



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 11:59 AM BST

PDB ID : 6TOT
Title : Crystal structure of the Orexin-1 receptor in complex with lemborexant
Authors : Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.
Deposited on : 2019-12-11
Resolution : 2.22 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

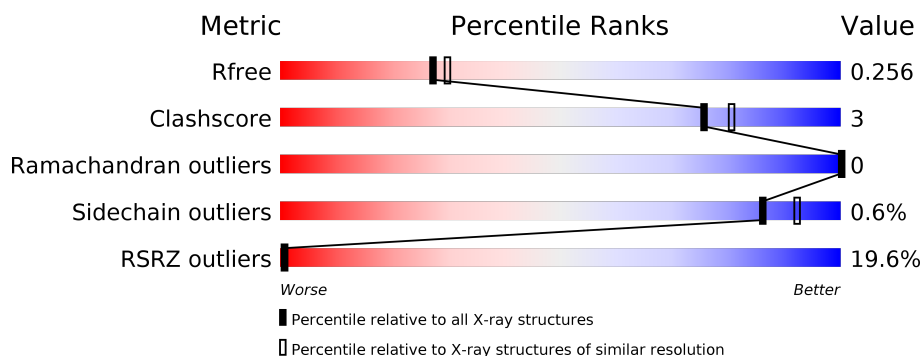
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 on 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	336	<div> <div>18%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	336	<div> <div>17%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5266 atoms, of which 40 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	300	Total	C	N	O	S	0	0	0
			2422	1611	400	394	17			
1	B	303	Total	C	N	O	S	0	0	0
			2404	1592	403	392	17			

There are 116 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	?	-	ALA	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	VAL	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ASN	deletion	UNP O43613
A	?	-	TRP	deletion	UNP O43613
A	?	-	LYS	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	SER	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613

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

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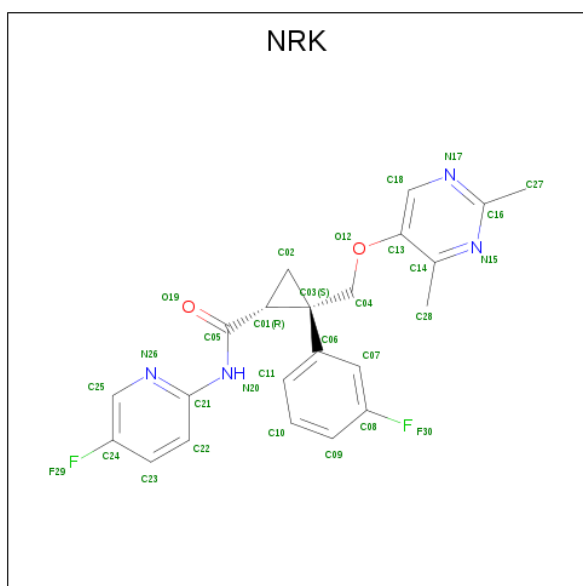
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	PHE	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	304	VAL	LEU	engineered mutation	UNP O43613
B	339	ALA	CYS	engineered mutation	UNP O43613
B	375	TRP	CYS	engineered mutation	UNP O43613
B	376	TRP	CYS	engineered mutation	UNP O43613
B	381	ALA	-	expression tag	UNP O43613
B	382	ALA	-	expression tag	UNP O43613
B	383	ALA	-	expression tag	UNP O43613
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613

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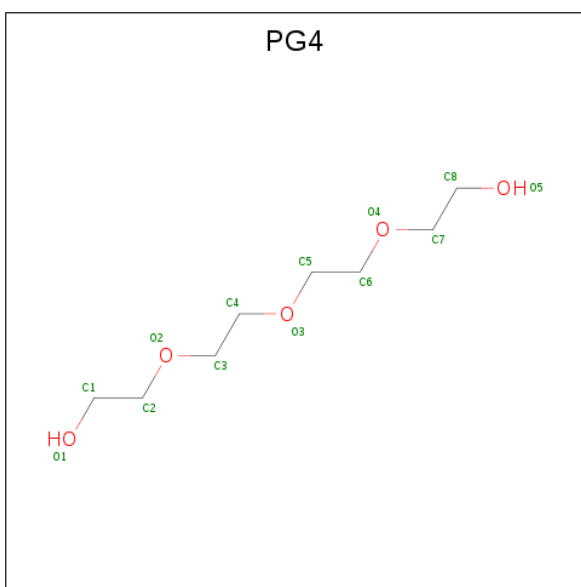
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is (1 {R},2 {S})-2-[(2,4-dimethylpyrimidin-5-yl)oxymethyl]- {N}-(5-fluoranylpyridin-2-yl)-2-(3-fluorophenyl)cyclopropane-1-carboxamide (three-letter code: NRK) (formula: C₂₂H₂₀F₂N₄O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			50	22	2	20	4	2		
2	B	1	Total	C	F	H	N	O	0	0
			50	22	2	20	4	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



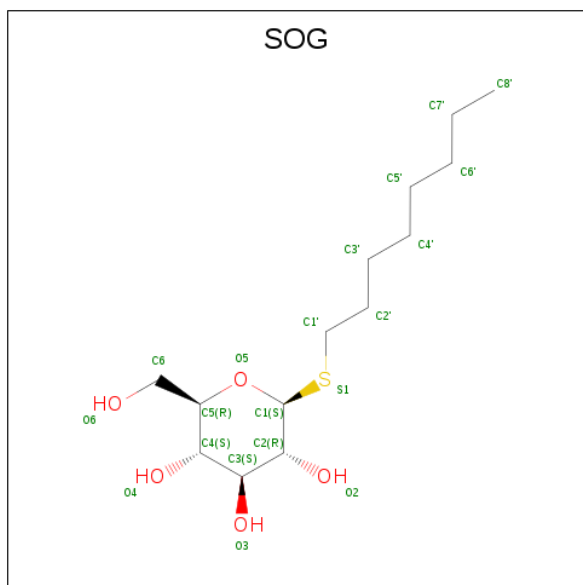
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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

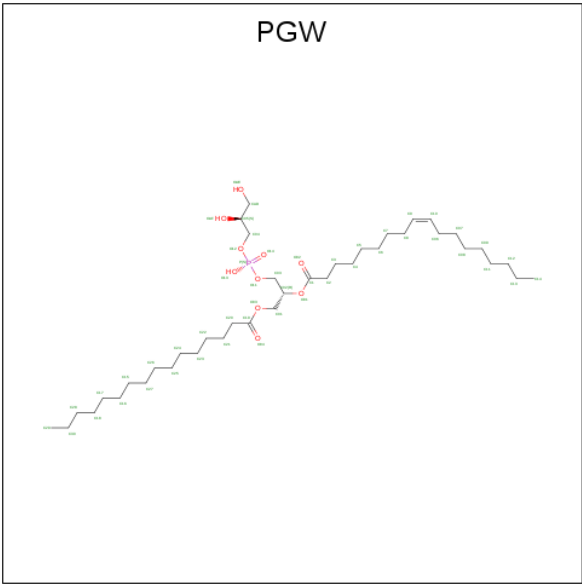
- Molecule 5 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula: $C_{14}H_{28}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	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
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			13	7	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			16	10	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(

hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



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

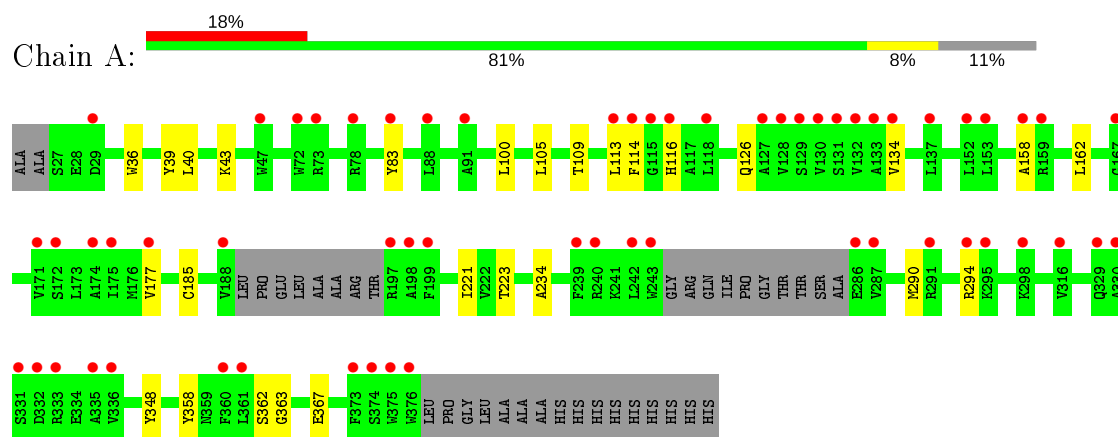
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total	O	0	0
			18	18		
7	B	25	Total	O	0	0
			25	25		

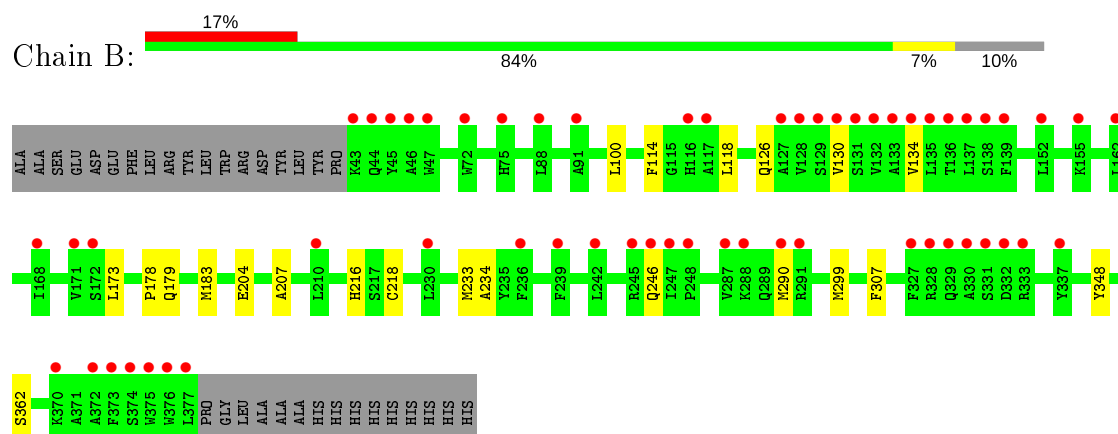
3 Residue-property plots

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	59.73Å 145.72Å 71.70Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	24.02 – 2.22 33.91 – 2.21	Depositor EDS
% Data completeness (in resolution range)	63.9 (24.02-2.22) 83.0 (33.91-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.206 , 0.239 0.230 , 0.256	Depositor DCC
R_{free} test set	2831 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5266	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: NRK, PGW, PG4, SO4, SOG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2491	0.62	0/3393
1	B	0.50	0/2470	0.63	0/3368
All	All	0.50	0/4961	0.62	0/6761

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2422	0	2464	20	0
1	B	2404	0	2474	14	0
2	A	30	20	0	0	0
2	B	30	20	0	0	0
3	A	13	0	18	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	73	0	95	0	0
5	B	89	0	112	1	0
6	A	102	0	152	6	0
7	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	25	0	0	0	0
All	All	5226	40	5315	33	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 3.

