



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:05 AM UTC

PDB ID : 6TP3 / pdb_00006tp3
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 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)
Xtrriage (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

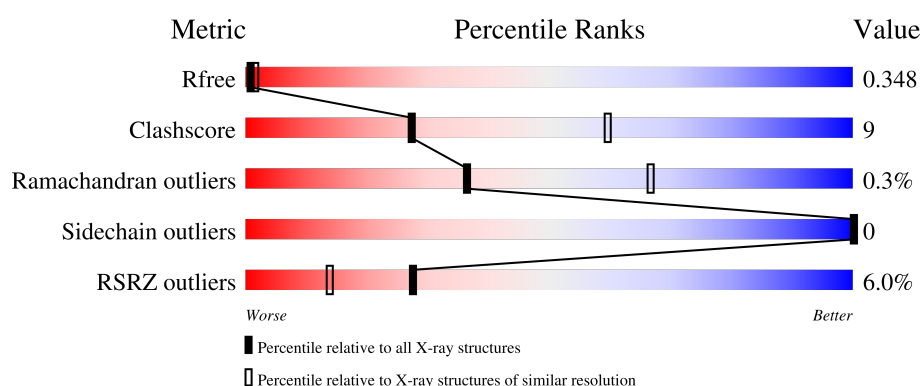
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (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 $\leq 5\%$. 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	3% 70% 13% 15%
1	B	368	7% 72% 11% 17%

2 Entry composition

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:

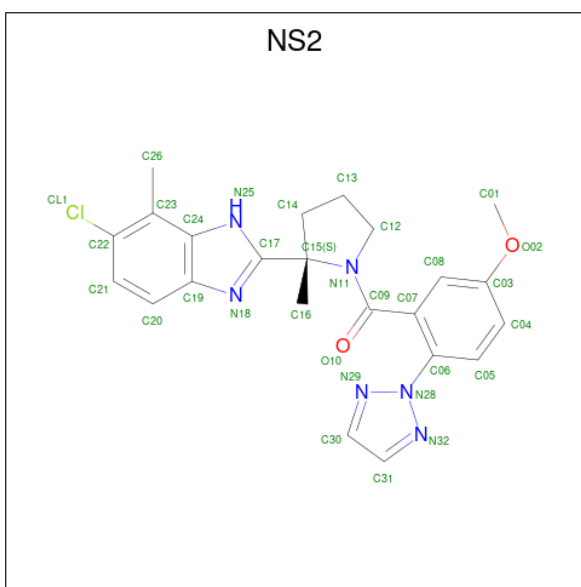
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU	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 (CCD ID: NS2) (formula: C₂₃H₂₃ClN₆O₂) (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 (CCD ID: SO4) (formula: O₄S).



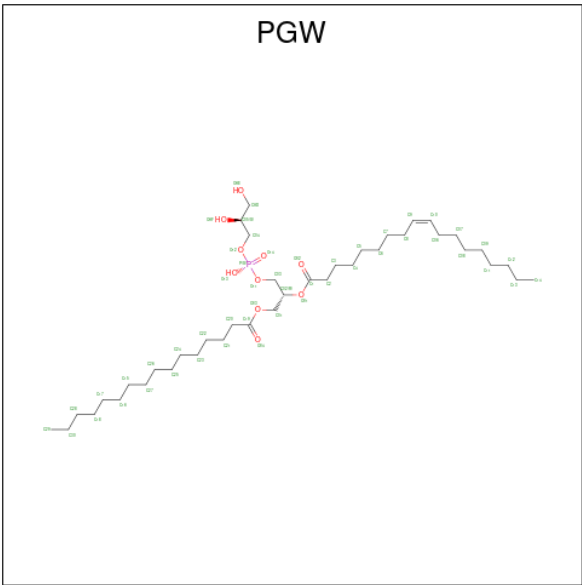
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		

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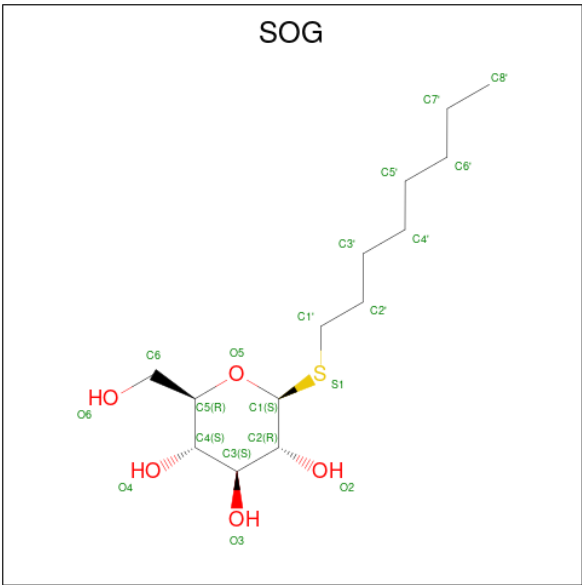
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- 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: C₄₀H₇₇O₁₀P).



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: C₁₄H₂₈O₅S).

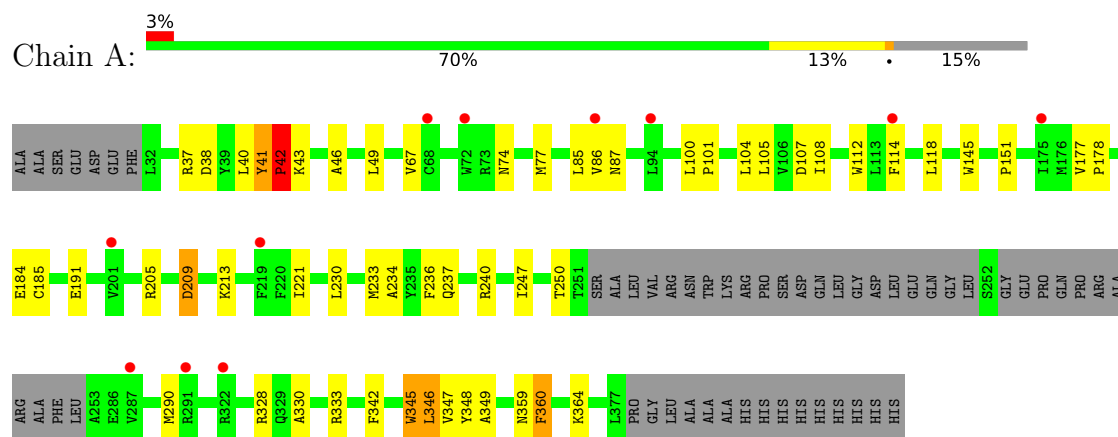


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			20	14	5	1		
			Total	C	O	S		
			20	14	5	1		
			Total	C	O	S		
5	A	1	20	14	5	1	0	0
			Total	C	O	S		
			14	8	5	1		
			Total	C	O	S		
			20	14	5	1		
5	A	1	Total	C	O	S	0	0
			20	14	5	1		
			Total	C	O	S		
			20	14	5	1		
			Total	C	O	S		
5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

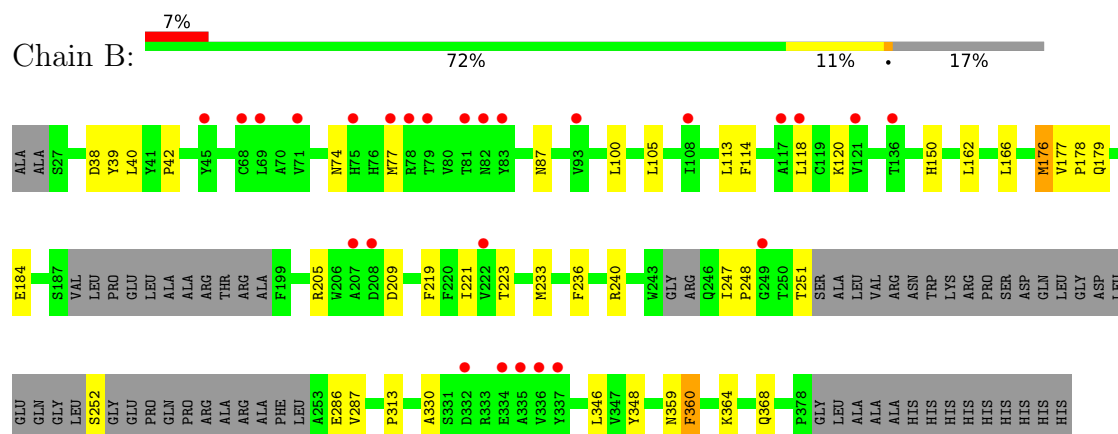
3 Residue-property plots [i](#)

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

• Molecule 1: Orexin receptor type 1



• Molecule 1: Orexin receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	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 25.86 – 3.04	Depositor EDS
% Data completeness (in resolution range)	58.6 (25.86-3.04) 77.6 (25.86-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.15 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.205 , 0.230 0.257 , 0.348	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)	0.24 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SOG, PGW, NS2, SO4

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	0.81	1/2587 (0.0%)	1.27	14/3529 (0.4%)
1	B	0.80	0/2538	1.22	7/3460 (0.2%)
All	All	0.81	1/5125 (0.0%)	1.24	21/6989 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	MET	SD-CE	6.28	1.95	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	VAL	N-CA-C	-11.61	99.28	110.42
1	A	345	TRP	N-CA-C	9.05	120.75	111.07
1	A	87	ASN	N-CA-C	-8.16	102.46	111.36
1	A	347	VAL	N-CA-CB	8.12	120.05	110.55
1	B	87	ASN	N-CA-C	-6.60	104.17	111.36
1	A	360	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	85	LEU	N-CA-C	5.87	118.46	111.71
1	B	360	PHE	CA-CB-CG	5.81	119.61	113.80
1	B	38	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	87	ASN	N-CA-CB	5.73	118.63	110.16
1	A	328	ARG	CA-C-N	5.63	130.35	121.56
1	A	328	ARG	C-N-CA	5.63	130.35	121.56
1	B	330	ALA	CA-C-N	5.50	129.94	121.19
1	B	330	ALA	C-N-CA	5.50	129.94	121.19
1	A	346	LEU	N-CA-C	5.45	119.19	112.54
1	A	42	PRO	CA-N-CD	5.36	119.50	112.00
1	A	209	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	151	PRO	N-CA-C	5.18	120.88	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	MET	CA-C-N	5.07	123.43	120.24
1	B	176	MET	C-N-CA	5.07	123.43	120.24
1	A	191	GLU	CB-CG-CD	5.00	121.11	112.60

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	60	2
1	B	2467	0	2508	42	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
4	B	51	0	76	2	0
5	A	134	0	181	6	0
5	B	102	0	121	6	0
All	All	5399	46	5543	100	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.

All (100) 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:233:MET:HE1	1:B:178:PRO:HB3	1.40	1.00
1:A:41:TYR:HB3	1:A:42:PRO:CD	1.92	1.00
1:A:41:TYR:CB	1:A:42:PRO:HD3	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:CB	1:A:42:PRO:CD	2.44	0.94
1:A:41:TYR:HD2	1:A:42:PRO:HD3	1.18	0.94
1:A:234:ALA:HB2	4:A:404:PGW:H7A	1.45	0.93
1:A:178:PRO:HB3	1:B:233:MET:HE1	1.52	0.91
1:A:41:TYR:CD2	1:A:42:PRO:CD	2.54	0.89
1:A:345:TRP:HE3	1:A:346:LEU:CD1	1.85	0.89
1:A:41:TYR:HB3	1:A:42:PRO:HD2	1.51	0.88
1:A:101:PRO:HB2	5:A:405:SOG:H8'1	1.55	0.87
1:A:41:TYR:HD2	1:A:42:PRO:CD	1.92	0.78
1:A:43:LYS:NZ	1:A:107:ASP:O	2.16	0.75
1:B:150:HIS:HE1	5:B:409:SOG:H1	1.52	0.73
1:A:345:TRP:CE3	1:A:346:LEU:CD1	2.64	0.72
1:B:184:GLU:HG3	1:B:205:ARG:HD2	1.72	0.71
1:B:120:LYS:HZ2	5:B:410:SOG:H6'1	1.56	0.70
1:A:41:TYR:HB3	1:A:42:PRO:HD3	1.65	0.68
1:A:145:TRP:HE1	1:A:237:GLN:HE21	1.43	0.67
1:B:150:HIS:CE1	5:B:409:SOG:H1	2.30	0.66
1:A:342:PHE:CZ	1:A:346:LEU:HD11	2.30	0.66
1:B:74:ASN:HB3	1:B:77:MET:HE2	1.77	0.65
1:A:346:LEU:HD12	1:A:346:LEU:N	2.12	0.65
1:A:49:LEU:HD23	1:A:108:ILE:CD1	2.27	0.65
1:A:74:ASN:HB3	1:A:77:MET:HE2	1.78	0.64
1:A:38:ASP:HA	5:A:411:SOG:H62	1.79	0.63
1:A:346:LEU:HA	1:A:349:ALA:HB3	1.81	0.63
1:A:114:PHE:HB3	1:A:118:LEU:HD12	1.82	0.61
1:B:247:ILE:N	1:B:248:PRO:HD3	2.15	0.61
1:B:251:THR:HB	1:B:286:GLU:CB	2.31	0.61
1:A:213:LYS:HD3	5:A:410:SOG:H2	1.84	0.59
1:A:359:ASN:HD22	1:A:360:PHE:HD1	1.49	0.59
1:B:114:PHE:HB3	1:B:118:LEU:HD12	1.84	0.59
1:A:77:MET:SD	1:A:364:LYS:HB3	2.44	0.58
1:A:49:LEU:HD23	1:A:108:ILE:HD11	1.85	0.58
1:B:251:THR:HG22	1:B:252:SER:N	2.19	0.57
1:B:77:MET:SD	1:B:364:LYS:HB3	2.45	0.56
1:A:342:PHE:O	1:A:346:LEU:HD13	2.05	0.56
1:B:251:THR:HB	1:B:286:GLU:HB2	1.86	0.56
1:B:247:ILE:HG23	1:B:247:ILE:O	2.06	0.55
1:A:43:LYS:H	1:A:46:ALA:HB2	1.72	0.55
1:A:346:LEU:HA	1:A:349:ALA:CB	2.37	0.54
1:B:74:ASN:HB2	1:B:368:GLN:NE2	2.23	0.54
1:B:120:LYS:NZ	5:B:410:SOG:H6'1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HG13	1:B:221:ILE:HD12	1.89	0.53
1:A:346:LEU:CD1	1:A:346:LEU:N	2.71	0.53
1:A:49:LEU:HD23	1:A:108:ILE:HD13	1.92	0.52
1:A:118:LEU:HD11	5:A:405:SOG:H1'1	1.91	0.52
1:A:342:PHE:CE2	1:A:346:LEU:HD21	2.46	0.51
1:B:105:LEU:HD21	1:B:113:LEU:HD12	1.92	0.51
1:A:346:LEU:CD1	1:A:346:LEU:H	2.24	0.50
1:A:342:PHE:CE1	1:A:346:LEU:HD11	2.47	0.49
1:A:112:TRP:CD1	1:A:185:CYS:HG	2.30	0.49
1:B:247:ILE:N	1:B:248:PRO:CD	2.77	0.48
1:A:209:ASP:HB2	5:A:407:SOG:O6	2.13	0.48
1:B:359:ASN:HD22	1:B:360:PHE:HD1	1.62	0.47
1:A:100:LEU:HD12	1:A:348:TYR:HB3	1.96	0.47
1:B:219:PHE:O	1:B:223:THR:HG23	2.15	0.47
1:B:209:ASP:HB2	5:B:404:SOG:H1'1	1.95	0.47
1:B:100:LEU:HD12	1:B:348:TYR:HB3	1.95	0.47
1:B:105:LEU:HD23	1:B:114:PHE:CZ	2.50	0.46
2:B:401:NS2:C09	2:B:401:NS2:N29	2.79	0.46
1:B:251:THR:HB	1:B:286:GLU:HB3	1.97	0.46
1:B:287:VAL:O	1:B:287:VAL:HG12	2.15	0.46
1:A:184:GLU:HG3	1:A:205:ARG:NE	2.31	0.45
1:A:330:ALA:HA	1:A:333:ARG:HG3	1.98	0.45
1:B:114:PHE:HA	5:B:408:SOG:H5	1.99	0.45
1:A:37:ARG:HA	1:A:40:LEU:HB2	1.99	0.45
2:A:401:NS2:N29	2:A:401:NS2:C09	2.80	0.45
1:A:67:VAL:HG12	1:A:86:VAL:HG12	2.00	0.44
1:A:233:MET:CE	1:B:178:PRO:HB3	2.29	0.44
1:A:177:VAL:N	1:A:178:PRO:HD2	2.31	0.44
1:B:39:TYR:C	1:B:42:PRO:HD2	2.43	0.44
1:B:233:MET:HE2	4:B:403:PGW:H3	1.99	0.44
1:A:247:ILE:HG23	1:A:250:THR:CG2	2.47	0.44
1:B:236:PHE:CE2	1:B:240:ARG:HD2	2.53	0.44
1:A:104:LEU:O	1:A:108:ILE:HG12	2.18	0.44
1:B:162:LEU:O	1:B:166:LEU:HD13	2.17	0.44
1:B:177:VAL:N	1:B:178:PRO:HD2	2.33	0.43
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.80	0.43
1:A:342:PHE:CZ	1:A:346:LEU:HD21	2.53	0.43
1:B:176:MET:O	1:B:179:GLN:HB3	2.19	0.43
1:B:251:THR:HG22	1:B:252:SER:H	1.80	0.43
1:A:230:LEU:HD13	4:A:404:PGW:H07A	2.01	0.43
1:B:247:ILE:HD11	1:B:287:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:CE2	1:A:240:ARG:HD2	2.55	0.42
5:A:409:SOG:H7'2	1:B:236:PHE:HB2	1.99	0.42
1:B:251:THR:CG2	1:B:252:SER:N	2.83	0.42
1:B:100:LEU:C	1:B:100:LEU:HD23	2.45	0.41
1:B:77:MET:HE1	1:B:368:GLN:HG3	2.03	0.41
1:A:100:LEU:C	1:A:100:LEU:HD23	2.46	0.41
1:A:178:PRO:HD3	4:B:403:PGW:H3A	2.01	0.41
1:A:41:TYR:HD2	1:A:42:PRO:CG	2.34	0.41
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.91	0.41
1:A:234:ALA:CB	4:A:404:PGW:H7A	2.34	0.41
1:B:313:PRO:HG2	1:B:346:LEU:HD12	2.03	0.40

