.88	0.18	44,79,147,155	0
5	SOG	A	410	20/20	0.88	0.16	86,113,128,128	0
4	PGW	A	404	51/51	0.88	0.17	49,77,145,148	0
3	SO4	A	402	5/5	0.89	0.09	95,97,104,108	0
5	SOG	A	405	20/20	0.89	0.14	73,110,123,123	0
6	NA	A	413	1/1	0.92	0.19	82,82,82,82	0
3	SO4	B	402	5/5	0.94	0.06	88,96,101,111	0

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

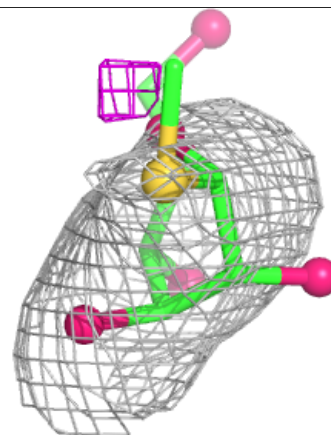
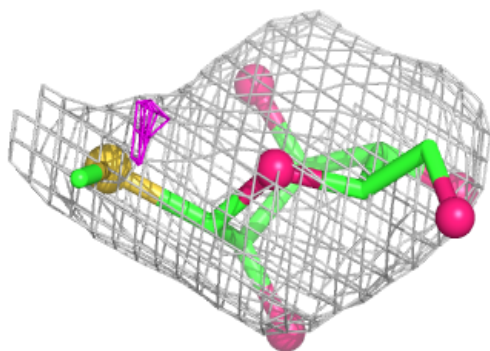
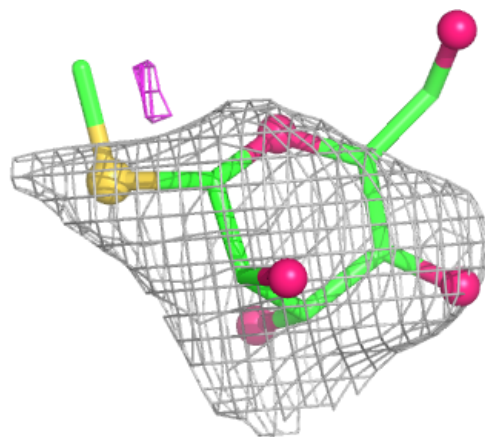
Electron density around SOG A 409:

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

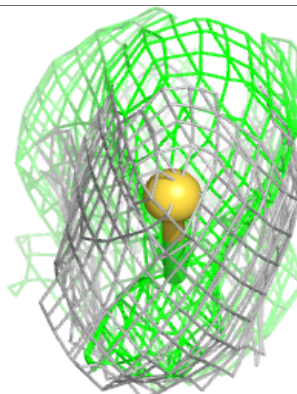
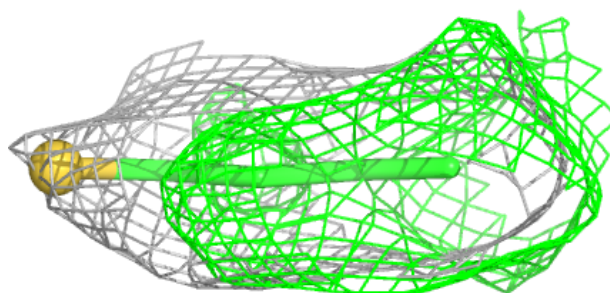
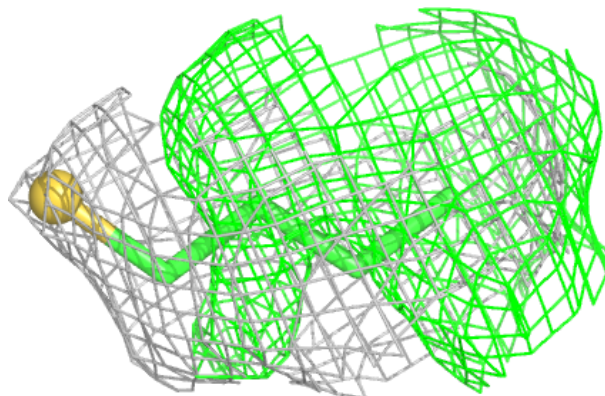


Electron density around SOG A 408:

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

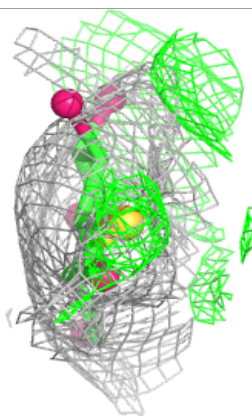
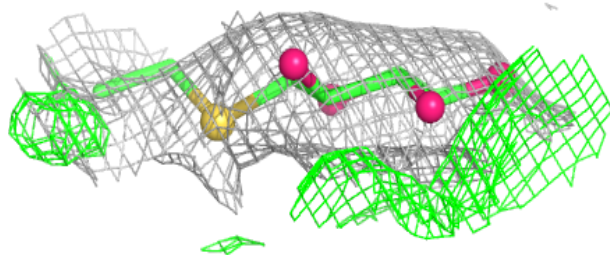
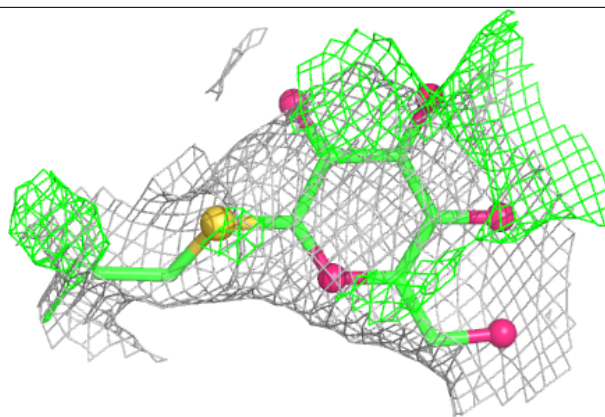
**Electron density around SOG A 411:**

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

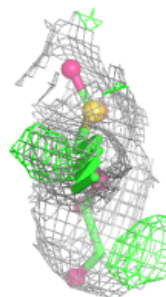
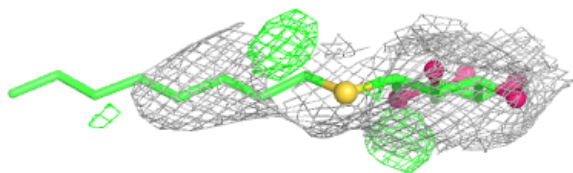
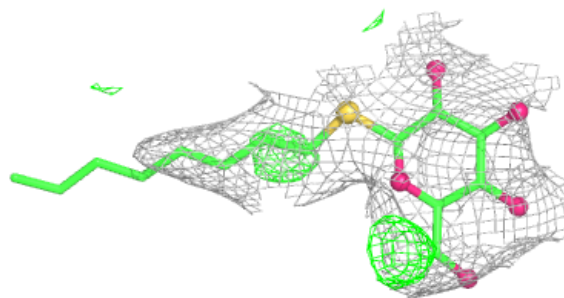


Electron density around SOG B 405:

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

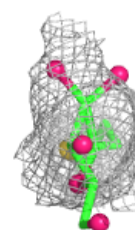
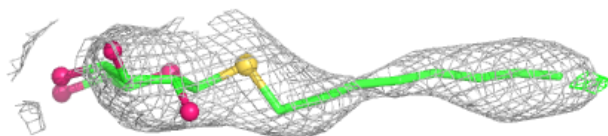
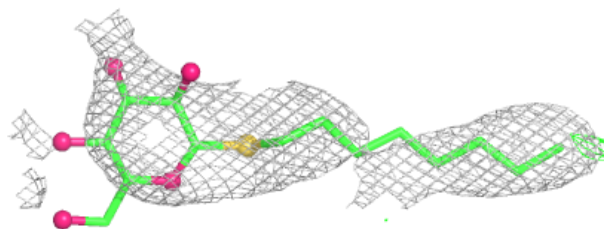
**Electron density around SOG B 409:**