All (33) 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:39:TYR:CE1	1:A:43:LYS:HD2	2.13	0.83
6:A:410:PGW:HADA	1:B:207:ALA:H	1.52	0.74
1:A:290:MET:CE	1:A:294:ARG:HH21	2.04	0.70
1:A:105:LEU:HD12	1:A:114:PHE:HZ	1.56	0.69
1:A:290:MET:HE2	1:A:294:ARG:HH21	1.59	0.67
6:A:409:PGW:H7A	1:B:234:ALA:HB2	1.77	0.66
1:A:105:LEU:HD12	1:A:114:PHE:CZ	2.31	0.65
1:A:234:ALA:HB2	6:A:410:PGW:H9	1.80	0.63
1:A:100:LEU:HD12	1:A:348:TYR:HB3	1.84	0.57
1:A:363:GLY:O	1:A:367:GLU:HG2	2.09	0.53
1:B:204:GLU:OE1	1:B:216:HIS:HE1	1.95	0.50
1:A:39:TYR:CE1	1:A:43:LYS:CD	2.89	0.49
1:A:290:MET:HE1	1:A:294:ARG:HH21	1.79	0.48
1:B:246:GLN:CD	1:B:290:MET:SD	2.93	0.47
1:B:134:VAL:HG22	1:B:307:PHE:CZ	2.49	0.46
1:B:179:GLN:O	1:B:183:MET:HG2	2.16	0.46
6:A:410:PGW:H20A	1:B:178:PRO:HB3	1.97	0.45
1:A:358:TYR:O	1:A:362:SER:HB3	2.17	0.45
1:A:36:TRP:HA	1:A:40:LEU:HB2	2.00	0.44
1:A:221:ILE:HG21	1:B:218:CYS:HA	2.00	0.43
1:A:134:VAL:HG21	1:A:223:THR:O	2.17	0.43
1:A:177:VAL:HG22	3:A:402:PG4:H62	2.01	0.43
1:A:109:THR:HG21	1:A:113:LEU:HD11	2.01	0.43
1:A:116:HIS:CD2	1:A:185:CYS:HB3	2.53	0.43
1:B:173:LEU:HB3	5:B:406:SOG:H8'2	2.00	0.42
1:A:83:TYR:CE1	1:A:158:ALA:HB1	2.55	0.41
1:A:234:ALA:CB	6:A:410:PGW:H9	2.47	0.41
1:B:114:PHE:HB3	1:B:118:LEU:HD12	2.02	0.41
6:A:409:PGW:H2A	1:B:233:MET:HB3	2.02	0.41
1:A:83:TYR:HE1	1:A:158:ALA:HB1	1.86	0.41
1:B:100:LEU:HD12	1:B:348:TYR:HB3	2.03	0.40
1:B:299:MET:SD	1:B:362:SER:HB2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:O	1:B:134:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/336 (88%)	289 (98%)	5 (2%)	0	100	100
1	B	301/336 (90%)	296 (98%)	5 (2%)	0	100	100
All	All	595/672 (88%)	585 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/279 (91%)	252 (99%)	2 (1%)	81	89
1	B	252/279 (90%)	251 (100%)	1 (0%)	91	95
All	All	506/558 (91%)	503 (99%)	3 (1%)	86	92

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

Mol	Chain	Res	Type
1	A	126	GLN
1	A	162	LEU
1	B	126	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	368	GLN
1	B	150	HIS
1	B	216	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	403	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	B	403	-	4,4,4	0.19	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SOG	A	407	-	12,13,20	0.64	0	16,18,25	1.34	2 (12%)
6	PGW	A	410	-	50,50,50	0.98	2 (4%)	53,56,56	1.00	2 (3%)
5	SOG	B	406	-	20,20,20	1.17	1 (5%)	24,25,25	1.25	3 (12%)
5	SOG	B	408	-	20,20,20	1.18	2 (10%)	24,25,25	0.94	2 (8%)
5	SOG	B	405	-	12,13,20	0.69	0	16,18,25	1.05	1 (6%)
5	SOG	A	408	-	20,20,20	1.04	2 (10%)	24,25,25	1.07	1 (4%)
6	PGW	A	409	-	50,50,50	1.00	2 (4%)	53,56,56	1.05	3 (5%)
2	NRK	A	401	-	31,33,33	1.37	5 (16%)	39,48,48	3.15	11 (28%)
5	SOG	A	405	-	20,20,20	0.91	1 (5%)	24,25,25	1.24	1 (4%)
5	SOG	B	404	-	20,20,20	1.00	2 (10%)	24,25,25	0.76	0
4	SO4	B	402	-	4,4,4	0.13	0	6,6,6	0.29	0
3	PG4	A	402	-	12,12,12	0.19	0	11,11,11	0.12	0
5	SOG	B	407	-	16,16,20	1.12	2 (12%)	20,21,25	0.97	1 (5%)
4	SO4	A	404	-	4,4,4	0.16	0	6,6,6	0.09	0
2	NRK	B	401	-	31,33,33	1.47	6 (19%)	39,48,48	3.30	14 (35%)
5	SOG	A	406	-	20,20,20	1.02	2 (10%)	24,25,25	1.06	1 (4%)

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	406	-	-	9/11/31/31	0/1/1/1
5	SOG	A	407	-	-	3/4/24/31	0/1/1/1
6	PGW	A	410	-	-	22/55/55/55	-
5	SOG	B	406	-	-	7/11/31/31	0/1/1/1
5	SOG	B	408	-	-	6/11/31/31	0/1/1/1
5	SOG	B	405	-	-	0/4/24/31	0/1/1/1
2	NRK	A	401	-	-	5/20/28/28	0/4/4/4
5	SOG	A	405	-	-	6/11/31/31	0/1/1/1
5	SOG	B	404	-	-	9/11/31/31	0/1/1/1
5	SOG	A	408	-	-	5/11/31/31	0/1/1/1
3	PG4	A	402	-	-	2/10/10/10	-
5	SOG	B	407	-	-	3/7/27/31	0/1/1/1
6	PGW	A	409	-	-	30/55/55/55	-
2	NRK	B	401	-	-	5/20/28/28	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	409	PGW	O01-C1	4.64	1.47	1.34
6	A	410	PGW	O01-C1	4.58	1.47	1.34
6	A	409	PGW	O03-C19	4.52	1.46	1.33
5	B	406	SOG	C1'-S1	-4.41	1.75	1.81
6	A	410	PGW	O03-C19	4.29	1.45	1.33
5	B	408	SOG	C1'-S1	-3.75	1.76	1.81
5	A	408	SOG	C1'-S1	-3.42	1.77	1.81
5	A	406	SOG	C1'-S1	-3.41	1.77	1.81
2	B	401	NRK	C18-C13	3.36	1.43	1.38
5	B	407	SOG	C1'-S1	-3.36	1.77	1.81
5	A	405	SOG	C1'-S1	-3.24	1.77	1.81
5	B	404	SOG	C1'-S1	-3.16	1.77	1.81
2	A	401	NRK	C18-C13	2.92	1.43	1.38
5	B	408	SOG	C1-S1	-2.58	1.76	1.80
2	A	401	NRK	C25-C24	2.50	1.40	1.37
2	A	401	NRK	C04-C03	2.39	1.57	1.54
2	B	401	NRK	C01-C05	2.23	1.56	1.51
2	B	401	NRK	C14-N15	2.22	1.37	1.34
5	B	404	SOG	C1-S1	-2.21	1.77	1.80
5	A	406	SOG	C1-S1	-2.19	1.77	1.80
2	B	401	NRK	C23-C24	2.19	1.41	1.37
2	B	401	NRK	C04-C03	2.15	1.57	1.54
2	A	401	NRK	C21-N26	2.13	1.38	1.34
2	B	401	NRK	C25-C24	2.13	1.40	1.37
5	B	407	SOG	C1-S1	-2.09	1.77	1.80
2	A	401	NRK	C23-C24	2.06	1.41	1.37
5	A	408	SOG	C1-S1	-2.03	1.77	1.80