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 ⓘ

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	312/368 (85%)	306 (98%)	4 (1%)	2 (1%)	21	53
1	B	301/368 (82%)	294 (98%)	7 (2%)	0	100	100
All	All	613/736 (83%)	600 (98%)	11 (2%)	2 (0%)	36	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO

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Mol	Chain	Res	Type
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	B	64	ASN
1	B	82	ASN
1	B	150	HIS
1	B	359	ASN

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

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	0.18	0	6,6,6	0.23	0
5	SOG	A	408	-	14,14,20	0.86	0	18,19,25	1.24	2 (11%)
2	NS2	B	401	-	35,36,36	2.78	14 (40%)	43,54,54	2.77	19 (44%)
5	SOG	B	409	-	11,12,20	0.95	0	15,17,25	1.75	2 (13%)
5	SOG	A	407	-	20,20,20	1.07	2 (10%)	24,25,25	1.60	5 (20%)
3	SO4	A	402	-	4,4,4	0.48	0	6,6,6	0.32	0
5	SOG	A	406	-	20,20,20	1.06	1 (5%)	24,25,25	1.47	4 (16%)
4	PGW	B	403	-	50,50,50	1.09	2 (4%)	53,56,56	1.04	3 (5%)
5	SOG	A	410	-	20,20,20	1.07	1 (5%)	24,25,25	0.97	1 (4%)
5	SOG	B	407	-	4,4,20	0.43	0	3,3,25	0.49	0
2	NS2	A	401	-	35,36,36	2.75	14 (40%)	43,54,54	2.69	19 (44%)
5	SOG	B	406	-	12,13,20	0.82	0	17,18,25	0.91	1 (5%)
5	SOG	B	410	-	20,20,20	0.87	1 (5%)	24,25,25	1.09	2 (8%)
5	SOG	A	411	-	20,20,20	0.96	1 (5%)	24,25,25	1.40	4 (16%)
5	SOG	B	408	-	11,12,20	1.09	0	15,17,25	1.43	3 (20%)
4	PGW	A	404	-	50,50,50	1.03	2 (4%)	53,56,56	1.10	4 (7%)
5	SOG	B	405	-	20,20,20	0.93	0	24,25,25	1.65	3 (12%)
5	SOG	B	404	-	20,20,20	1.00	1 (5%)	24,25,25	1.95	5 (20%)
5	SOG	A	409	-	20,20,20	0.85	1 (5%)	24,25,25	1.43	3 (12%)
5	SOG	A	405	-	20,20,20	1.05	1 (5%)	24,25,25	1.36	4 (16%)
3	SO4	A	403	-	4,4,4	0.24	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	A	410	-	-	5/11/31/31	0/1/1/1
5	SOG	B	408	-	-	1/2/22/31	0/1/1/1
5	SOG	A	406	-	-	7/11/31/31	0/1/1/1
4	PGW	B	403	-	-	29/55/55/55	-
5	SOG	B	407	-	-	2/2/2/31	-
4	PGW	A	404	-	-	30/55/55/55	-
2	NS2	A	401	-	-	5/15/33/33	0/5/5/5
5	SOG	A	408	-	-	1/5/25/31	0/1/1/1
2	NS2	B	401	-	-	5/15/33/33	0/5/5/5
5	SOG	B	405	-	-	8/11/31/31	0/1/1/1
5	SOG	B	406	-	-	2/4/24/31	0/1/1/1
5	SOG	B	410	-	-	5/11/31/31	0/1/1/1
5	SOG	B	404	-	-	7/11/31/31	0/1/1/1
5	SOG	B	409	-	-	1/2/22/31	0/1/1/1
5	SOG	A	409	-	-	7/11/31/31	0/1/1/1
5	SOG	A	411	-	-	4/11/31/31	0/1/1/1
5	SOG	A	405	-	-	6/11/31/31	0/1/1/1
5	SOG	A	407	-	-	7/11/31/31	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NS2	C17-N25	9.91	1.46	1.35
2	A	401	NS2	C17-N25	9.27	1.45	1.35
2	A	401	NS2	C12-N11	5.89	1.54	1.47
2	B	401	NS2	C09-N11	5.54	1.44	1.35
2	A	401	NS2	C09-N11	5.46	1.44	1.35
4	B	403	PGW	O01-C1	5.06	1.48	1.34
4	B	403	PGW	O03-C19	4.89	1.47	1.33
2	B	401	NS2	C12-N11	4.73	1.53	1.47
4	A	404	PGW	O03-C19	4.70	1.47	1.33
4	A	404	PGW	O01-C1	4.49	1.47	1.34
2	A	401	NS2	C21-C20	-4.36	1.31	1.38
2	B	401	NS2	C21-C20	-4.33	1.31	1.38
2	B	401	NS2	N28-N29	4.07	1.38	1.33
5	A	410	SOG	C1'-S1	-3.47	1.76	1.81
2	A	401	NS2	C16-C15	3.43	1.58	1.53
2	A	401	NS2	N28-N29	3.35	1.38	1.33
5	A	406	SOG	C1'-S1	-3.29	1.76	1.81
2	A	401	NS2	C05-C06	3.23	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	SOG	C1'-S1	-3.19	1.76	1.81
5	A	405	SOG	C1'-S1	-3.05	1.77	1.81
5	A	411	SOG	C1'-S1	-3.03	1.77	1.81
2	A	401	NS2	C14-C15	-2.95	1.51	1.54
5	A	407	SOG	C1'-S1	-2.88	1.77	1.81
2	B	401	NS2	C16-C15	2.81	1.57	1.53
2	A	401	NS2	C24-N25	2.80	1.44	1.38
2	B	401	NS2	C15-N11	-2.69	1.44	1.48
2	B	401	NS2	C14-C15	-2.64	1.51	1.54
2	B	401	NS2	C24-N25	2.64	1.44	1.38
2	A	401	NS2	C26-C23	-2.62	1.46	1.51
5	B	410	SOG	C1'-S1	-2.60	1.77	1.81
2	B	401	NS2	C05-C06	2.58	1.43	1.39
2	B	401	NS2	C26-C23	-2.55	1.46	1.51
5	A	407	SOG	O5-C1	2.41	1.46	1.42
2	A	401	NS2	N28-N32	2.39	1.36	1.33
2	A	401	NS2	C05-C04	2.29	1.42	1.38
2	A	401	NS2	C06-N28	2.26	1.45	1.43
2	B	401	NS2	N28-N32	2.25	1.36	1.33
5	A	409	SOG	C1'-S1	-2.22	1.78	1.81
2	B	401	NS2	C05-C04	2.21	1.42	1.38
2	B	401	NS2	C06-N28	2.19	1.45	1.43
2	A	401	NS2	C31-C30	2.05	1.44	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NS2	C14-C15-N11	7.70	106.56	101.67
2	A	401	NS2	C14-C15-N11	7.32	106.32	101.67
2	B	401	NS2	C21-C22-CL1	-6.72	105.19	118.42
2	A	401	NS2	C21-C22-CL1	-6.13	106.34	118.42
5	B	404	SOG	C1-O5-C5	5.69	122.77	112.56
5	B	405	SOG	C1-O5-C5	5.33	122.12	112.56
2	A	401	NS2	N25-C17-N18	-5.03	108.36	114.05
2	A	401	NS2	C08-C07-C06	-4.86	113.04	118.76
2	B	401	NS2	C08-C07-C06	-4.85	113.05	118.76
2	A	401	NS2	C07-C08-C03	4.85	127.31	119.41
2	B	401	NS2	C23-C22-CL1	4.84	127.84	119.54
2	B	401	NS2	N25-C17-N18	-4.81	108.62	114.05
2	B	401	NS2	C07-C08-C03	4.80	127.23	119.41
2	A	401	NS2	C23-C22-CL1	4.63	127.48	119.54
5	A	407	SOG	C1-O5-C5	4.61	120.84	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	409	SOG	C4-C3-C2	4.39	118.54	110.83
4	A	404	PGW	O01-C1-C2	4.14	120.44	111.48
4	B	403	PGW	O01-C1-C2	4.14	120.43	111.48
5	A	409	SOG	C3-C4-C5	-3.91	103.14	110.23
5	B	404	SOG	O5-C1-C2	3.88	115.67	110.32
5	B	405	SOG	C1'-S1-C1	3.86	108.79	100.45
2	A	401	NS2	C20-C19-C24	3.76	123.68	120.24
2	B	401	NS2	C20-C19-C24	3.76	123.68	120.24
2	A	401	NS2	C16-C15-C14	-3.75	108.51	111.87
2	A	401	NS2	O10-C09-N11	-3.70	115.78	122.28
2	B	401	NS2	O10-C09-N11	-3.63	115.90	122.28
5	A	406	SOG	C1'-S1-C1	3.50	108.02	100.45
5	B	404	SOG	O5-C5-C4	3.49	115.98	109.70
5	A	405	SOG	C3-C4-C5	3.43	116.45	110.23
5	A	411	SOG	C3-C4-C5	3.43	116.44	110.23
5	B	404	SOG	C3-C4-C5	3.42	116.43	110.23
2	B	401	NS2	C16-C15-C14	-3.33	108.89	111.87
5	A	405	SOG	C4-C3-C2	3.27	116.57	110.83
5	A	408	SOG	C4-C3-C2	3.27	116.56	110.83
2	B	401	NS2	C15-C17-N18	-3.24	118.88	125.16
5	A	406	SOG	C4-C3-C2	3.22	116.48	110.83
4	A	404	PGW	O03-C19-C20	3.21	121.63	111.83
5	B	409	SOG	C3-C4-C5	3.20	116.04	110.23
2	B	401	NS2	C13-C12-N11	3.20	106.88	103.32
2	A	401	NS2	C13-C12-N11	3.18	106.85	103.32
5	B	410	SOG	O5-C1-C2	-3.18	105.93	110.32
2	B	401	NS2	C05-C04-C03	-3.15	116.13	119.73
2	A	401	NS2	C15-C17-N18	-3.14	119.08	125.16
2	A	401	NS2	C05-C04-C03	-3.11	116.18	119.73
5	B	408	SOG	C3-C4-C5	3.05	115.76	110.23
2	B	401	NS2	C26-C23-C22	3.04	125.51	121.86
5	A	411	SOG	C1-O5-C5	2.99	117.92	112.56
5	A	407	SOG	C1'-S1-C1	2.97	106.86	100.45
2	A	401	NS2	C19-N18-C17	2.96	110.30	105.16
5	B	405	SOG	O5-C1-S1	-2.88	102.02	109.94
2	B	401	NS2	C19-N18-C17	2.83	110.06	105.16
5	A	407	SOG	O5-C1-C2	2.81	114.19	110.32
5	B	408	SOG	C4-C3-C2	2.80	115.74	110.83
5	A	409	SOG	O5-C5-C6	2.65	113.01	106.44
2	B	401	NS2	C21-C22-C23	2.63	126.59	122.86
5	A	409	SOG	C6-C5-C4	2.62	119.44	113.02
2	A	401	NS2	C05-C06-N28	-2.60	115.39	118.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	PGW	O03-C19-C20	2.55	119.61	111.83
4	B	403	PGW	C01-O03-C19	2.54	126.40	117.12
2	A	401	NS2	C26-C23-C22	2.49	124.85	121.86
5	A	410	SOG	C1-O5-C5	2.48	117.01	112.56
2	B	401	NS2	C24-C23-C22	-2.45	113.79	116.68
5	A	405	SOG	O5-C5-C4	2.45	114.11	109.70
4	A	404	PGW	O03-C19-O04	-2.41	117.60	123.63
5	A	406	SOG	C1-O5-C5	-2.40	108.26	112.56
5	A	407	SOG	C1-C2-C3	2.36	115.17	110.55
5	A	408	SOG	C1-C2-C3	2.34	115.13	110.55
2	A	401	NS2	C05-C06-C07	2.30	122.69	119.16
5	A	406	SOG	O5-C5-C6	2.29	112.12	106.44
2	B	401	NS2	C05-C06-C07	2.28	122.67	119.16
5	B	410	SOG	C4-C3-C2	2.28	114.83	110.83
5	A	411	SOG	C4-C3-C2	2.26	114.81	110.83
5	B	408	SOG	O2-C2-C1	2.22	114.25	110.30
2	B	401	NS2	C05-C06-N28	-2.22	115.83	118.39
5	A	411	SOG	O5-C5-C4	2.18	113.62	109.70
4	A	404	PGW	O01-C1-O02	-2.16	118.66	123.70
5	B	406	SOG	C4-C3-C2	2.13	114.57	110.83
5	B	404	SOG	C1'-S1-C1	2.12	105.04	100.45
2	A	401	NS2	C21-C22-C23	2.10	125.84	122.86
2	A	401	NS2	C24-C23-C22	-2.08	114.23	116.68
5	A	405	SOG	C1'-S1-C1	2.05	104.89	100.45
5	A	407	SOG	C4-C3-C2	2.05	114.43	110.83
2	A	401	NS2	O10-C09-C07	-2.04	116.06	120.06
2	B	401	NS2	O10-C09-C07	-2.00	116.13	120.06

There are no chirality outliers.