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

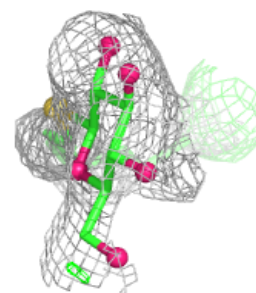
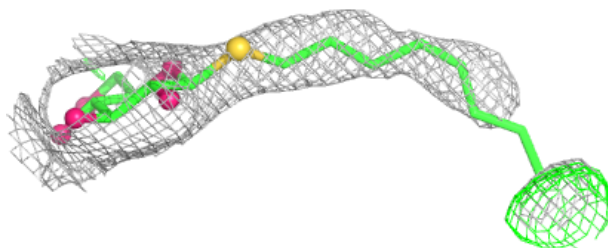
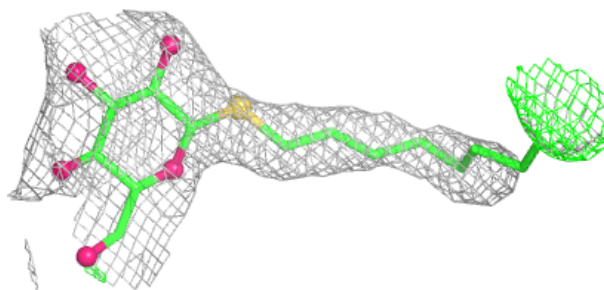


Electron density around SOG A 407:

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

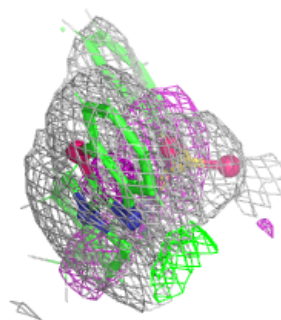
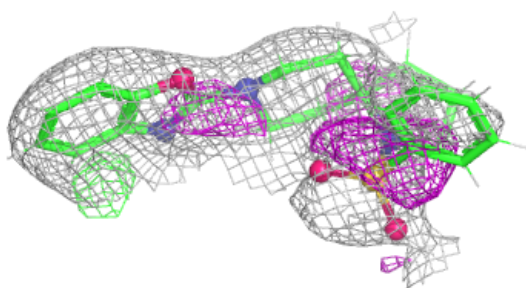
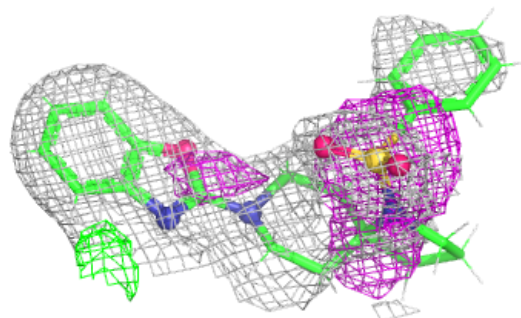
**Electron density around SOG B 408:**

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

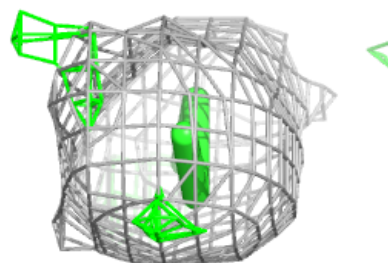
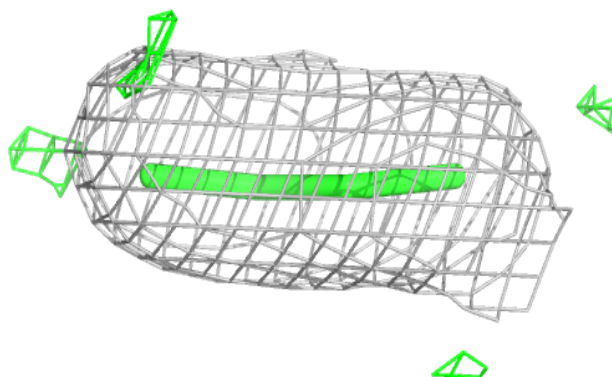
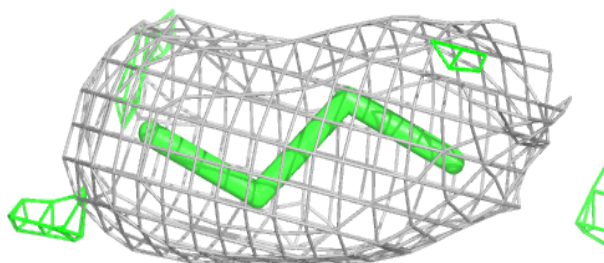


Electron density around NV8 B 401:

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

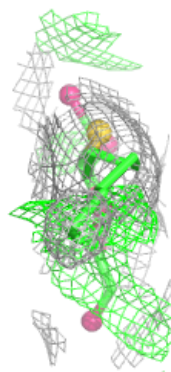
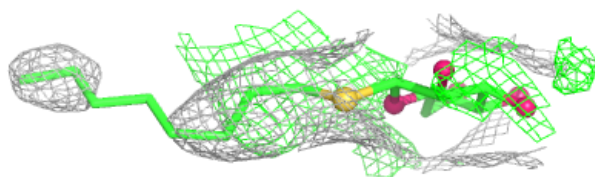
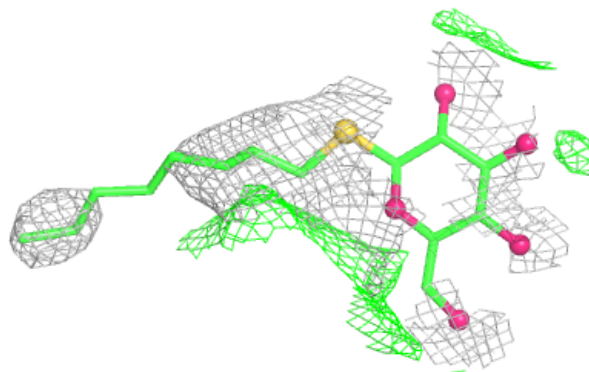
**Electron density around SOG A 412:**

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

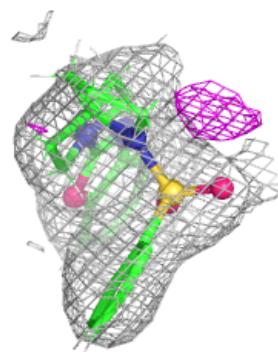
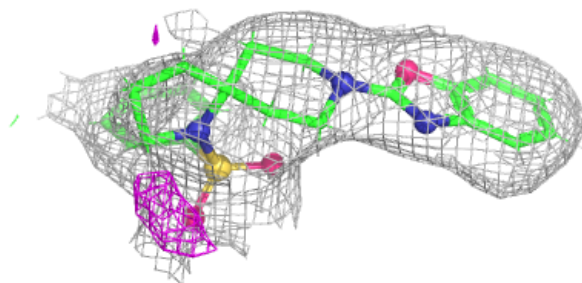
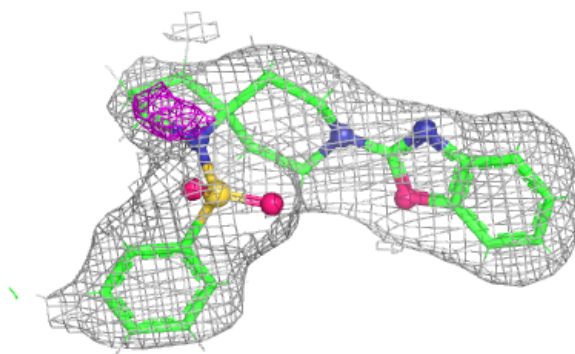


Electron density around SOG A 406:

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

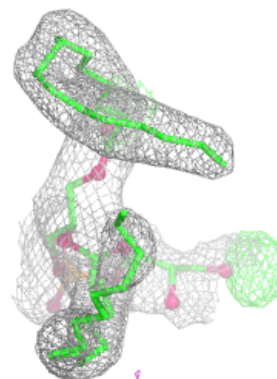
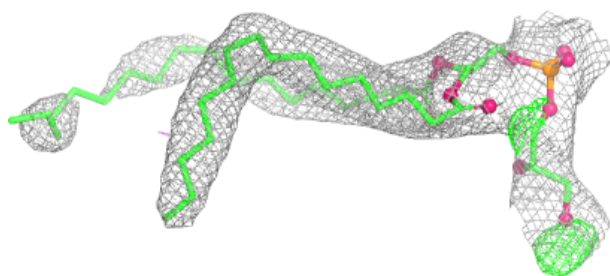
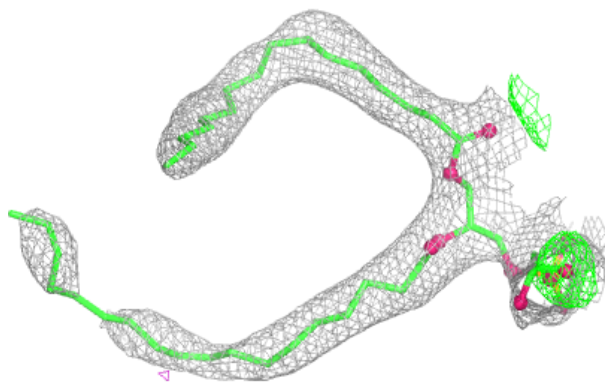
**Electron density around NV8 A 401:**