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NRK	C01-C05-N20	14.00	128.95	114.38
2	A	401	NRK	C01-C05-N20	12.58	127.47	114.38
2	A	401	NRK	O19-C05-C01	-8.20	110.86	122.25
2	B	401	NRK	C23-C24-C25	-6.94	117.90	121.54
2	B	401	NRK	C02-C01-C05	6.58	131.50	118.65
2	B	401	NRK	O19-C05-C01	-6.45	113.29	122.25
2	A	401	NRK	C23-C24-C25	-6.37	118.20	121.54
2	A	401	NRK	C02-C01-C05	6.01	130.37	118.65
6	A	410	PGW	O01-C1-C2	4.32	120.81	111.50
6	A	409	PGW	O01-C1-C2	4.06	120.24	111.50
5	A	405	SOG	C1'-S1-C1	3.85	107.29	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NRK	C03-C01-C05	-3.49	112.55	119.42
2	B	401	NRK	C24-C25-N26	3.29	123.44	121.46
5	B	406	SOG	C3-C4-C5	3.24	116.02	110.24
6	A	409	PGW	O03-C19-C20	3.16	121.82	111.91
5	A	406	SOG	C1-O5-C5	3.10	118.29	112.58
5	A	407	SOG	C3-C4-C5	3.00	115.58	110.24
5	A	407	SOG	C4-C3-C2	2.98	116.02	110.82
5	B	405	SOG	C1-O5-C5	2.94	118.01	112.58
2	A	401	NRK	C02-C03-C06	2.93	125.48	118.85
2	B	401	NRK	O19-C05-N20	-2.91	117.68	123.93
2	B	401	NRK	F29-C24-C23	2.90	123.46	118.54
2	A	401	NRK	C18-C13-C14	-2.83	114.41	118.41
2	B	401	NRK	C09-C08-C07	-2.81	119.64	123.29
5	B	406	SOG	C4-C3-C2	2.72	115.57	110.82
2	B	401	NRK	C06-C07-C08	2.69	121.22	118.30
6	A	410	PGW	O03-C19-C20	2.56	119.95	111.91
2	B	401	NRK	C18-C13-C14	-2.52	114.84	118.41
2	B	401	NRK	C02-C03-C04	-2.49	112.03	117.48
5	B	406	SOG	C1'-S1-C1	2.47	104.72	100.09
2	A	401	NRK	C22-C21-N26	-2.38	118.85	122.57
2	A	401	NRK	C24-C25-N26	2.37	122.88	121.46
5	B	407	SOG	C4-C3-C2	2.36	114.95	110.82
2	B	401	NRK	C04-O12-C13	2.35	123.41	117.67
2	A	401	NRK	C28-C14-C13	2.31	124.29	120.28
2	B	401	NRK	C28-C14-C13	2.28	124.25	120.28
2	A	401	NRK	C25-N26-C21	2.26	120.11	117.82
5	B	408	SOG	C1-O5-C5	2.22	116.67	112.58
5	B	408	SOG	C3-C4-C5	2.13	114.03	110.24
5	A	408	SOG	C1-C2-C3	-2.12	106.40	110.59
2	B	401	NRK	C22-C21-N26	-2.09	119.30	122.57
6	A	409	PGW	C03-C02-C01	-2.04	106.97	111.79

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	SOG	O5-C1-S1-C1'
6	A	410	PGW	C03-O11-P-O13
6	A	409	PGW	C03-O11-P-O12
6	A	409	PGW	C04-O12-P-O14
2	A	401	NRK	C02-C01-C05-O19
2	A	401	NRK	C02-C01-C05-N20

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Mol	Chain	Res	Type	Atoms
2	A	401	NRK	C03-C01-C05-O19
2	A	401	NRK	C03-C01-C05-N20
5	B	406	SOG	C2-C1-S1-C1'
5	B	406	SOG	O5-C1-S1-C1'
5	B	404	SOG	O5-C1-S1-C1'
5	B	407	SOG	C2'-C1'-S1-C1
2	B	401	NRK	C02-C01-C05-O19
2	B	401	NRK	C02-C01-C05-N20
2	B	401	NRK	C03-C01-C05-O19
2	B	401	NRK	C03-C01-C05-N20
5	A	406	SOG	C2'-C1'-S1-C1
5	A	408	SOG	S1-C1'-C2'-C3'
5	A	407	SOG	O5-C5-C6-O6
6	A	410	PGW	O12-C04-C05-OAF
5	A	406	SOG	O5-C5-C6-O6
5	A	408	SOG	O5-C5-C6-O6
5	A	405	SOG	O5-C5-C6-O6
5	B	406	SOG	O5-C5-C6-O6
6	A	410	PGW	O12-C04-C05-CAD
6	A	410	PGW	C20-C19-O03-C01
5	B	404	SOG	O5-C5-C6-O6
6	A	409	PGW	C19-C20-C21-C22
6	A	410	PGW	O04-C19-O03-C01
5	B	408	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	C19-C20-C21-C22
5	A	406	SOG	C4-C5-C6-O6
5	A	406	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	C6-C7-C8-C9
6	A	410	PGW	C03-O11-P-O12
5	A	405	SOG	C1'-C2'-C3'-C4'
5	B	404	SOG	C1'-C2'-C3'-C4'
6	A	409	PGW	C1-C2-C3-C4
5	A	407	SOG	C4-C5-C6-O6
5	A	406	SOG	C1'-C2'-C3'-C4'
5	B	404	SOG	C3'-C4'-C5'-C6'
5	B	404	SOG	C4'-C5'-C6'-C7'
5	A	406	SOG	C2'-C3'-C4'-C5'
6	A	409	PGW	C5-C6-C7-C8
6	A	409	PGW	C05-C04-O12-P
5	B	404	SOG	C2'-C3'-C4'-C5'
5	A	406	SOG	C3'-C4'-C5'-C6'
6	A	409	PGW	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	408	SOG	C4'-C5'-C6'-C7'
6	A	410	PGW	O02-C1-O01-C02
6	A	410	PGW	C21-C22-C23-C24
6	A	409	PGW	C16-C15-C27-C26
6	A	410	PGW	C22-C23-C24-C25
5	A	405	SOG	C4'-C5'-C6'-C7'
6	A	410	PGW	C08-C09-C11-C12
5	B	407	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	C2-C1-O01-C02
6	A	409	PGW	C2-C1-O01-C02
6	A	409	PGW	C08-C09-C11-C12
5	B	407	SOG	O5-C5-C6-O6
6	A	410	PGW	C09-C11-C12-C13
6	A	410	PGW	C27-C15-C16-C17
6	A	409	PGW	O02-C1-O01-C02
6	A	409	PGW	C04-O12-P-O11
6	A	410	PGW	C2-C3-C4-C5
5	A	405	SOG	C2'-C3'-C4'-C5'
5	B	408	SOG	O5-C5-C6-O6
5	B	406	SOG	C4-C5-C6-O6
5	A	405	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	C25-C26-C27-C15
5	A	405	SOG	C4-C5-C6-O6
6	A	409	PGW	C3-C4-C5-C6
6	A	409	PGW	C11-C12-C13-C14
5	A	406	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	C01-C02-C03-O11
5	B	404	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	O03-C01-C02-C03
5	A	406	SOG	C4'-C5'-C6'-C7'
6	A	410	PGW	C16-C15-C27-C26
6	A	409	PGW	C6-C7-C8-C9
5	B	408	SOG	C2'-C1'-S1-C1
6	A	409	PGW	C4-C5-C6-C7
6	A	409	PGW	C20-C19-O03-C01
3	A	402	PG4	C3-C4-O3-C5
5	A	408	SOG	C4-C5-C6-O6
6	A	409	PGW	O01-C02-C03-O11
6	A	410	PGW	O03-C01-C02-O01
5	B	404	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	C15-C16-C17-C18
6	A	409	PGW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	A	410	PGW	C05-C04-O12-P
5	B	408	SOG	C3'-C4'-C5'-C6'
6	A	409	PGW	C03-O11-P-O13
6	A	409	PGW	C04-O12-P-O13
6	A	409	PGW	O04-C19-O03-C01
5	B	406	SOG	C2'-C3'-C4'-C5'
5	B	408	SOG	C4'-C5'-C6'-C7'
6	A	410	PGW	C24-C25-C26-C27
5	A	408	SOG	C1'-C2'-C3'-C4'
6	A	410	PGW	C04-O12-P-O11
5	B	408	SOG	C2'-C3'-C4'-C5'
6	A	409	PGW	C20-C21-C22-C23
6	A	409	PGW	C03-C02-O01-C1
5	B	404	SOG	C4-C5-C6-O6
6	A	409	PGW	C7-C8-C9-C10
6	A	409	PGW	O01-C1-C2-C3
5	B	406	SOG	C5'-C6'-C7'-C8'
3	A	402	PG4	C6-C5-O3-C4
2	B	401	NRK	C03-C04-O12-C13
5	B	406	SOG	C4'-C5'-C6'-C7'
6	A	409	PGW	O02-C1-C2-C3
2	A	401	NRK	C03-C04-O12-C13

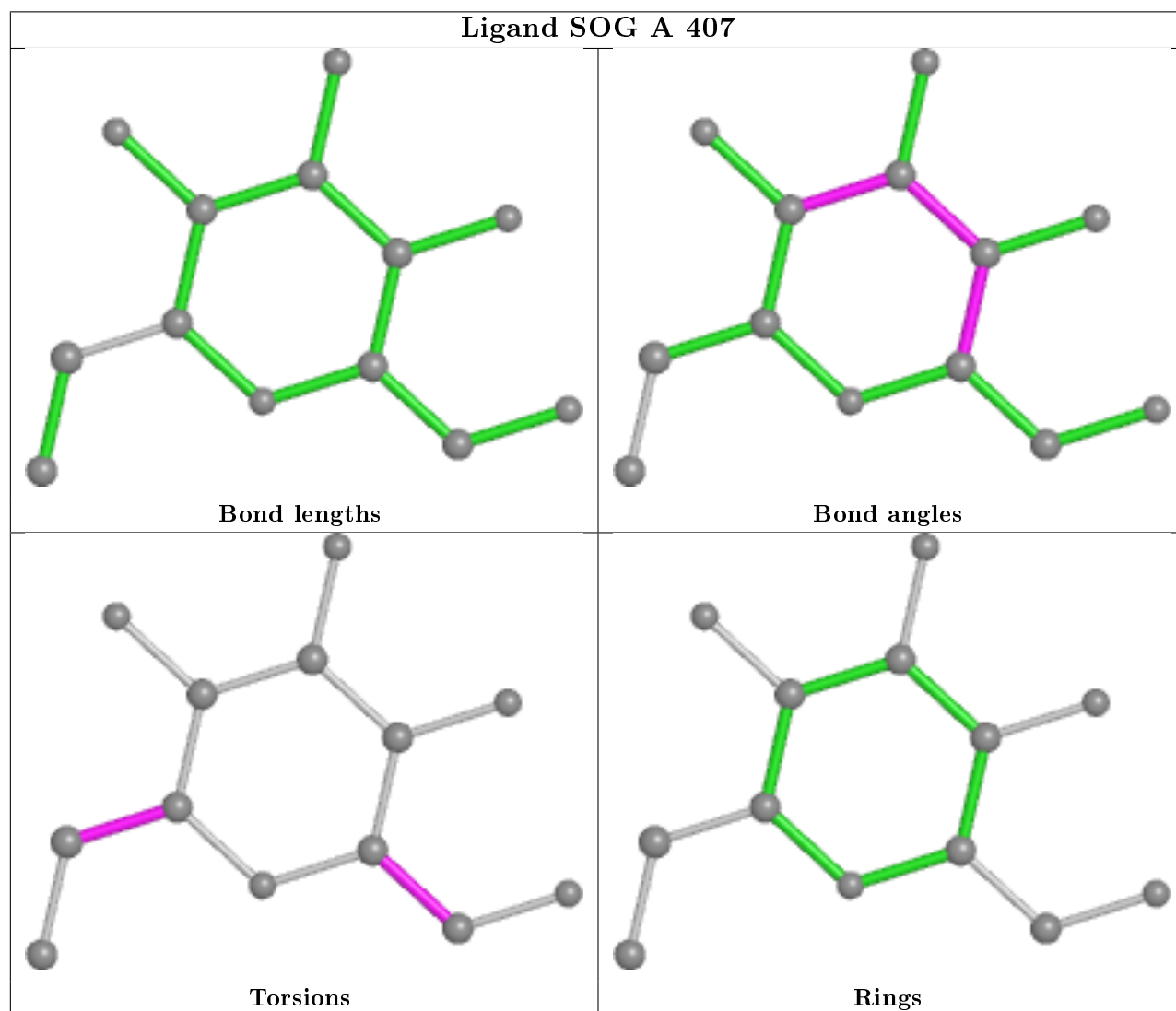
There are no ring outliers.