All (132) 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	A	401	NS2	C14-C15-C17-N25
2	B	401	NS2	C07-C09-N11-C12
2	B	401	NS2	C07-C09-N11-C15
2	B	401	NS2	O10-C09-N11-C12
2	B	401	NS2	O10-C09-N11-C15
2	B	401	NS2	C14-C15-C17-N25

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Mol	Chain	Res	Type	Atoms
4	A	404	PGW	C04-C05-CAD-OAE
4	B	403	PGW	C04-C05-CAD-OAE
5	A	407	SOG	O5-C1-S1-C1'
5	A	409	SOG	O5-C1-S1-C1'
5	B	405	SOG	C2-C1-S1-C1'
5	B	405	SOG	O5-C1-S1-C1'
4	A	404	PGW	O04-C19-O03-C01
4	A	404	PGW	C20-C19-O03-C01
5	A	409	SOG	C4-C5-C6-O6
5	A	410	SOG	O5-C5-C6-O6
5	B	405	SOG	C4-C5-C6-O6
4	B	403	PGW	O12-C04-C05-CAD
5	A	410	SOG	C4-C5-C6-O6
4	B	403	PGW	O12-C04-C05-OAF
4	A	404	PGW	C2-C1-O01-C02
5	A	409	SOG	O5-C5-C6-O6
5	B	408	SOG	O5-C5-C6-O6
4	B	403	PGW	C1-C2-C3-C4
5	B	405	SOG	O5-C5-C6-O6
4	A	404	PGW	O12-C04-C05-OAF
5	B	406	SOG	C4-C5-C6-O6
4	A	404	PGW	O02-C1-O01-C02
5	A	405	SOG	O5-C5-C6-O6
5	A	409	SOG	S1-C1'-C2'-C3'
5	B	404	SOG	S1-C1'-C2'-C3'
4	A	404	PGW	O12-C04-C05-CAD
5	A	406	SOG	C1'-C2'-C3'-C4'
5	A	407	SOG	C1'-C2'-C3'-C4'
5	A	411	SOG	O5-C5-C6-O6
5	A	411	SOG	C1'-C2'-C3'-C4'
5	B	405	SOG	C1'-C2'-C3'-C4'
5	B	404	SOG	O5-C5-C6-O6
5	A	405	SOG	C1'-C2'-C3'-C4'
5	B	410	SOG	C1'-C2'-C3'-C4'
4	A	404	PGW	C09-C11-C12-C13
5	B	410	SOG	C2'-C3'-C4'-C5'
4	B	403	PGW	C17-C18-C28-C30
5	A	411	SOG	C3'-C4'-C5'-C6'
5	B	405	SOG	C3'-C4'-C5'-C6'
4	A	404	PGW	C15-C16-C17-C18
4	A	404	PGW	C24-C25-C26-C27
4	B	403	PGW	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	404	PGW	C21-C22-C23-C24
4	B	403	PGW	C20-C21-C22-C23
4	B	403	PGW	C25-C26-C27-C15
4	A	404	PGW	OAF-C05-CAD-OAE
4	B	403	PGW	OAF-C05-CAD-OAE
4	A	404	PGW	C2-C3-C4-C5
4	B	403	PGW	C06-C07-C08-C09
5	A	406	SOG	S1-C1'-C2'-C3'
5	B	404	SOG	C1'-C2'-C3'-C4'
5	A	406	SOG	C3'-C4'-C5'-C6'
4	B	403	PGW	C08-C09-C11-C12
4	A	404	PGW	C4-C5-C6-C7
4	A	404	PGW	C27-C15-C16-C17
5	B	405	SOG	C4'-C5'-C6'-C7'
4	A	404	PGW	C23-C24-C25-C26
5	A	410	SOG	C2'-C3'-C4'-C5'
5	A	407	SOG	C2'-C3'-C4'-C5'
4	B	403	PGW	C23-C24-C25-C26
5	A	409	SOG	C3'-C4'-C5'-C6'
4	B	403	PGW	C22-C23-C24-C25
4	A	404	PGW	C07-C08-C09-C11
5	B	407	SOG	C2'-C1'-S1-C1
4	A	404	PGW	C16-C15-C27-C26
5	A	407	SOG	S1-C1'-C2'-C3'
5	B	404	SOG	C4'-C5'-C6'-C7'
4	A	404	PGW	C20-C21-C22-C23
4	A	404	PGW	O03-C01-C02-O01
4	A	404	PGW	C3-C4-C5-C6
4	B	403	PGW	C4-C5-C6-C7
5	A	405	SOG	C4'-C5'-C6'-C7'
5	A	406	SOG	O5-C5-C6-O6
4	A	404	PGW	C22-C23-C24-C25
5	B	410	SOG	C4'-C5'-C6'-C7'
5	B	406	SOG	O5-C5-C6-O6
4	B	403	PGW	C2-C3-C4-C5
4	A	404	PGW	O03-C01-C02-C03
4	A	404	PGW	C6-C7-C8-C9
4	B	403	PGW	C21-C22-C23-C24
4	B	403	PGW	C6-C7-C8-C9
5	A	405	SOG	C5'-C6'-C7'-C8'
5	A	410	SOG	C5'-C6'-C7'-C8'
4	B	403	PGW	C16-C15-C27-C26

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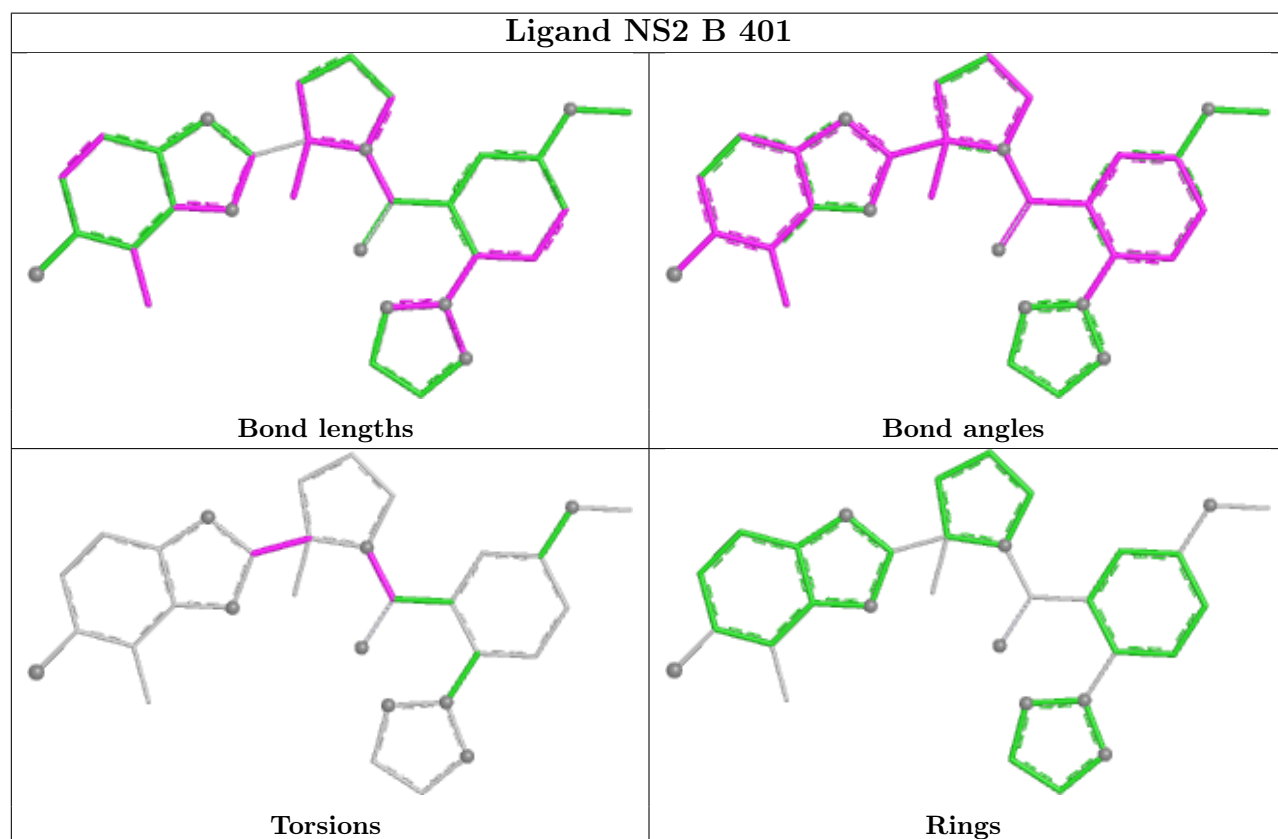
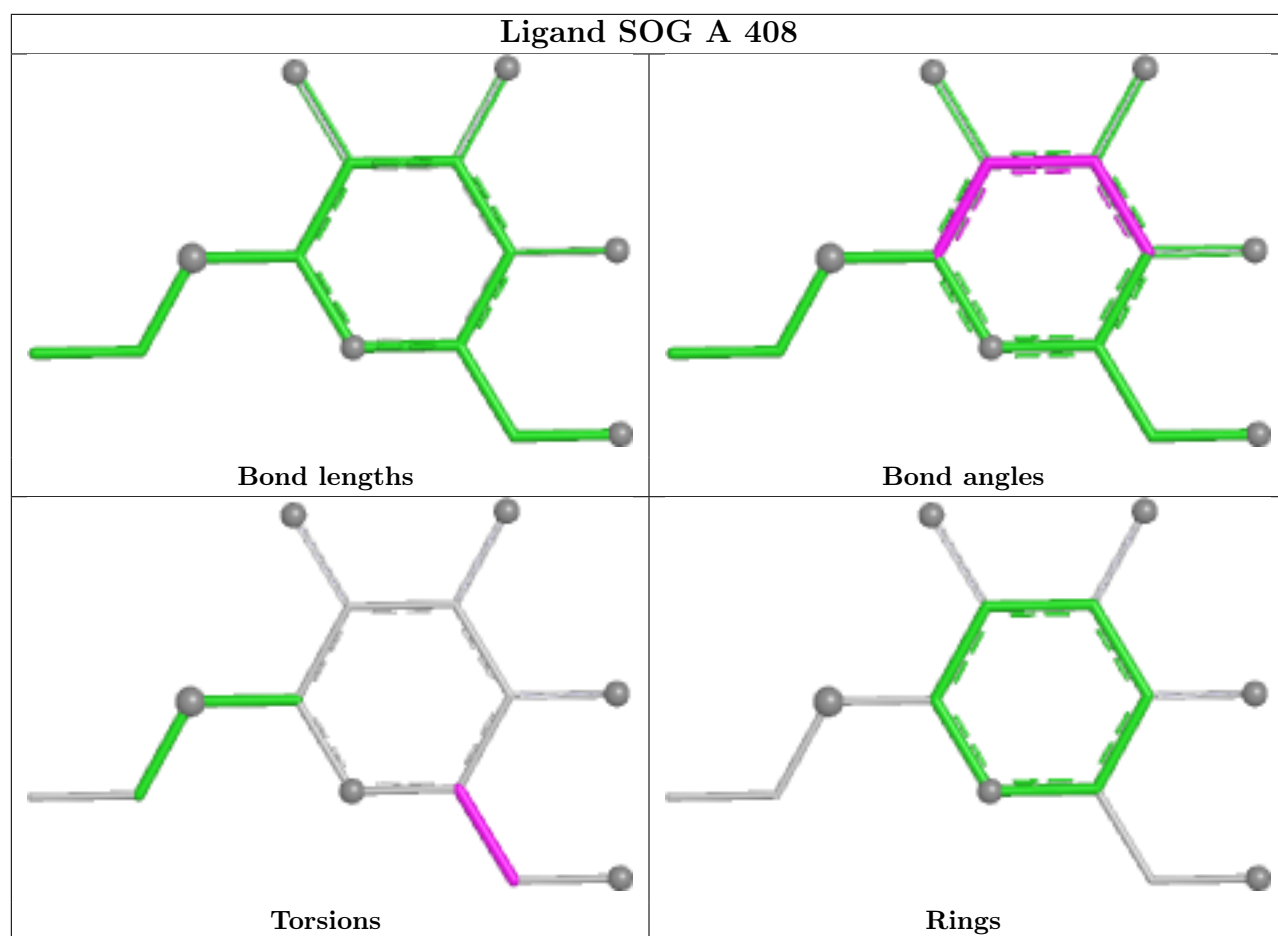
Mol	Chain	Res	Type	Atoms
4	B	403	PGW	C11-C12-C13-C14
5	B	409	SOG	O5-C5-C6-O6
4	B	403	PGW	C18-C28-C30-C29
5	A	406	SOG	C5'-C6'-C7'-C8'
4	B	403	PGW	C01-C02-C03-O11
4	B	403	PGW	C27-C15-C16-C17
5	B	404	SOG	C5'-C6'-C7'-C8'
5	B	404	SOG	C3'-C4'-C5'-C6'
4	A	404	PGW	C06-C07-C08-C09
4	B	403	PGW	O01-C02-C03-O11
4	A	404	PGW	C02-C03-O11-P
5	A	406	SOG	C2'-C3'-C4'-C5'
4	A	404	PGW	C16-C17-C18-C28
5	A	409	SOG	C2'-C3'-C4'-C5'
5	A	407	SOG	C2-C1-S1-C1'
5	B	407	SOG	S1-C1'-C2'-C3'
5	A	408	SOG	O5-C5-C6-O6
5	A	405	SOG	C2'-C3'-C4'-C5'
4	A	404	PGW	C03-O11-P-O14
4	A	404	PGW	C04-O12-P-O14
4	B	403	PGW	C07-C08-C09-C11
4	B	403	PGW	C05-C04-O12-P
5	A	411	SOG	S1-C1'-C2'-C3'
5	B	405	SOG	C5'-C6'-C7'-C8'
4	B	403	PGW	C09-C11-C12-C13
4	A	404	PGW	C5-C6-C7-C8
5	B	410	SOG	C5'-C6'-C7'-C8'
5	A	410	SOG	S1-C1'-C2'-C3'
5	A	407	SOG	O5-C5-C6-O6
5	A	407	SOG	C3'-C4'-C5'-C6'
4	B	403	PGW	C19-C20-C21-C22
4	B	403	PGW	C7-C8-C9-C10
5	A	405	SOG	C2'-C1'-S1-C1
5	A	409	SOG	C2'-C1'-S1-C1
5	B	404	SOG	C2'-C1'-S1-C1
5	B	410	SOG	C2'-C1'-S1-C1
4	B	403	PGW	O03-C19-C20-C21
5	A	406	SOG	C4'-C5'-C6'-C7'