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

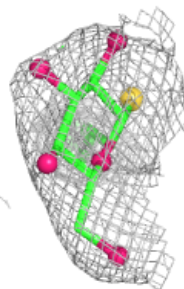
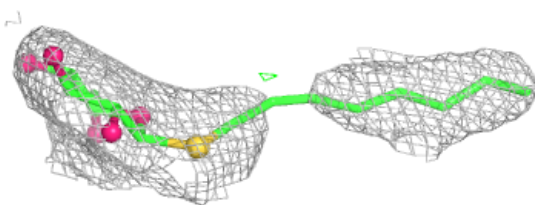
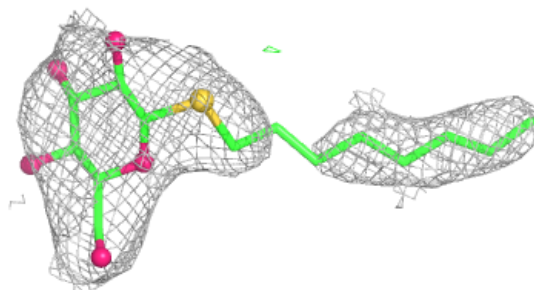


Electron density around PGW B 404:

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

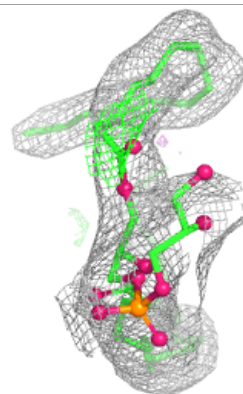
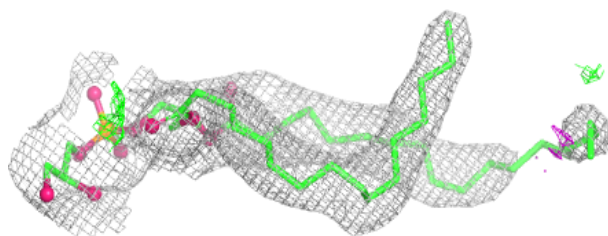
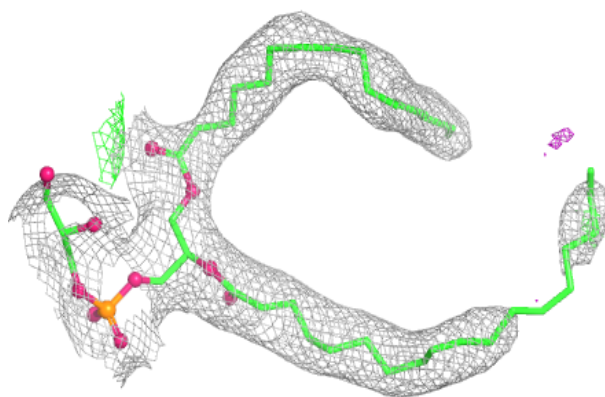
**Electron density around SOG A 410:**

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

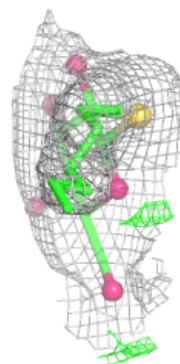
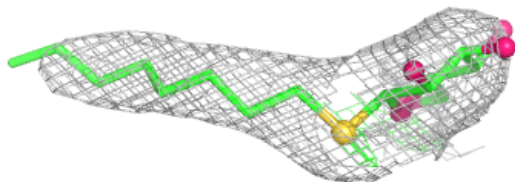
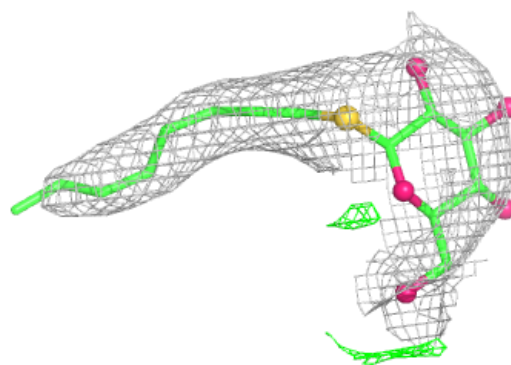


Electron density around PGW A 404:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.