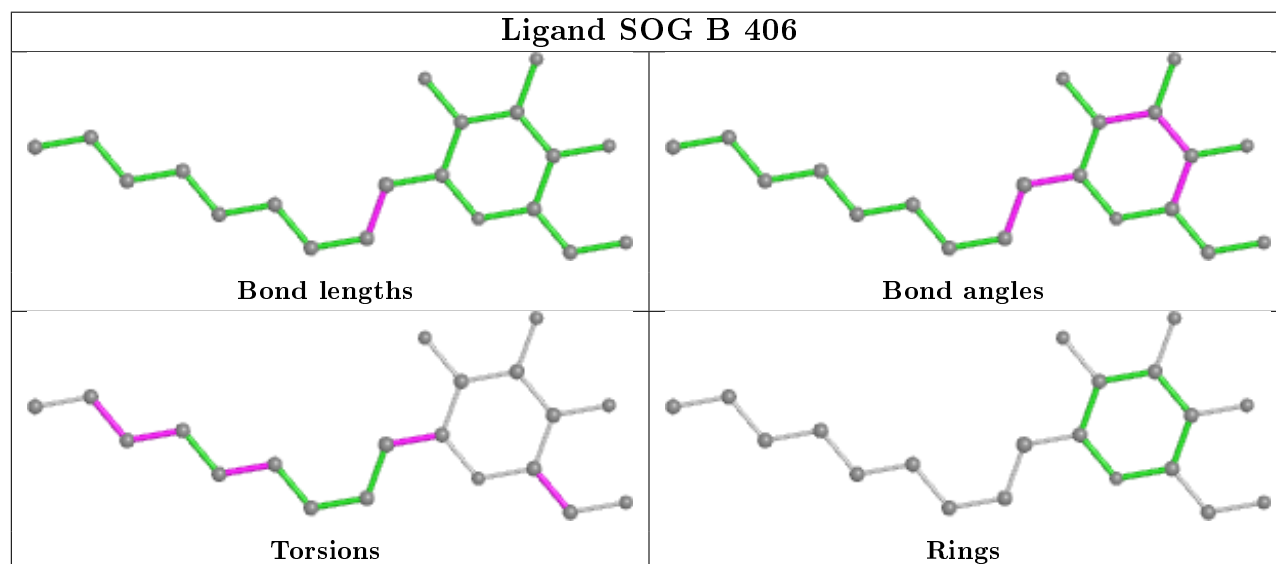
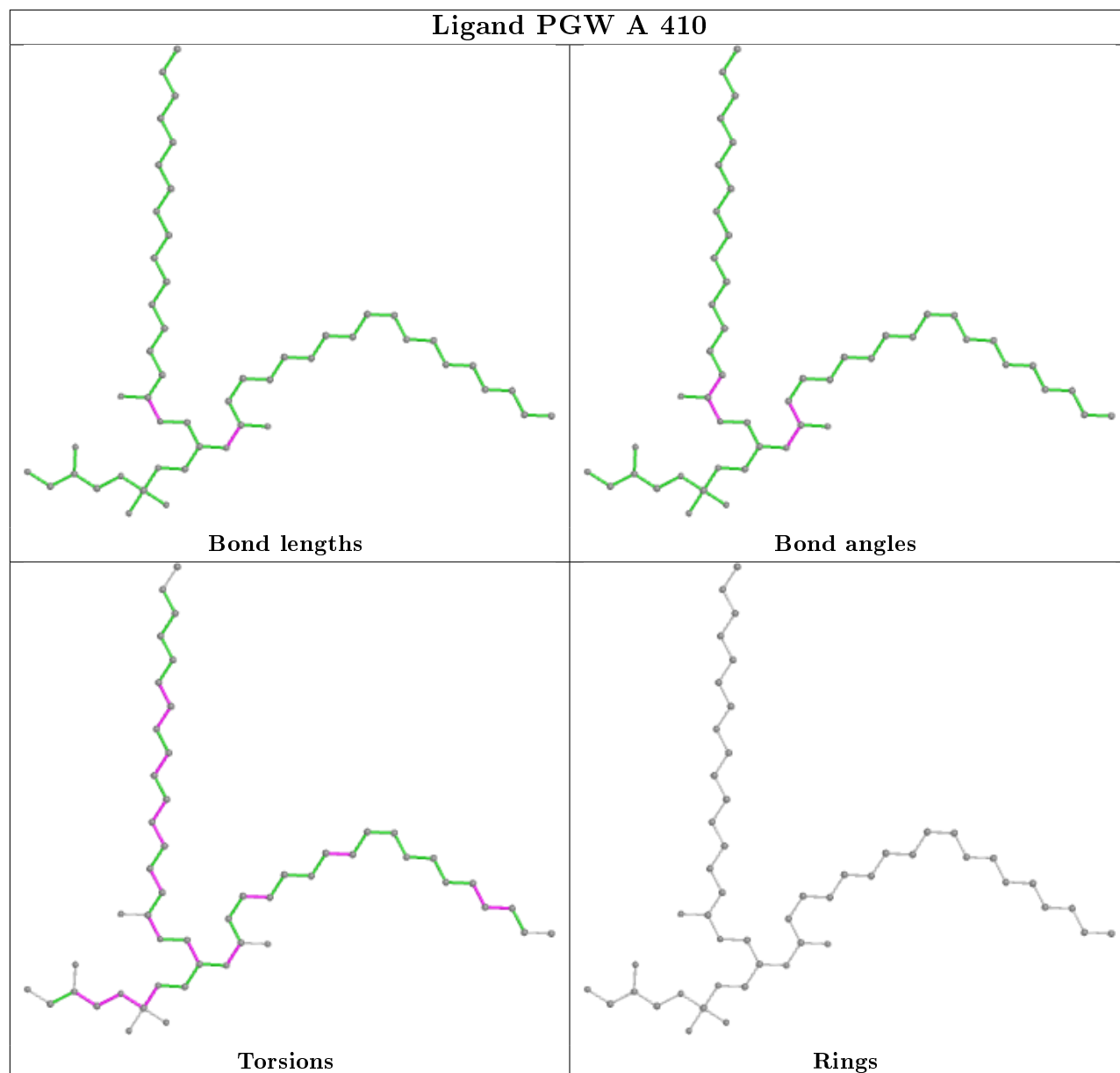
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	410	PGW	4	0
5	B	406	SOG	1	0
6	A	409	PGW	2	0
3	A	402	PG4	1	0

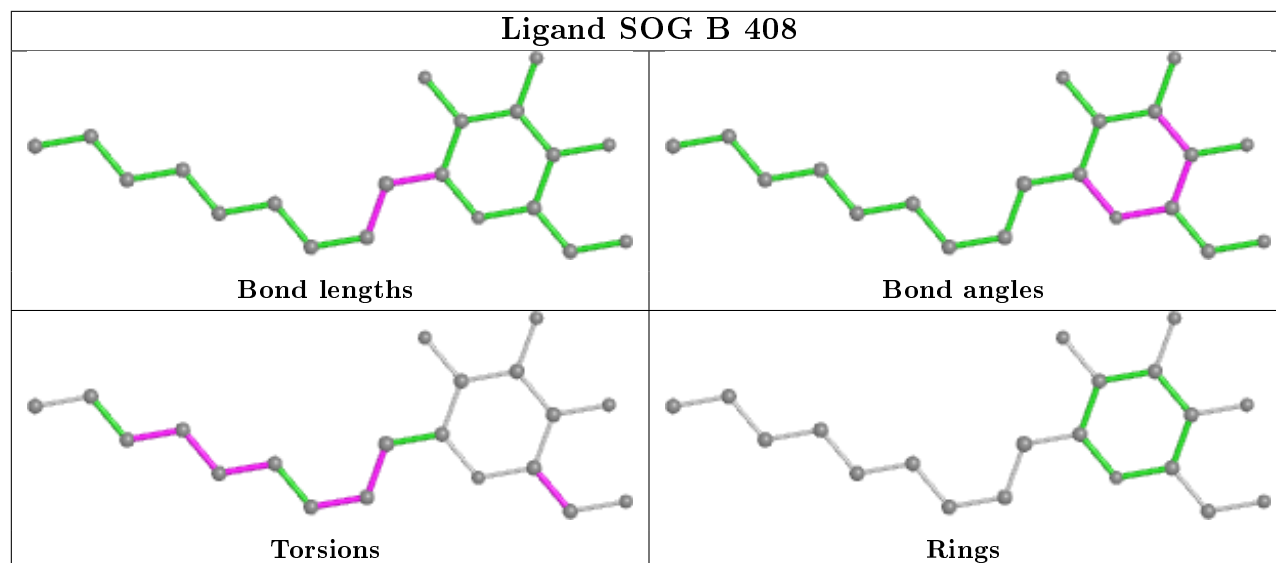
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