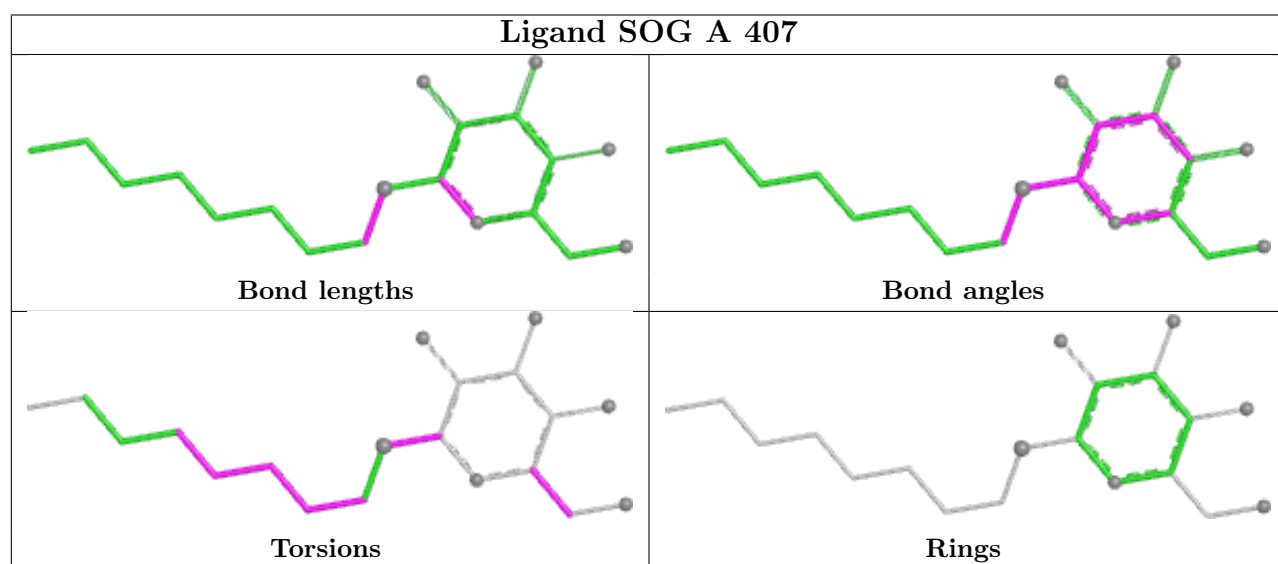
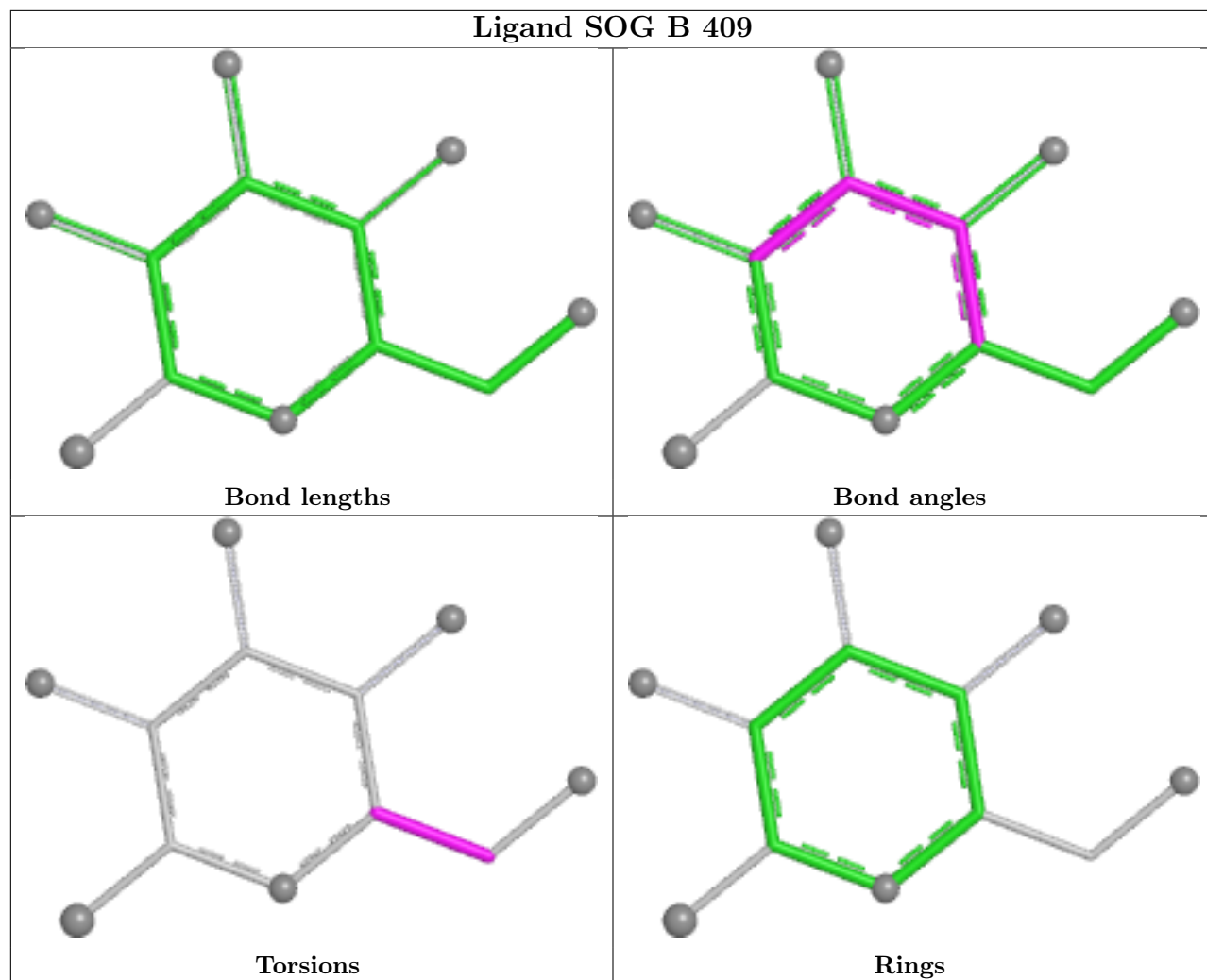
There are no ring outliers.

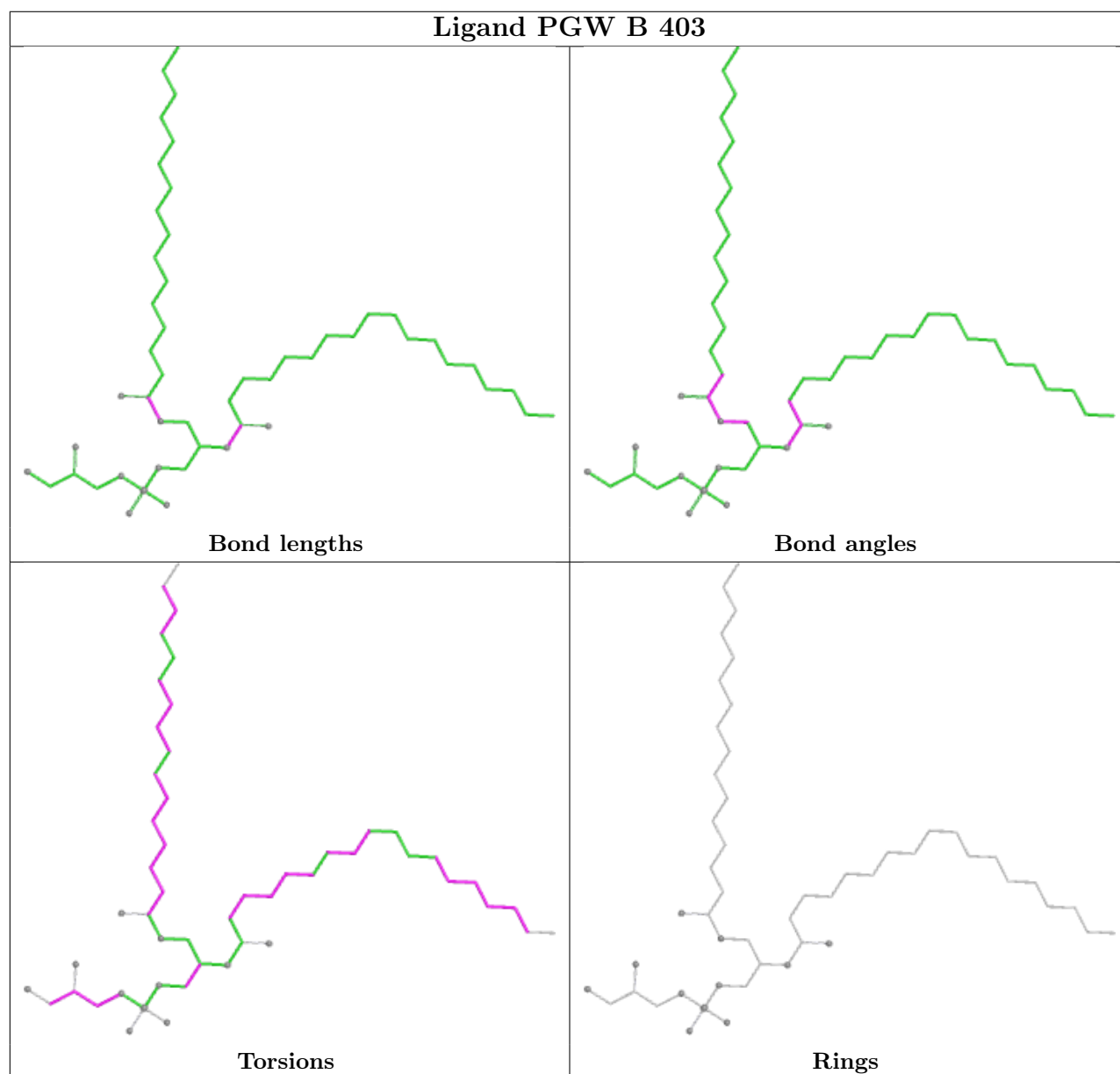
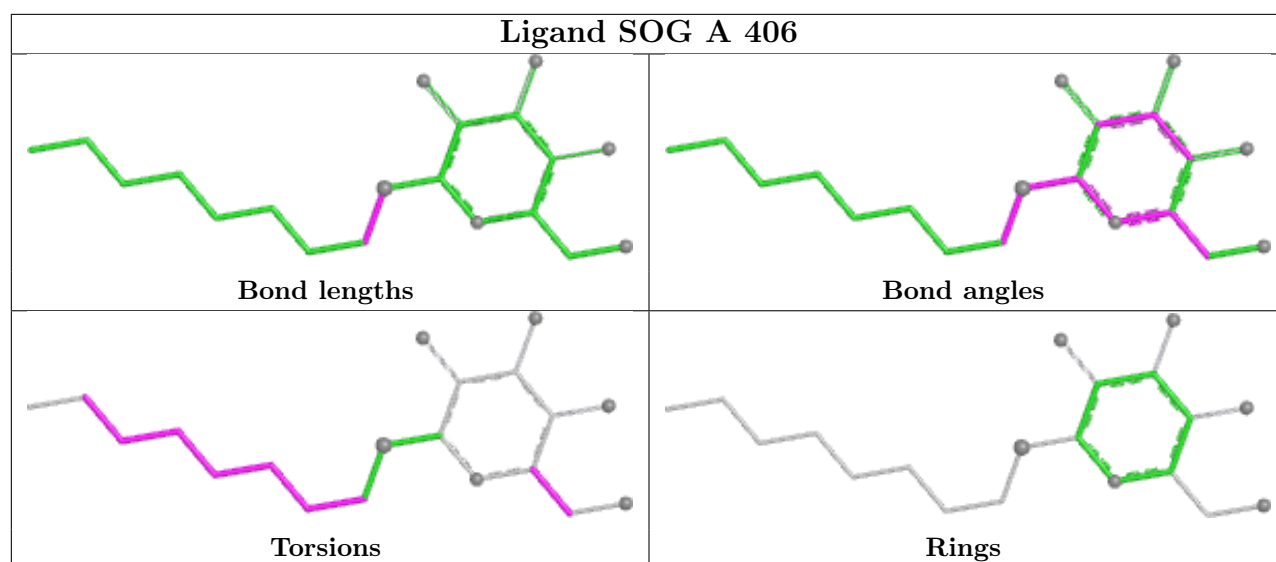
13 monomers are involved in 19 short contacts:

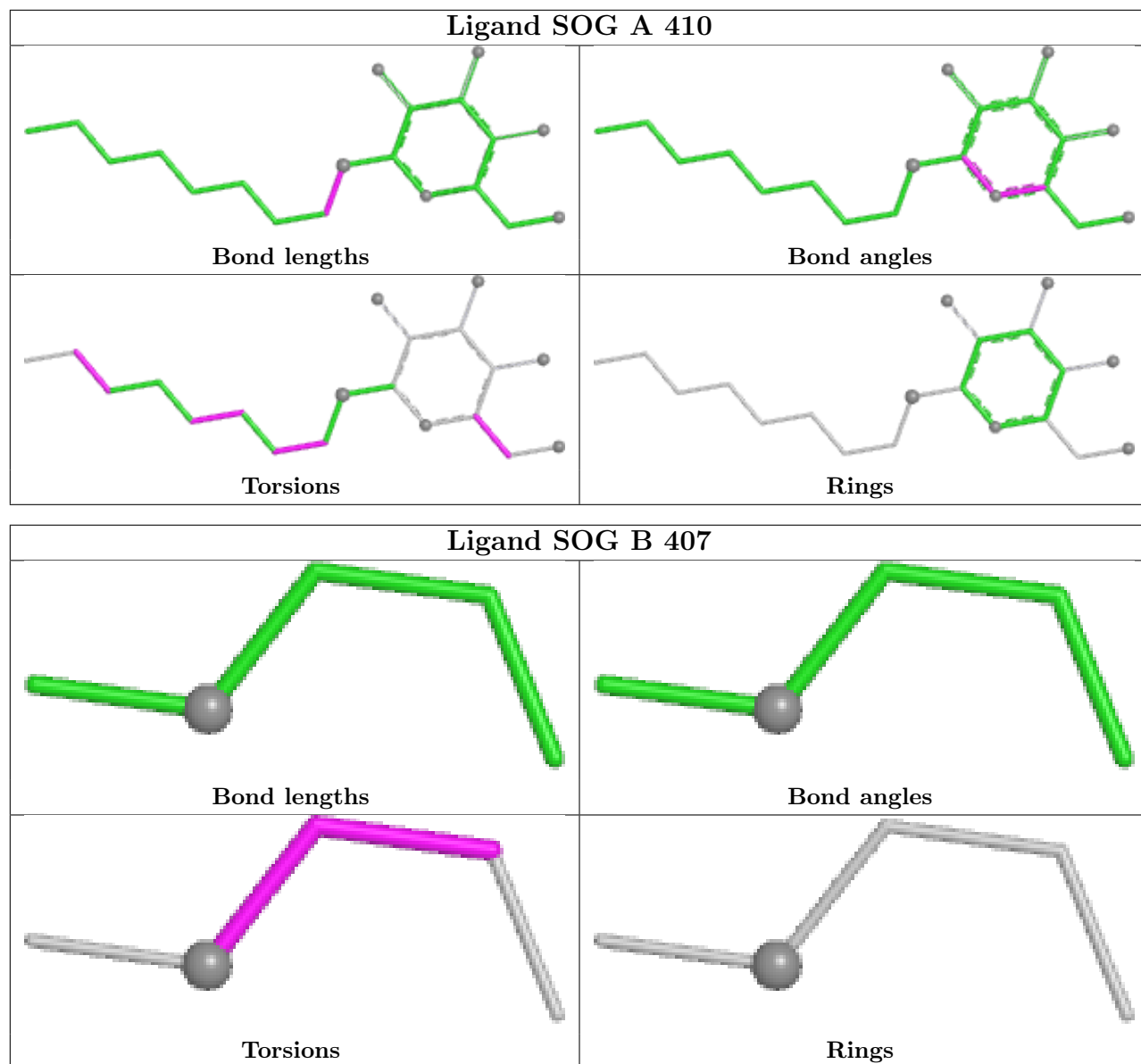
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NS2	1	0
5	B	409	SOG	2	0
5	A	407	SOG	1	0
4	B	403	PGW	2	0
5	A	410	SOG	1	0
2	A	401	NS2	1	0
5	B	410	SOG	2	0
5	A	411	SOG	1	0
5	B	408	SOG	1	0
4	A	404	PGW	3	0
5	B	404	SOG	1	0
5	A	409	SOG	1	0
5	A	405	SOG	2	0

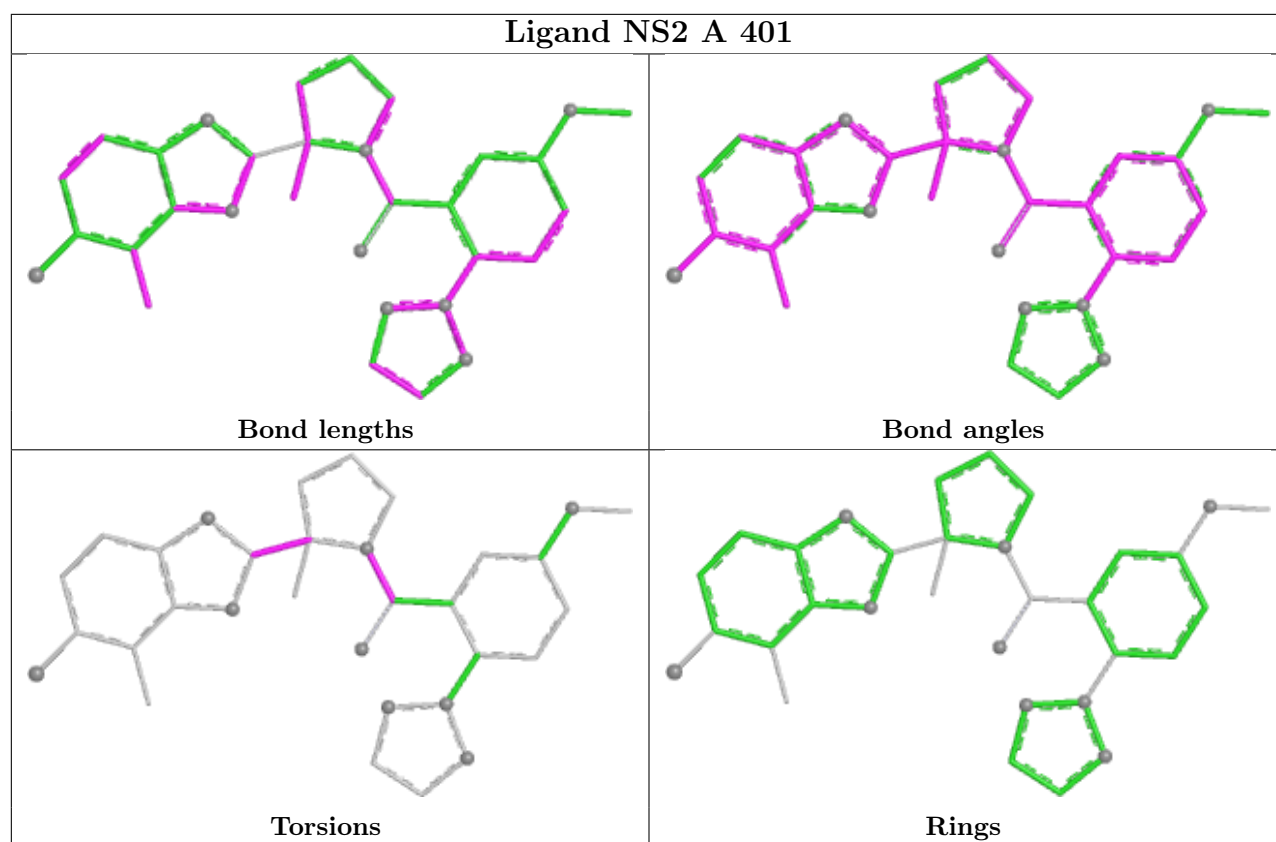
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

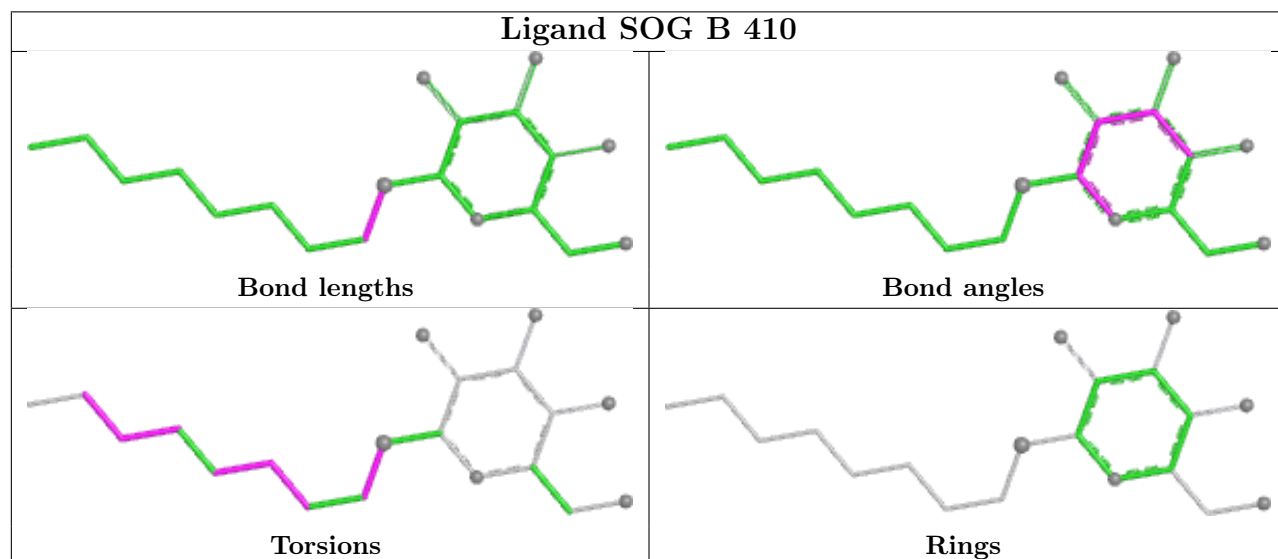
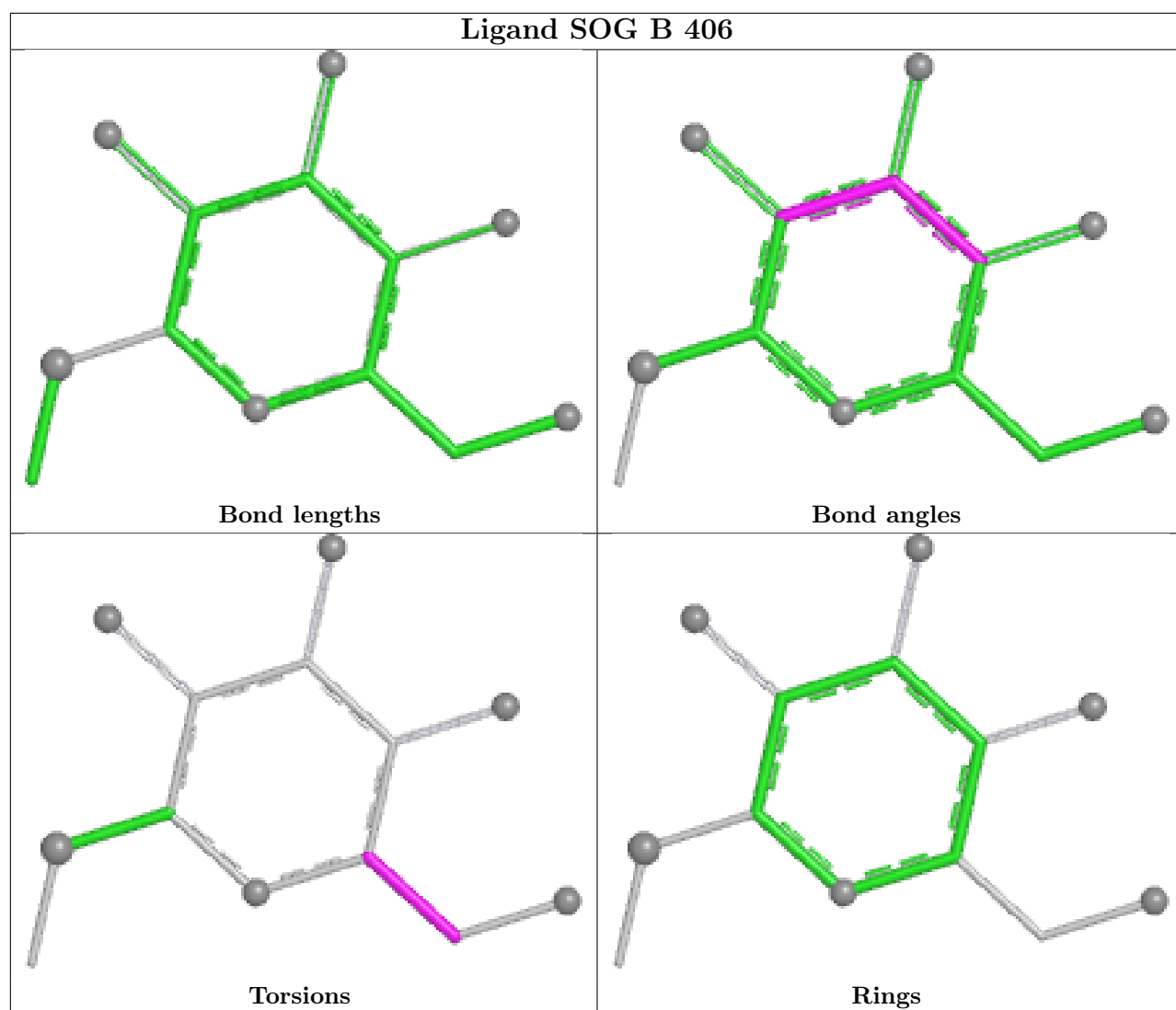