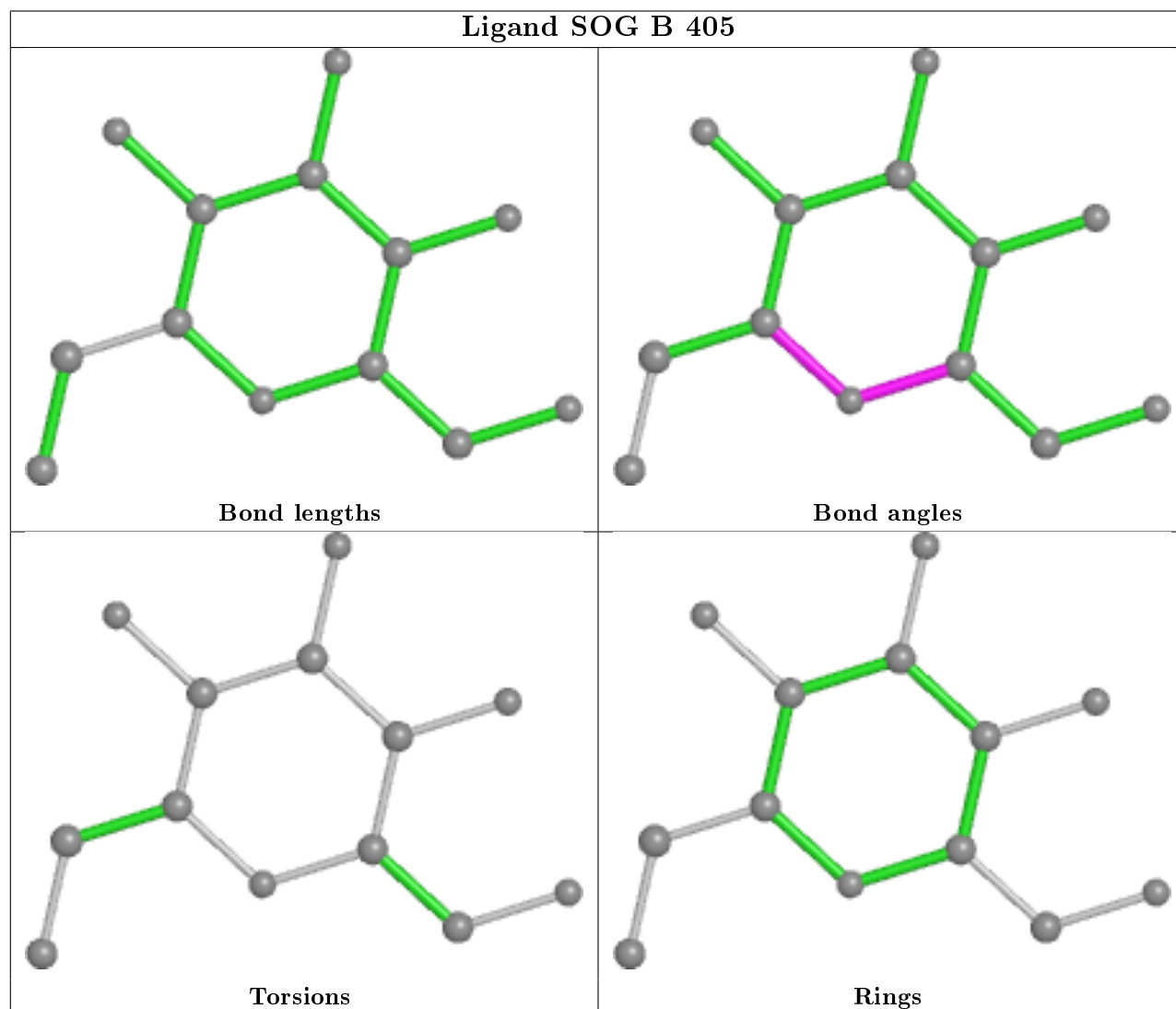




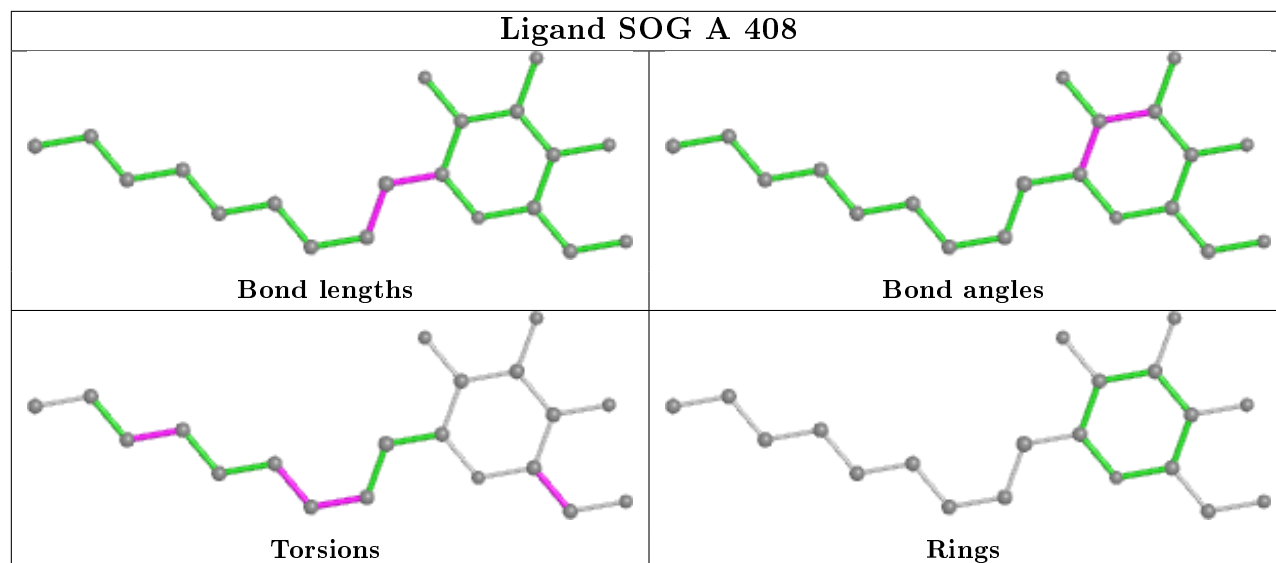
Ligand SOG B 408



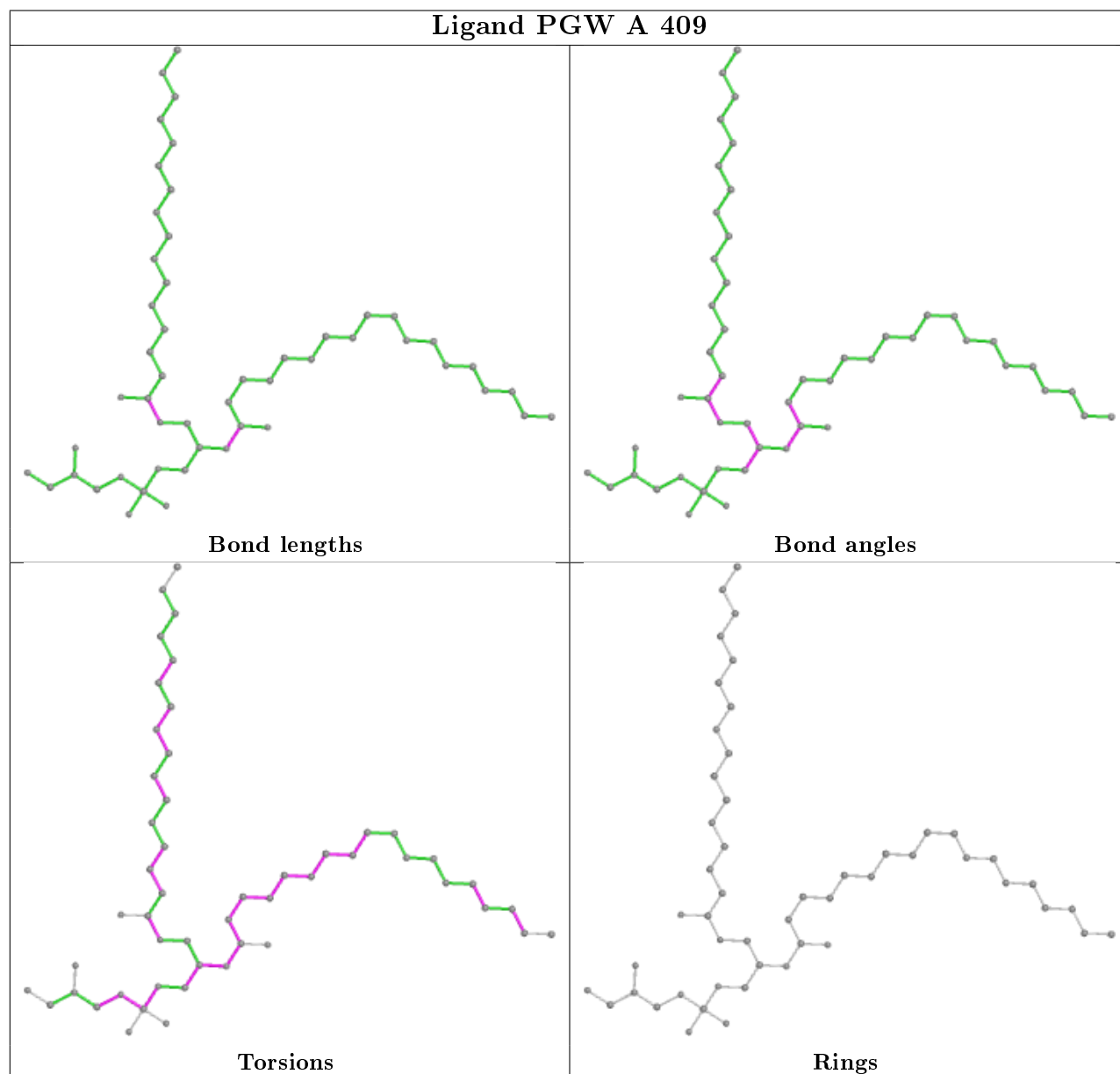
Ligand SOG B 405

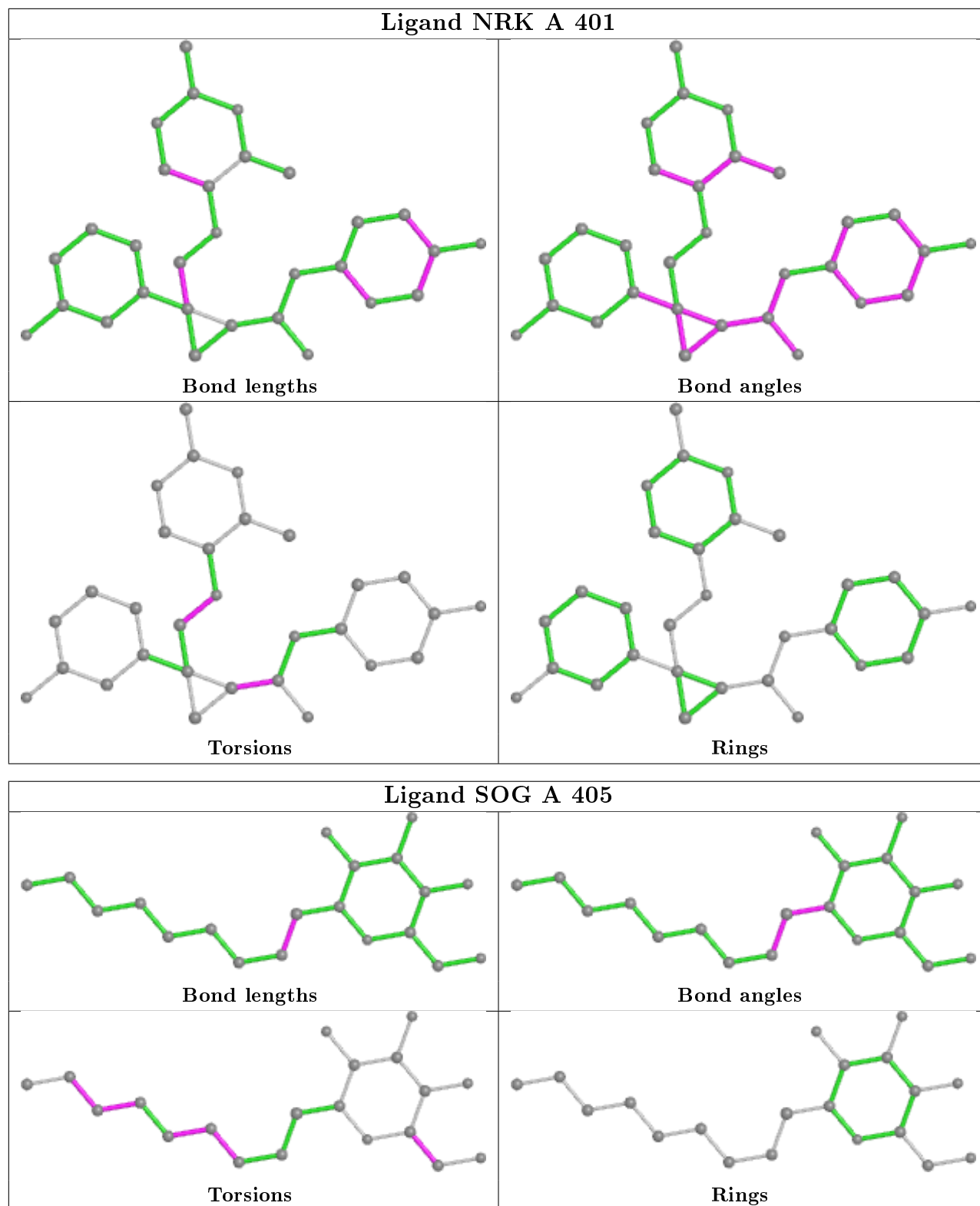


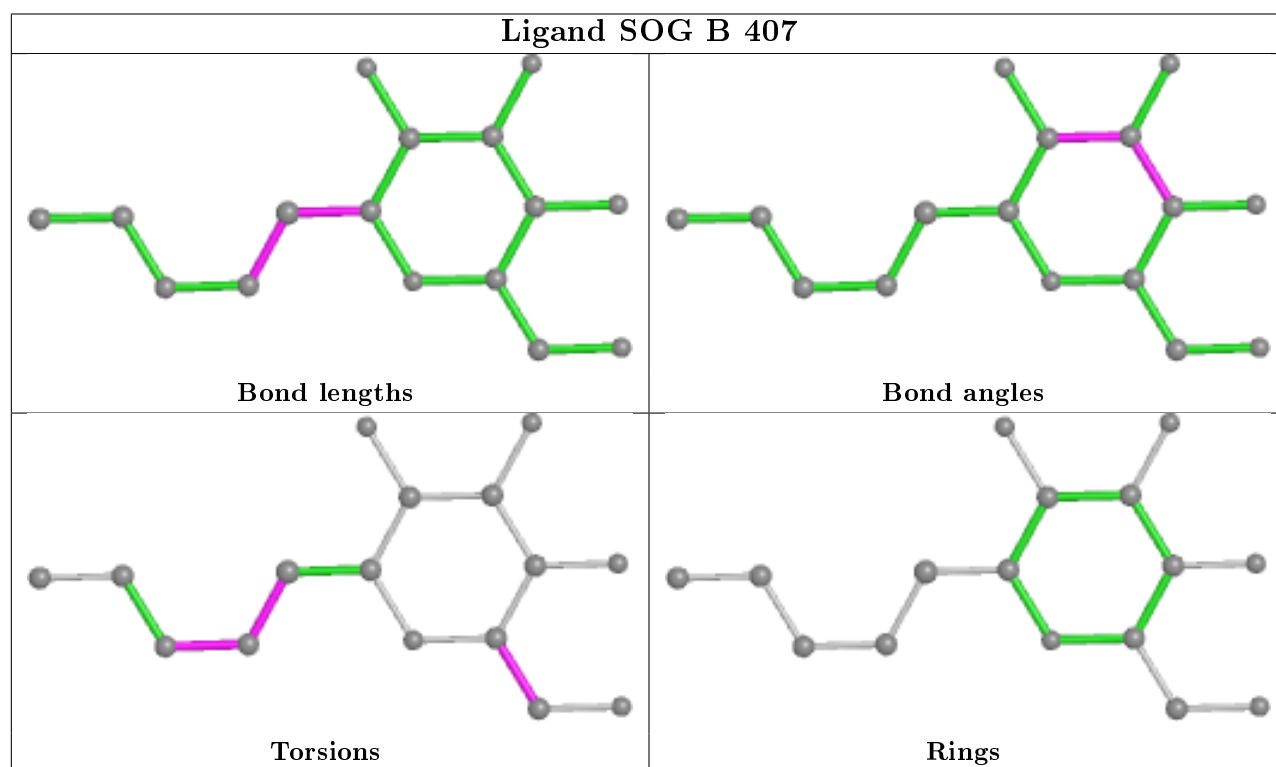
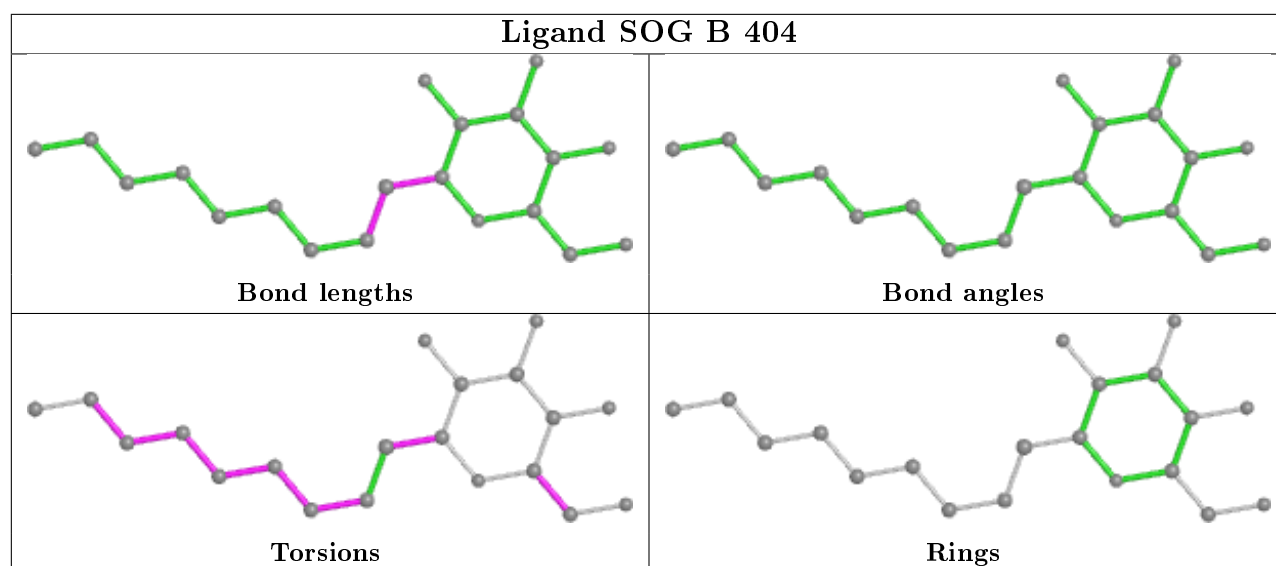
Ligand SOG A 408