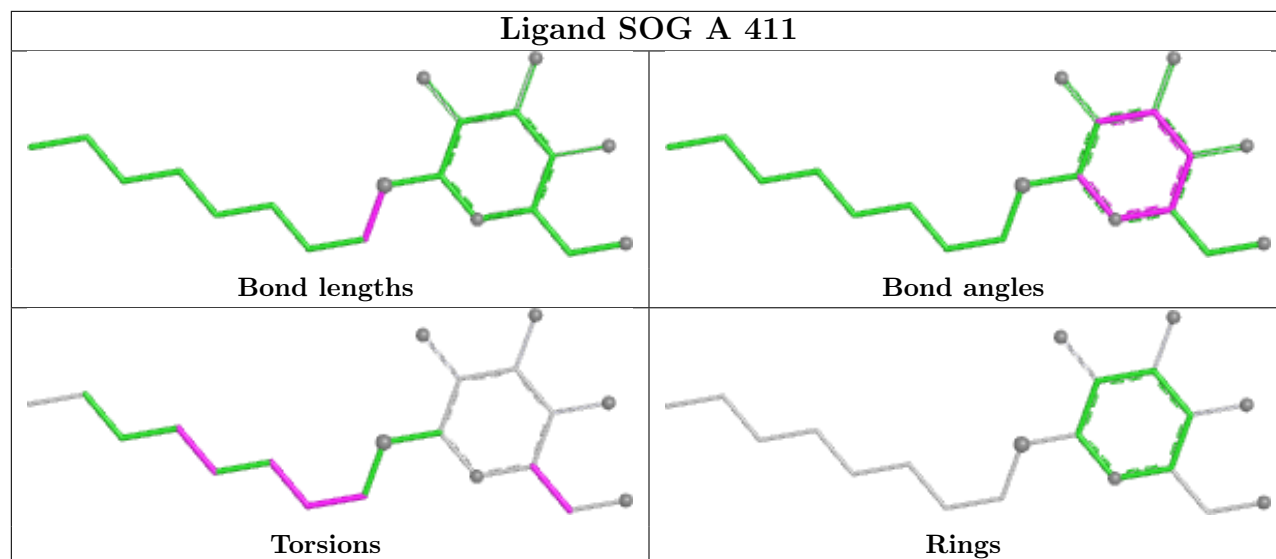




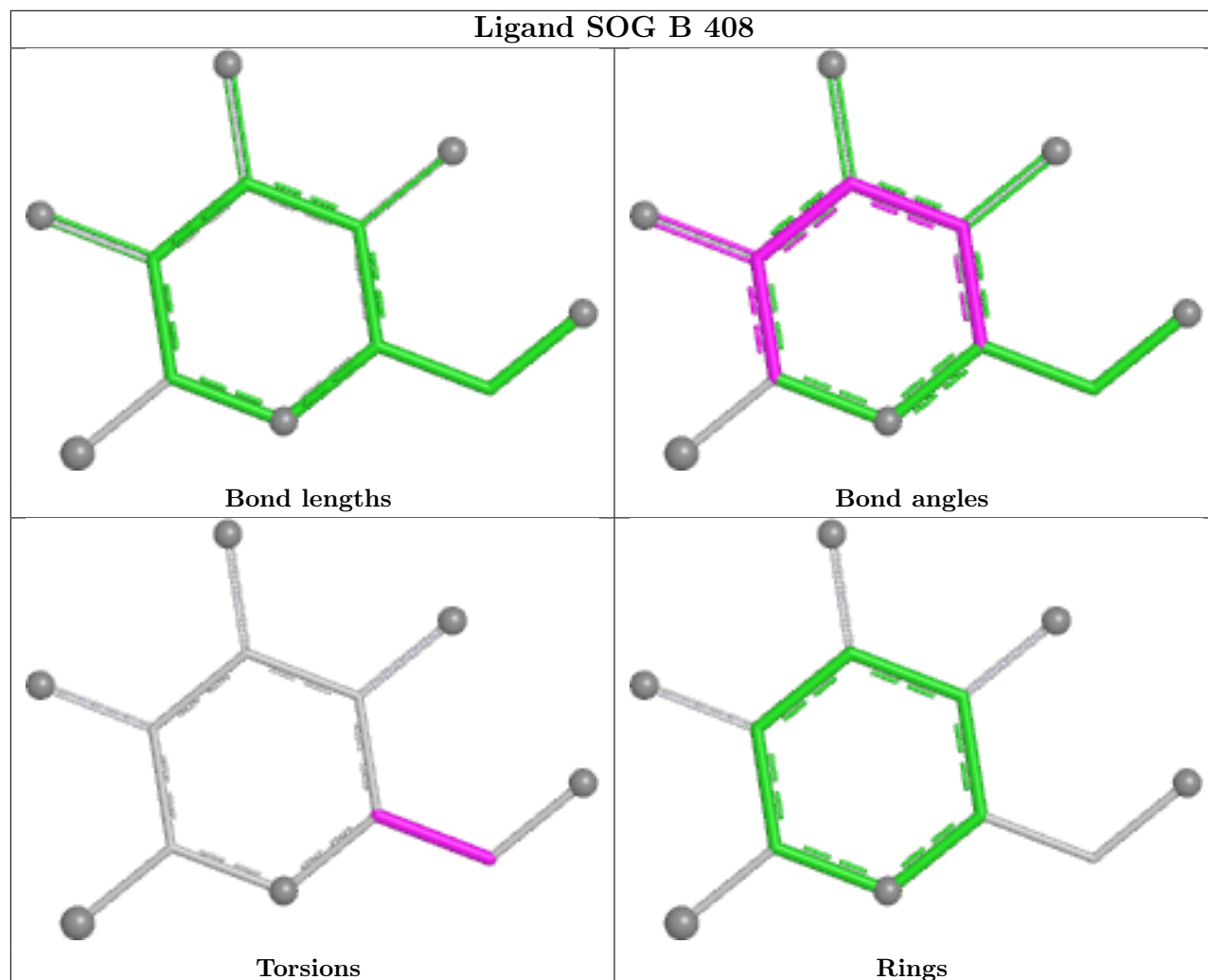


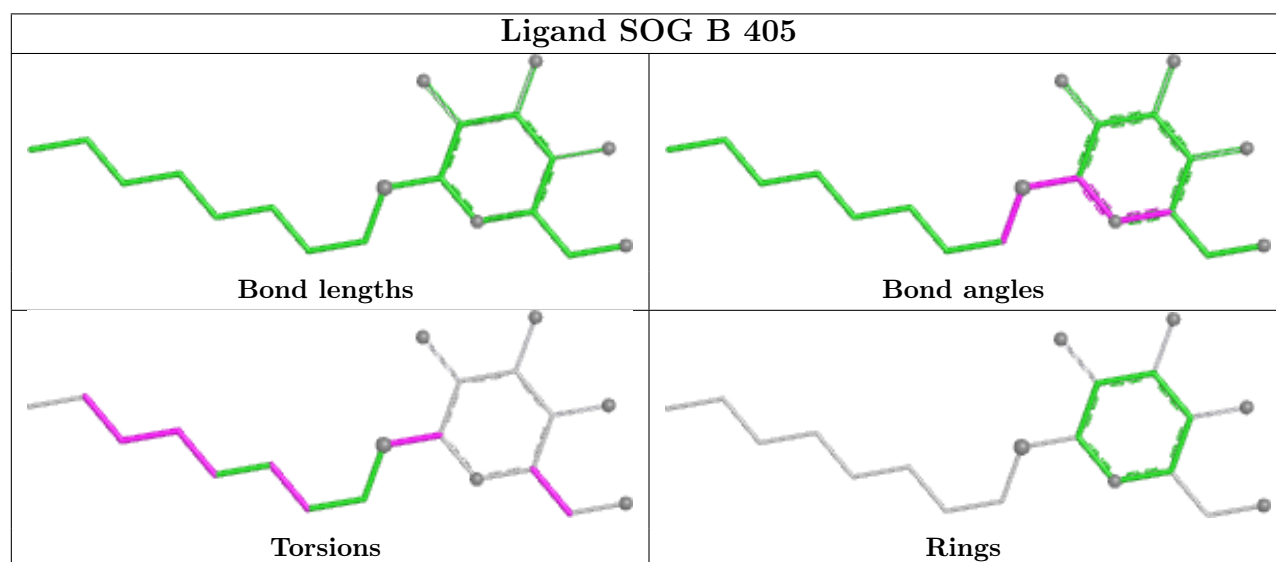
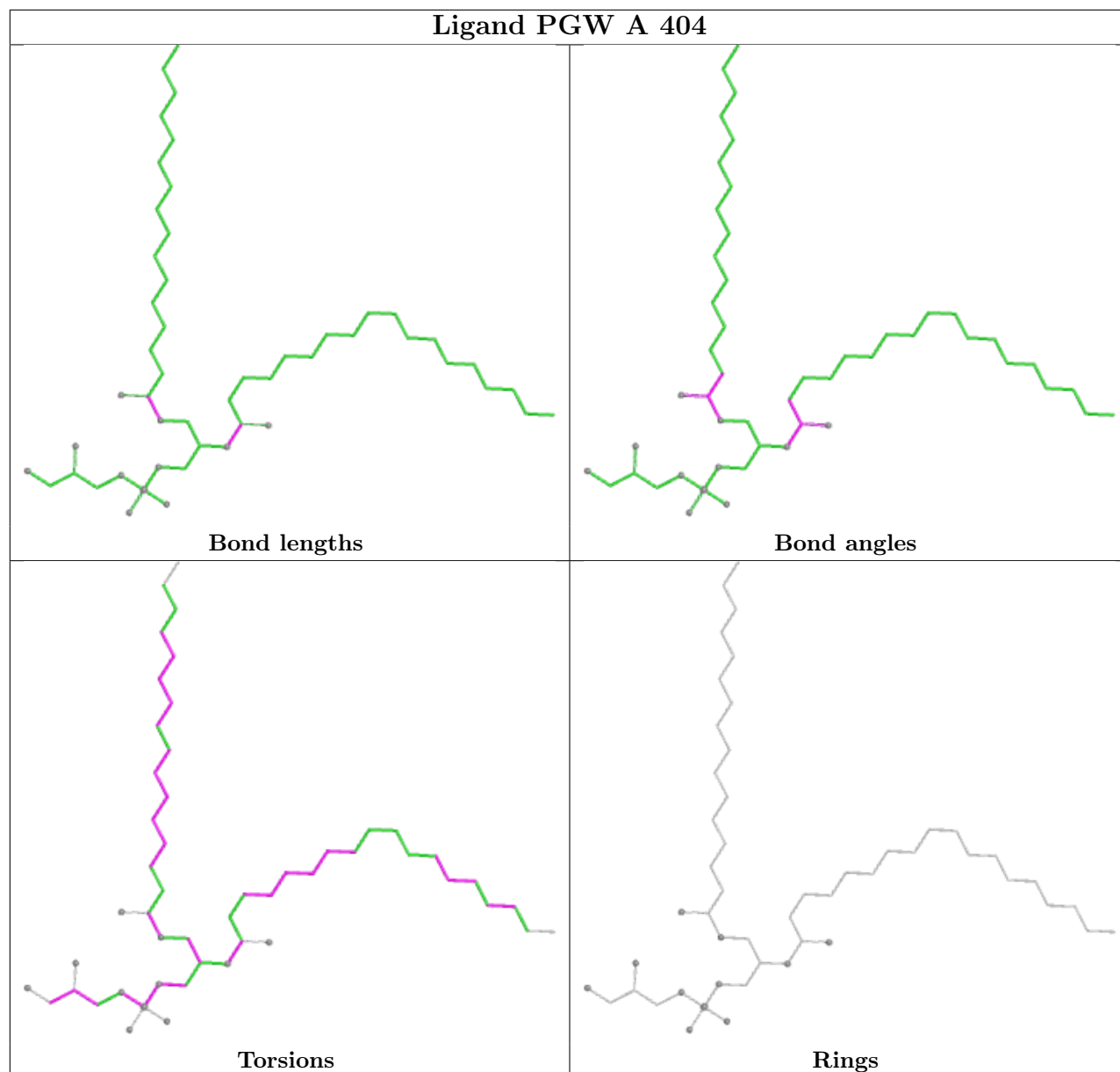


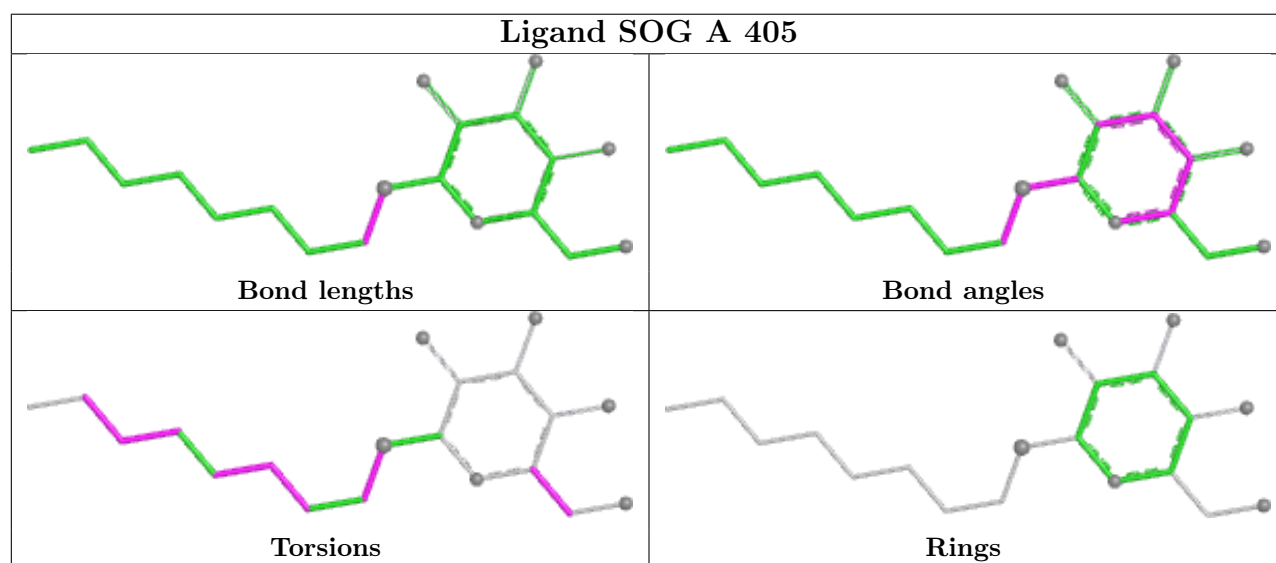
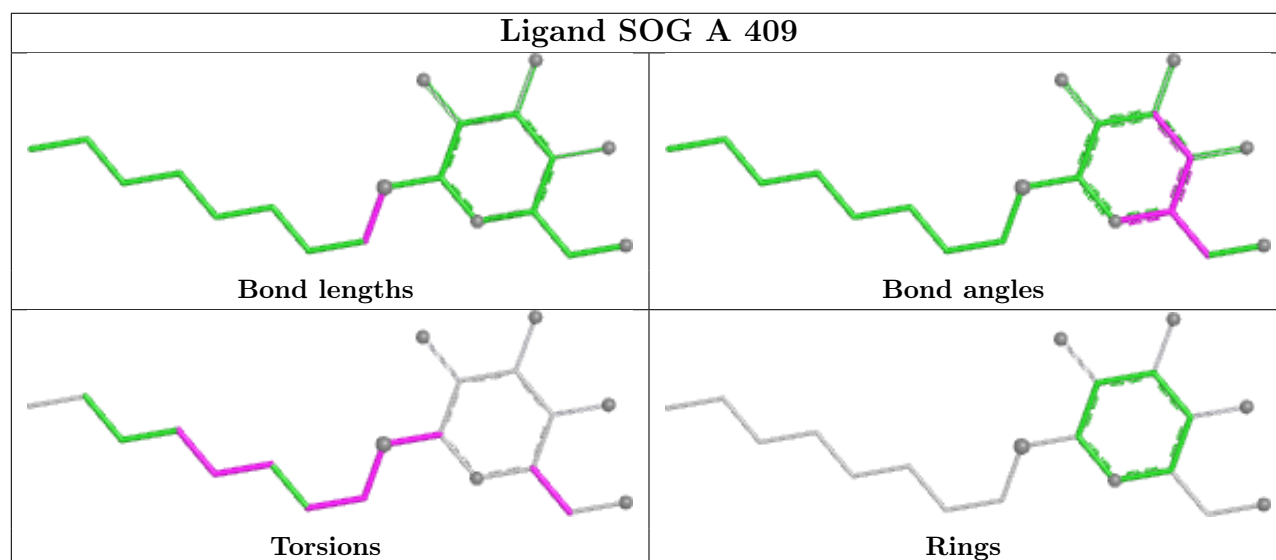
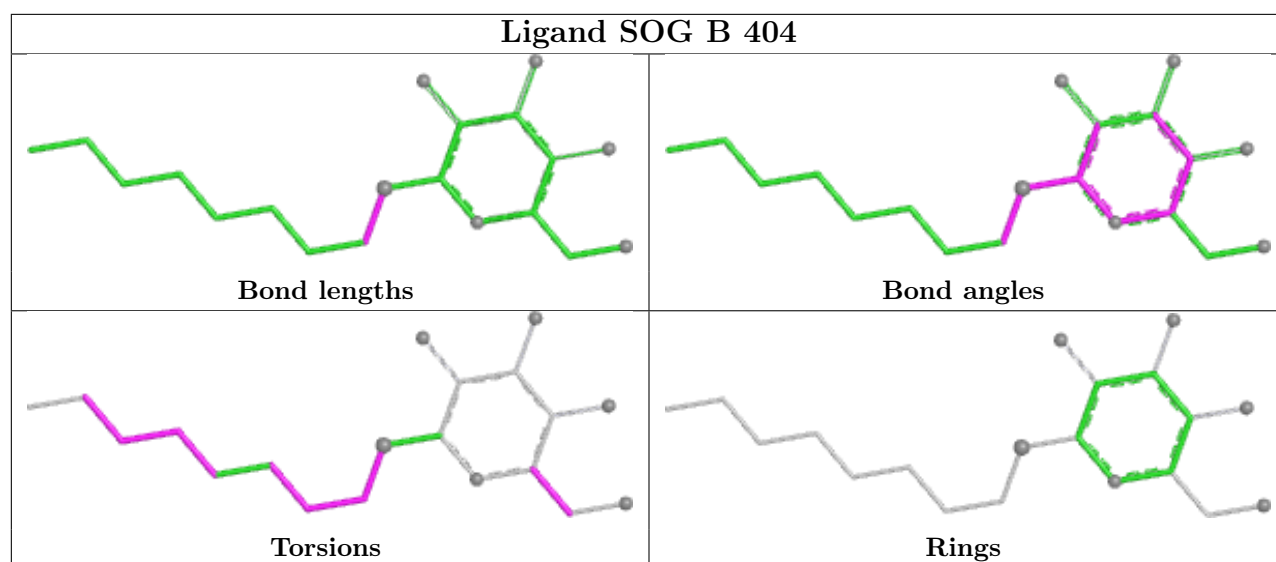
Ligand SOG A 411



Ligand SOG B 408







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	314/368 (85%)	-0.14	11 (3%) 47 26	60, 112, 191, 245	0
1	B	307/368 (83%)	0.14	26 (8%) 16 8	30, 108, 182, 221	0
All	All	621/736 (84%)	0.00	37 (5%) 27 14	30, 109, 190, 245	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	TRP	6.9
1	B	332	ASP	6.4
1	B	75	HIS	6.1
1	B	78	ARG	5.7
1	B	335	ALA	5.0
1	B	117	ALA	4.6
1	B	334	GLU	4.6
1	B	249	GLY	4.6
1	B	71	VAL	4.5
1	B	82	ASN	4.5
1	A	114	PHE	4.0
1	A	68	CYS	3.9
1	A	287	VAL	3.9
1	A	201	VAL	3.8
1	B	93	VAL	3.7
1	B	83	TYR	3.4
1	B	81	THR	3.3
1	B	79	THR	3.2
1	B	121	VAL	3.2
1	A	94	LEU	3.0
1	B	69	LEU	2.8
1	B	118	LEU	2.8
1	B	207	ALA	2.8
1	B	208	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	2.6
1	A	86	VAL	2.6
1	A	291	ARG	2.6
1	B	68	CYS	2.5
1	B	108	ILE	2.5
1	A	219	PHE	2.5
1	B	222	VAL	2.4
1	B	77	MET	2.4
1	B	336	VAL	2.3
1	B	337	TYR	2.3
1	B	45	TYR	2.2
1	A	322	ARG	2.2
1	B	136	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SOG	B	406	13/20	0.05	0.09	221,224,227,227	0
5	SOG	A	408	14/20	0.34	0.08	204,206,207,208	0
5	SOG	B	410	20/20	0.46	0.17	138,149,156,158	0
5	SOG	B	409	12/20	0.50	0.15	182,185,186,187	0
5	SOG	A	407	20/20	0.63	0.11	138,168,173,173	0
5	SOG	B	408	12/20	0.64	0.09	139,148,152,154	0
3	SO4	B	402	5/5	0.69	0.16	170,170,170,170	0
5	SOG	B	404	20/20	0.72	0.10	140,150,155,155	0
5	SOG	A	410	20/20	0.78	0.12	152,158,161,162	0
3	SO4	A	403	5/5	0.78	0.09	197,197,198,198	0

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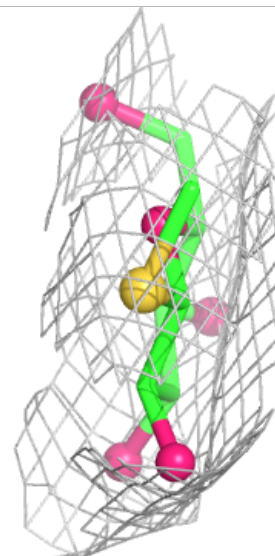
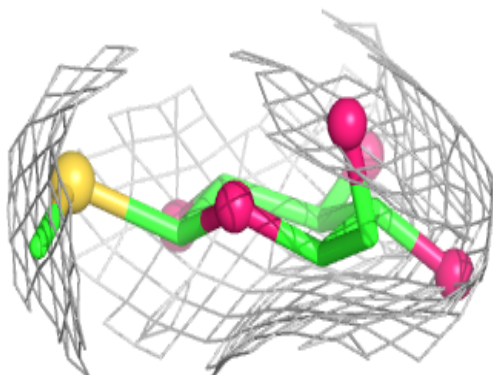
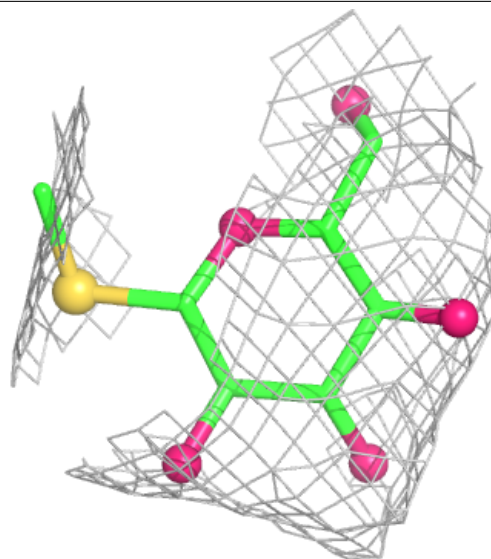
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SOG	A	411	20/20	0.79	0.09	166,183,185,185	0
5	SOG	A	409	20/20	0.79	0.11	111,143,151,151	0
3	SO4	A	402	5/5	0.83	0.12	146,147,148,151	0
4	PGW	B	403	51/51	0.89	0.17	60,82,162,162	0
5	SOG	A	406	20/20	0.89	0.10	70,107,119,119	0
2	NS2	A	401	32/32	0.90	0.13	62,90,129,129	0
5	SOG	B	405	20/20	0.90	0.07	71,130,140,140	0
5	SOG	A	405	20/20	0.90	0.10	121,133,136,137	0
4	PGW	A	404	51/51	0.91	0.13	49,101,160,163	0
2	NS2	B	401	32/32	0.93	0.10	61,79,105,105	0
5	SOG	B	407	5/20	0.95	0.17	131,134,144,144	0

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

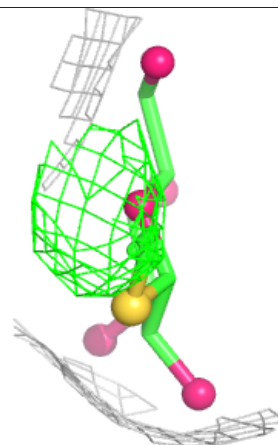
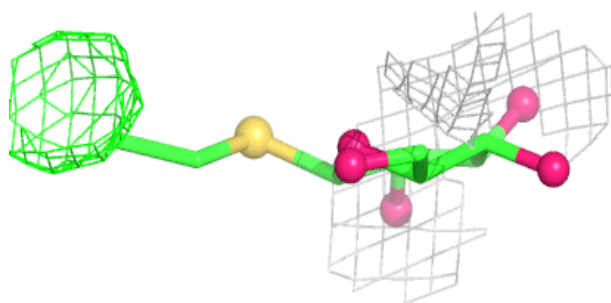
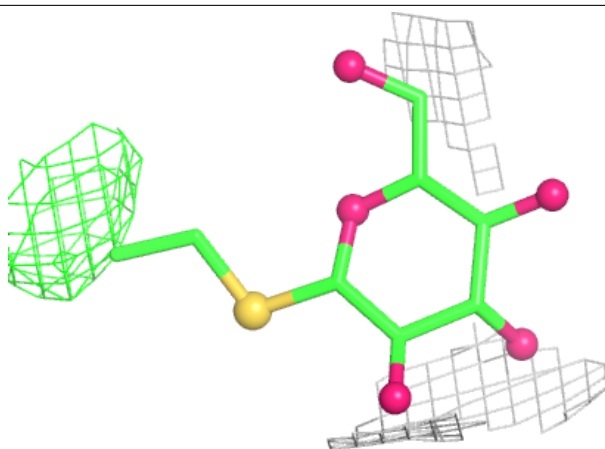
Electron density around SOG B 406:

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



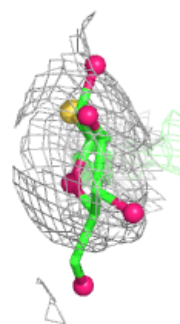
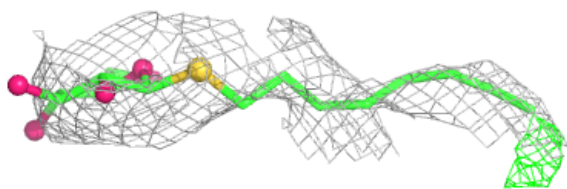
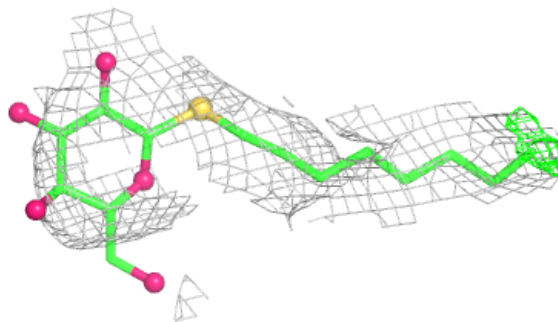
Electron density around SOG A 408:

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



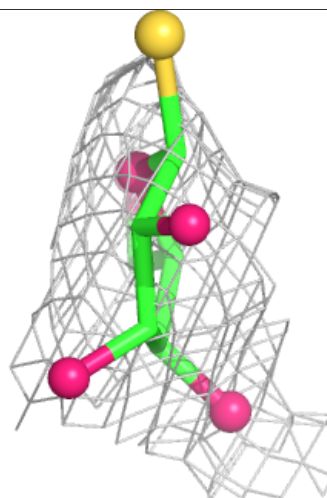
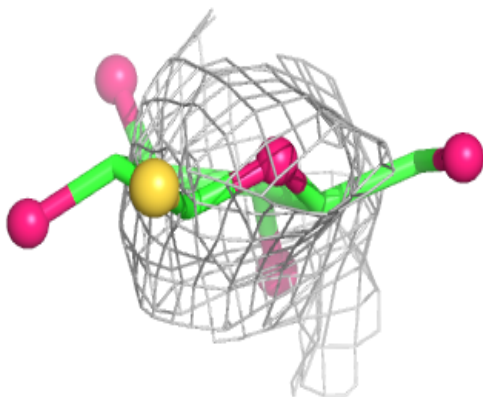
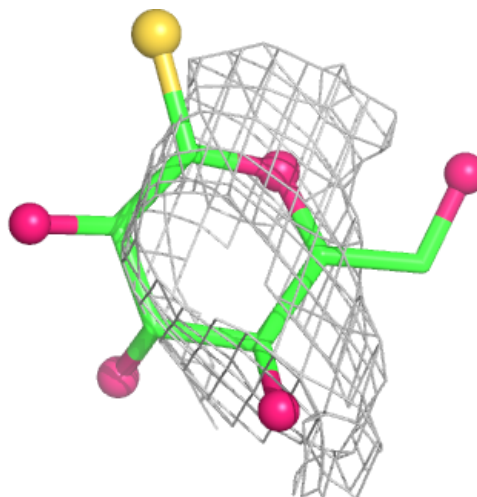
Electron density around SOG B 410:

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



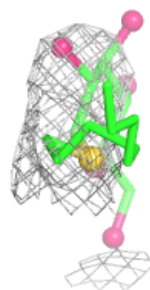
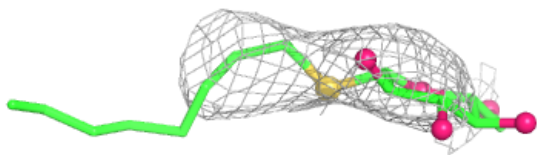
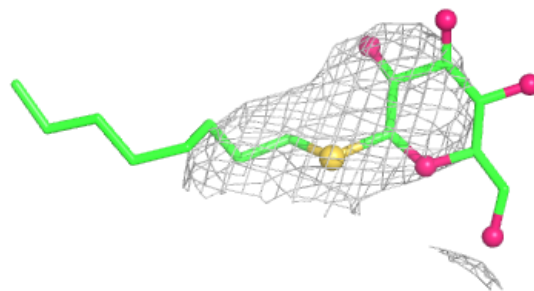
Electron density around SOG B 409:

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



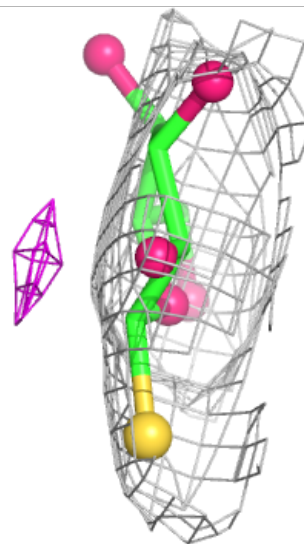
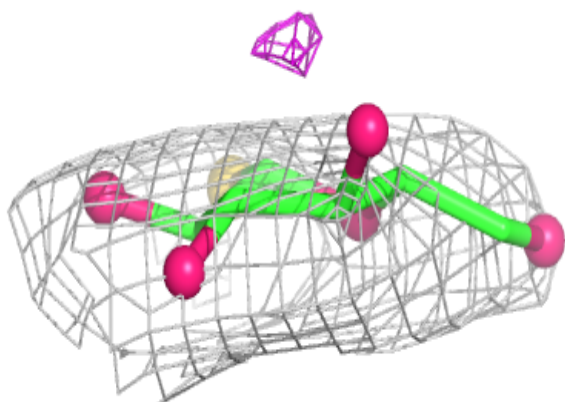
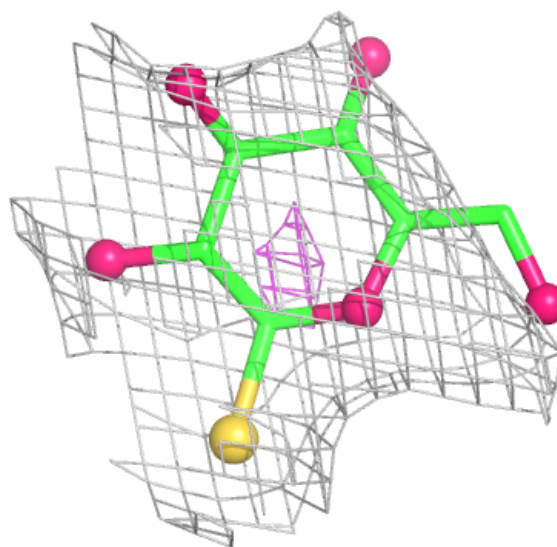
Electron density around SOG A 407:

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



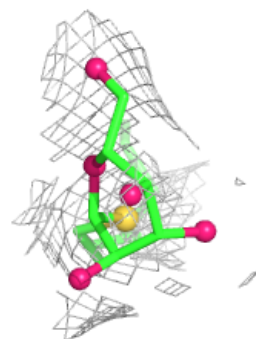
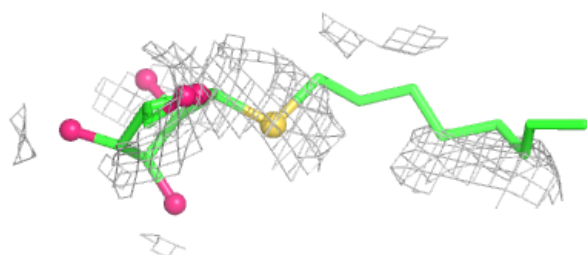
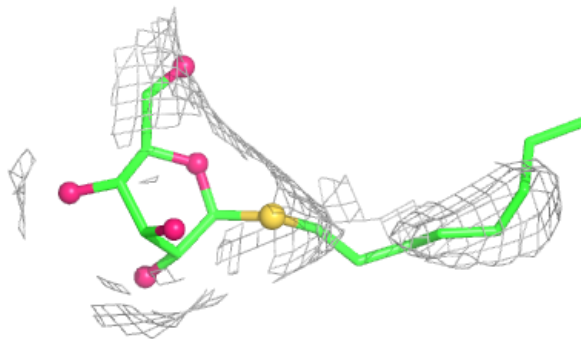
Electron density around SOG B 408:

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

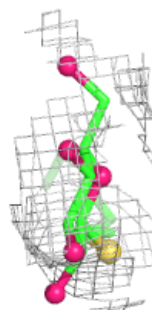
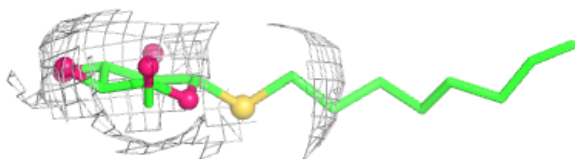
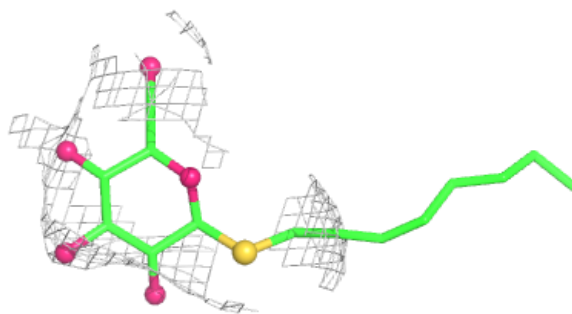


Electron density around SOG B 404:

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

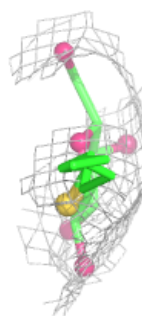
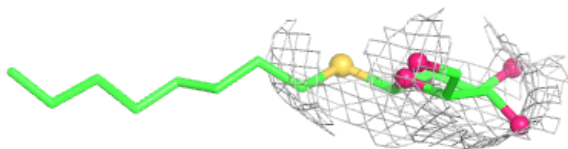
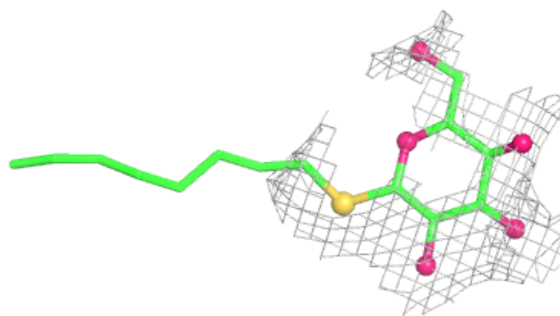
**Electron density around SOG A 410:**

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

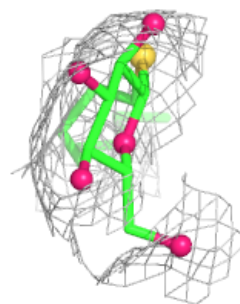
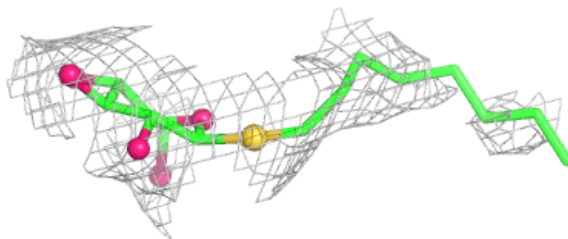
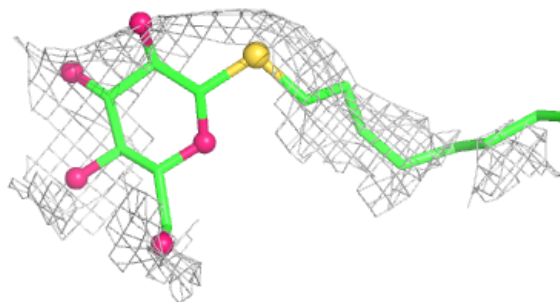


Electron density around SOG A 411:

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

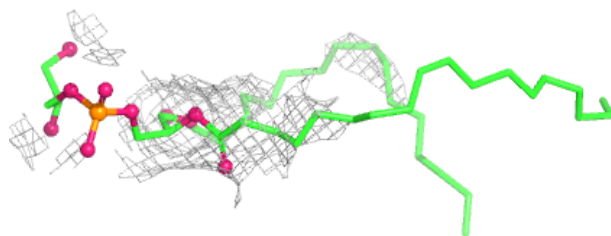
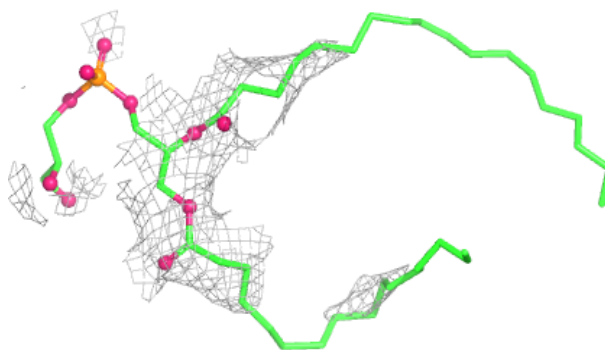
**Electron density around SOG A 409:**

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

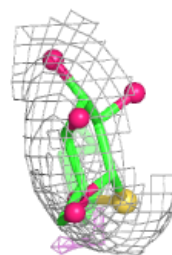
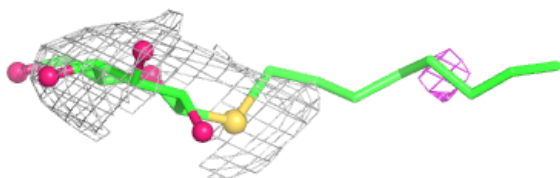
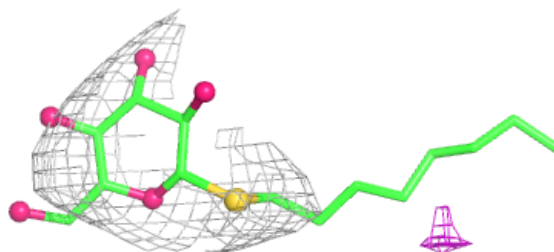


Electron density around PGW B 403:

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

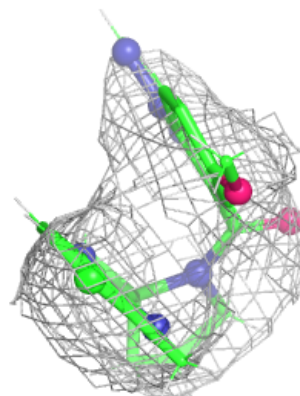
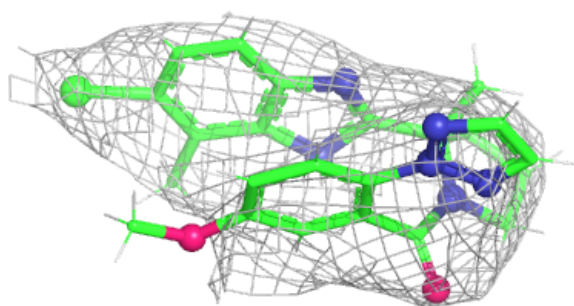
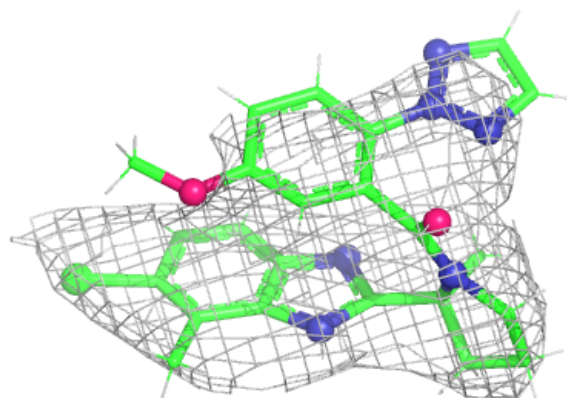
**Electron density around SOG A 406:**

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

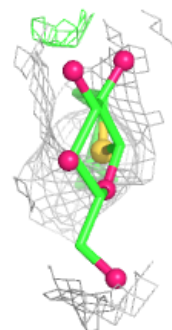
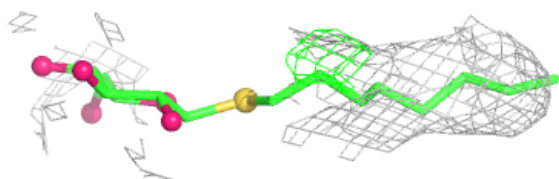
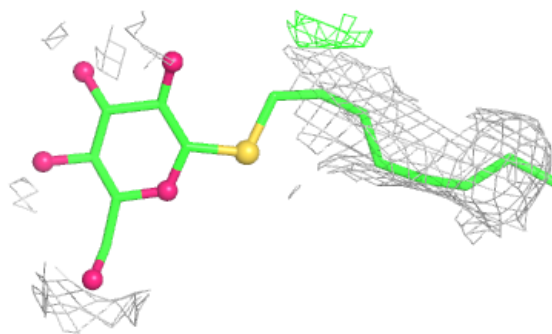


Electron density around NS2 A 401:

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

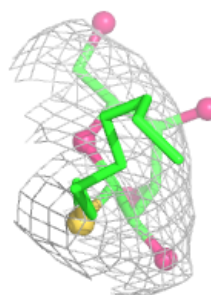
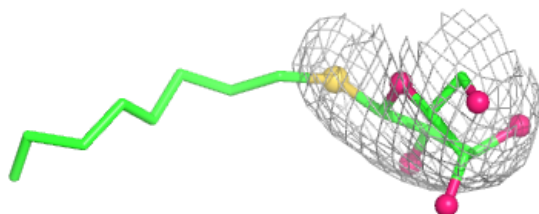
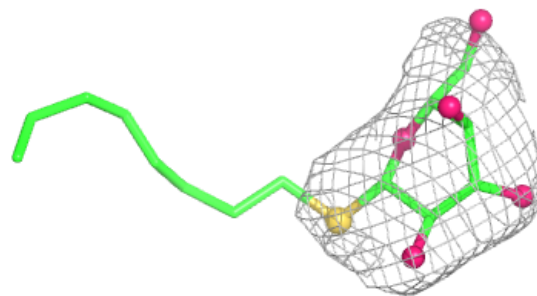
**Electron density around SOG B 405:**

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

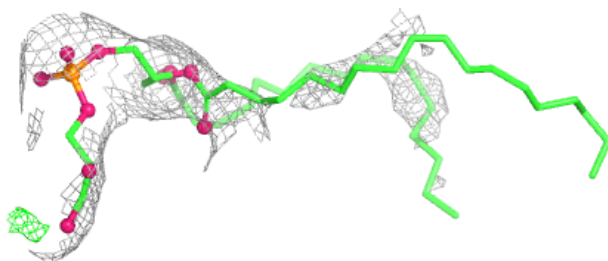
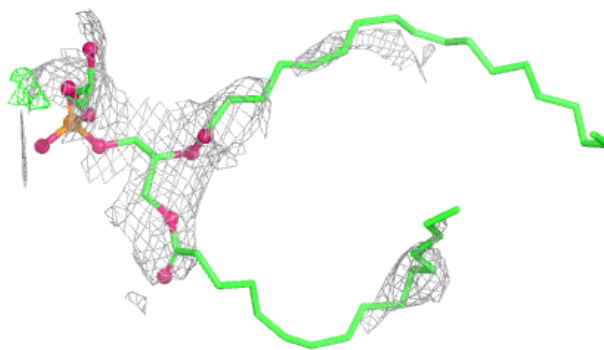


Electron density around SOG A 405:

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

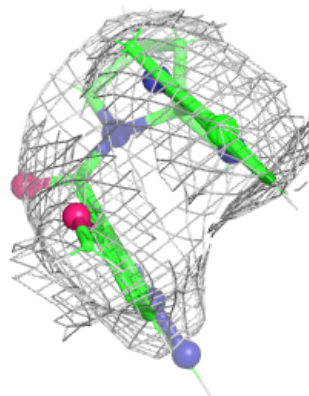
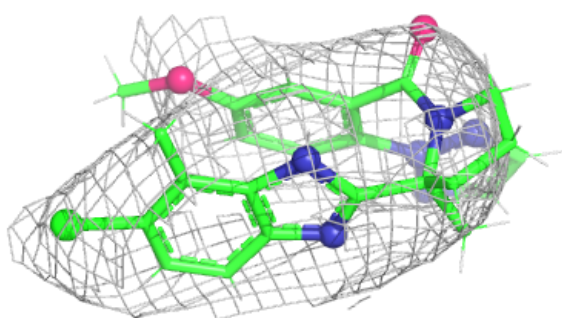
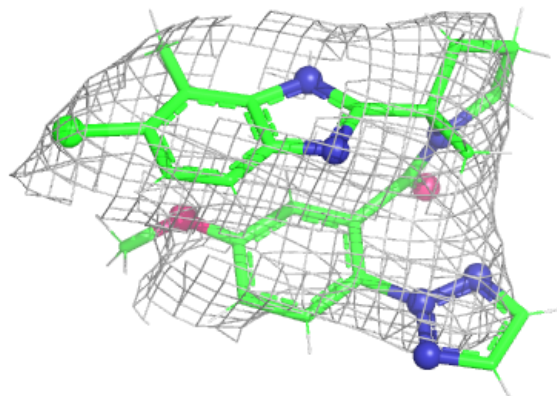
**Electron density around PGW A 404:**

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

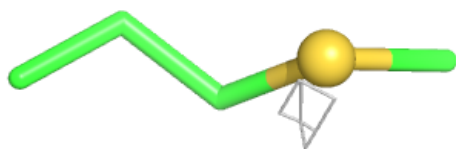
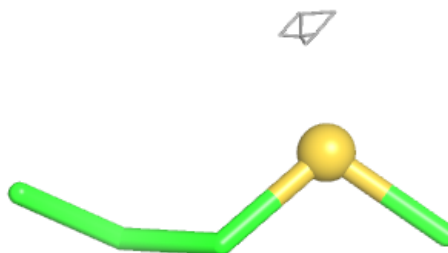


Electron density around NS2 B 401:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.