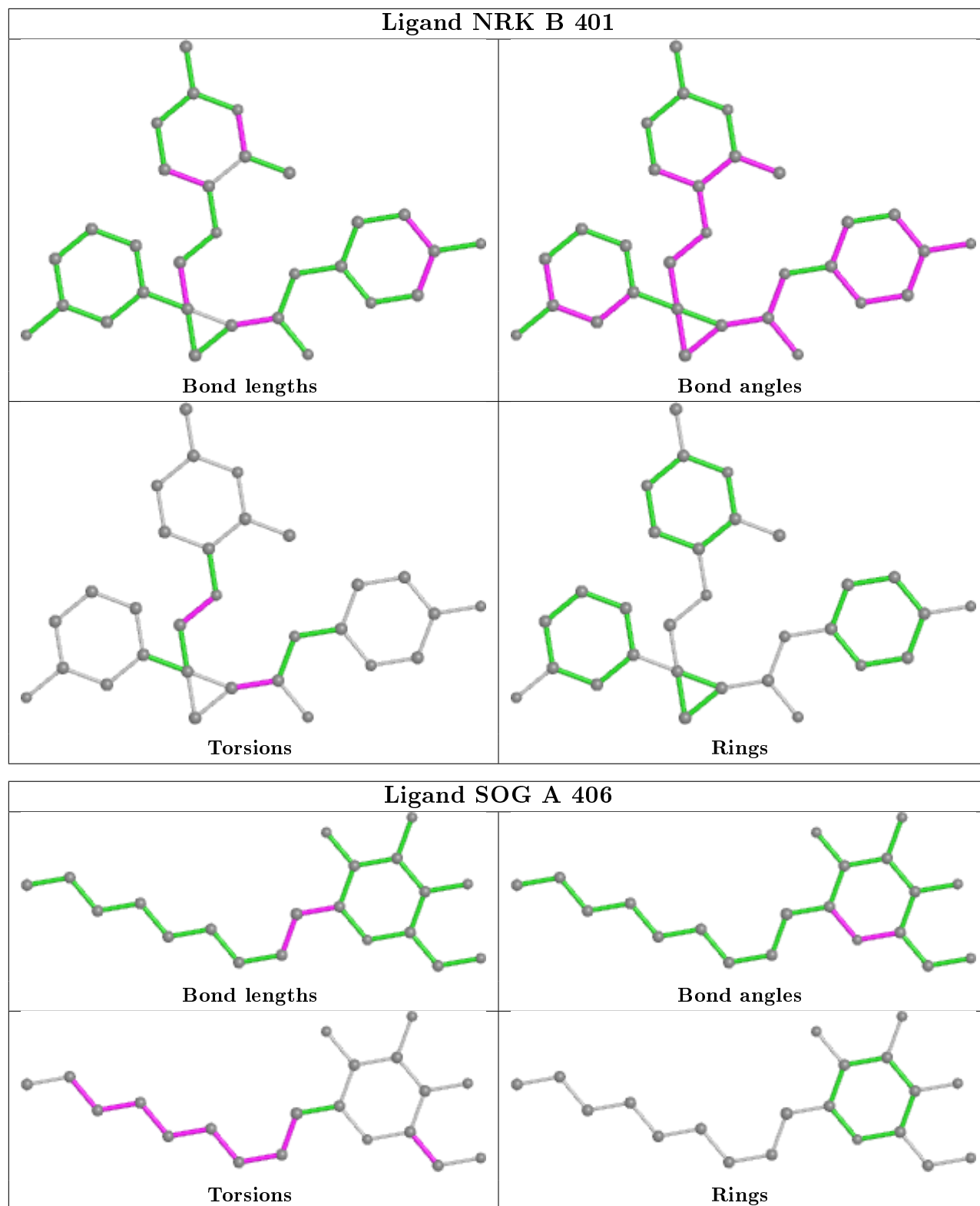


Ligand PGW A 409









5.7 Other polymers ⓘ

There are no such residues in this entry.







5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	300/336 (89%)	0.88	60 (20%)  	38, 63, 119, 158	0
1	B	303/336 (90%)	0.94	58 (19%)  	40, 61, 111, 159	0
All	All	603/672 (89%)	0.91	118 (19%)  	38, 62, 116, 159	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	8.6
1	B	287	VAL	7.7
1	B	45	TYR	7.3
1	A	330	ALA	7.0
1	B	246	GLN	6.8
1	B	47	TRP	6.8
1	A	197	ARG	6.5
1	B	376	TRP	6.3
1	B	245	ARG	6.3
1	B	329	GLN	5.8
1	A	333	ARG	5.8
1	B	43	LYS	5.8
1	B	375	TRP	5.3
1	B	247	ILE	5.1
1	A	329	GLN	5.1
1	A	361	LEU	4.8
1	B	337	TYR	4.8
1	A	198	ALA	4.8
1	B	290	MET	4.7
1	A	331	SER	4.5
1	A	199	PHE	4.4
1	A	73	ARG	4.4
1	B	328	ARG	4.4
1	A	152	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	72	TRP	4.3
1	A	47	TRP	4.1
1	B	242	LEU	4.1
1	B	370	LYS	4.0
1	B	134	VAL	4.0
1	B	152	LEU	4.0
1	B	333	ARG	3.9
1	B	377	LEU	3.9
1	B	330	ALA	3.8
1	A	332	ASP	3.7
1	A	175	ILE	3.7
1	A	83	TYR	3.6
1	B	130	VAL	3.6
1	A	373	PHE	3.5
1	A	287	VAL	3.5
1	B	44	GLN	3.5
1	B	155	LYS	3.5
1	A	116	HIS	3.4
1	B	332	ASP	3.4
1	B	288	LYS	3.4
1	B	129	SER	3.3
1	B	133	ALA	3.3
1	B	132	VAL	3.3
1	A	243	TRP	3.2
1	A	158	ALA	3.2
1	B	248	PRO	3.2
1	B	88	LEU	3.1
1	B	135	LEU	3.1
1	A	172	SER	3.1
1	A	130	VAL	3.0
1	A	298	LYS	3.0
1	A	132	VAL	3.0
1	A	114	PHE	3.0
1	B	162	LEU	3.0
1	B	91	ALA	3.0
1	B	117	ALA	2.9
1	A	115	GLY	2.9
1	A	88	LEU	2.9
1	A	376	TRP	2.9
1	B	210	LEU	2.8
1	B	374	SER	2.8
1	B	136	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	128	VAL	2.8
1	B	171	VAL	2.8
1	A	174	ALA	2.8
1	A	239	PHE	2.8
1	B	172	SER	2.7
1	B	139	PHE	2.7
1	A	295	LYS	2.7
1	A	128	VAL	2.7
1	A	286	GLU	2.7
1	B	291	ARG	2.6
1	A	171	VAL	2.6
1	B	373	PHE	2.6
1	B	131	SER	2.6
1	B	331	SER	2.6
1	A	133	ALA	2.6
1	A	159	ARG	2.6
1	B	230	LEU	2.5
1	A	72	TRP	2.5
1	B	372	ALA	2.5
1	B	239	PHE	2.5
1	B	168	ILE	2.5
1	A	291	ARG	2.4
1	A	242	LEU	2.4
1	A	374	SER	2.4
1	A	153	LEU	2.4
1	B	46	ALA	2.4
1	A	316	VAL	2.3
1	A	78	ARG	2.3
1	A	360	PHE	2.3
1	B	127	ALA	2.3
1	A	113	LEU	2.3
1	A	335	ALA	2.3
1	A	294	ARG	2.3
1	A	167	GLY	2.3
1	A	177	VAL	2.3
1	B	75	HIS	2.3
1	B	116	HIS	2.3
1	B	327	PHE	2.3
1	A	137	LEU	2.2
1	B	137	LEU	2.2
1	A	336	VAL	2.2
1	A	91	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	2.1
1	B	138	SER	2.1
1	A	129	SER	2.1
1	A	127	ALA	2.1
1	A	131	SER	2.1
1	B	236	PHE	2.1
1	A	240	ARG	2.0
1	A	118	LEU	2.0
1	A	375	TRP	2.0
1	A	29	ASP	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 monosaccharides 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.

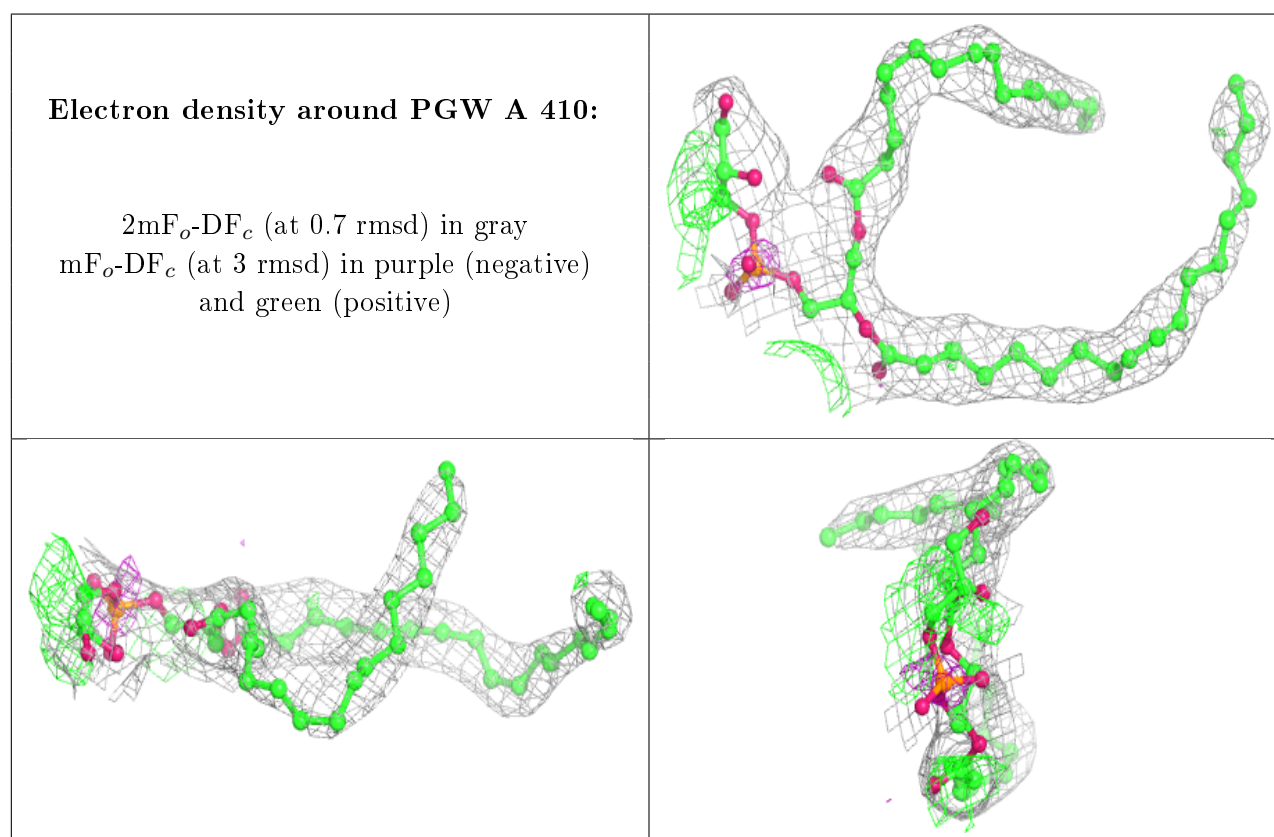
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG4	A	402	13/13	0.56	0.38	87,94,102,102	0
6	PGW	A	410	51/51	0.75	0.23	42,74,115,118	0
6	PGW	A	409	51/51	0.76	0.30	47,72,119,120	0
5	SOG	A	408	20/20	0.76	0.22	98,116,120,121	0
5	SOG	B	407	16/20	0.77	0.28	105,125,128,129	0
5	SOG	A	407	13/20	0.79	0.27	126,128,132,132	0
5	SOG	B	408	20/20	0.81	0.31	65,101,106,107	0
5	SOG	B	404	20/20	0.81	0.34	94,100,102,103	0
5	SOG	B	405	13/20	0.84	0.21	113,116,118,119	0
4	SO4	B	403	5/5	0.87	0.12	119,120,122,122	0
5	SOG	A	406	20/20	0.88	0.19	57,102,108,109	0
5	SOG	B	406	20/20	0.89	0.31	58,89,93,95	0
4	SO4	A	404	5/5	0.91	0.13	138,139,139,140	0

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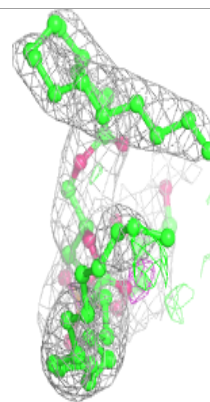
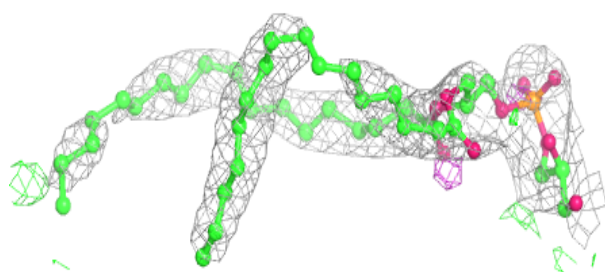
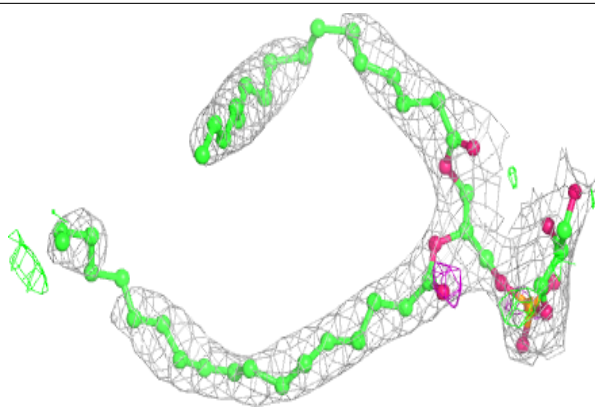
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NRK	A	401	30/30	0.91	0.15	44,45,51,66	0
4	SO4	A	403	5/5	0.93	0.11	112,112,113,114	0
2	NRK	B	401	30/30	0.93	0.14	44,45,49,60	0
5	SOG	A	405	20/20	0.93	0.16	55,63,73,73	0
4	SO4	B	402	5/5	0.97	0.07	89,90,91,93	0

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.

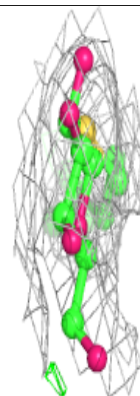
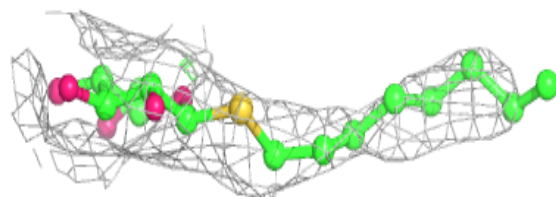
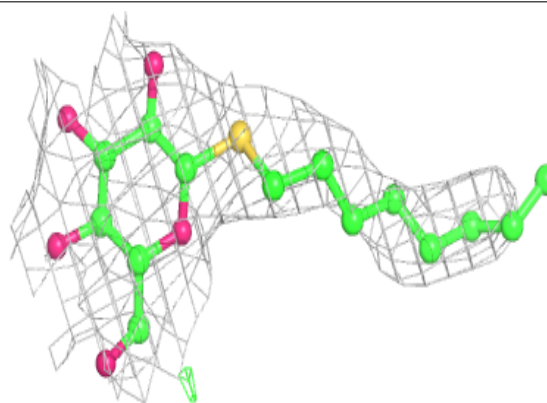


Electron density around PGW A 409:

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

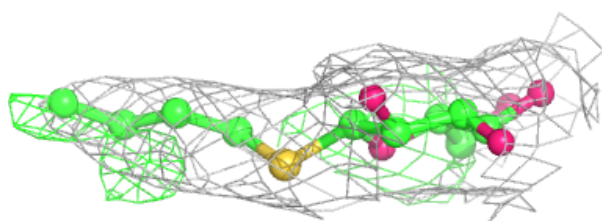
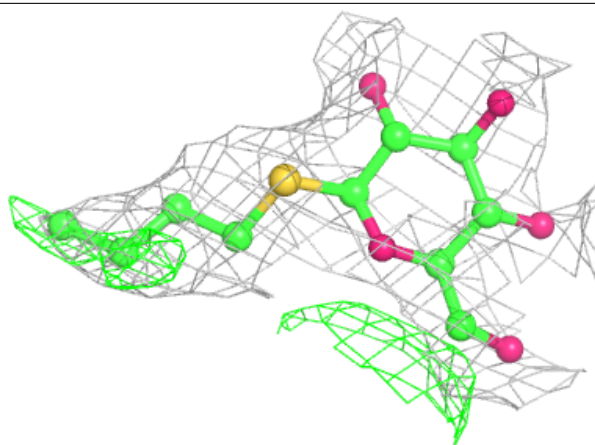
**Electron density around SOG A 408:**

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



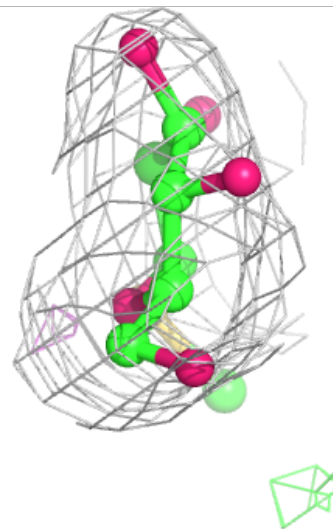
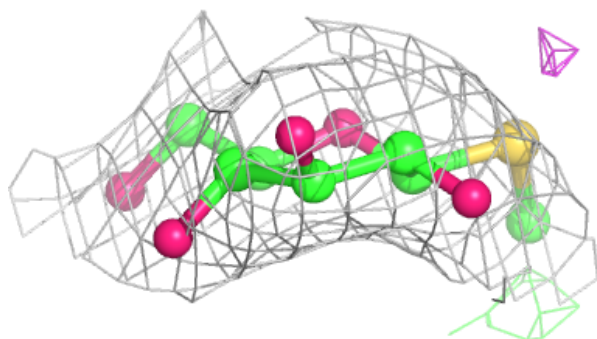
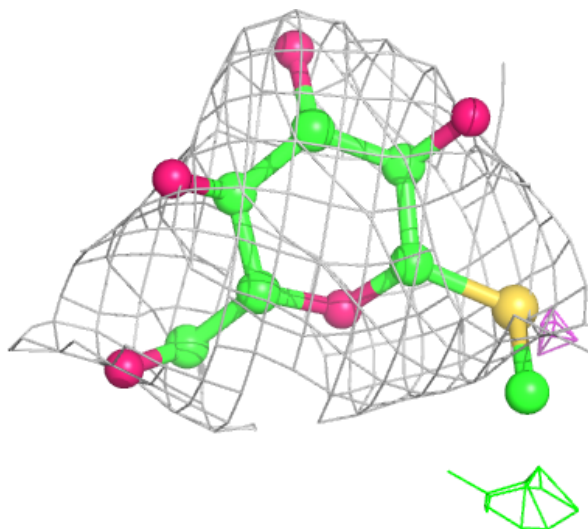
Electron density around SOG B 407:

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



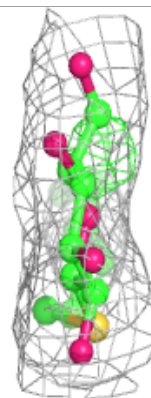
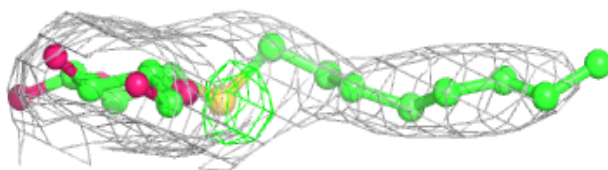
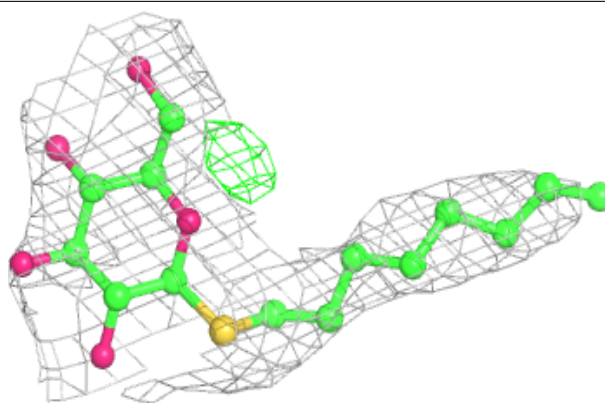
Electron density around SOG A 407:

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

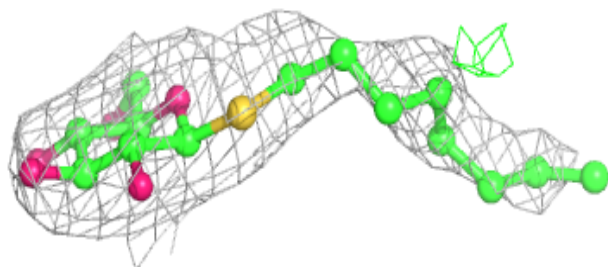
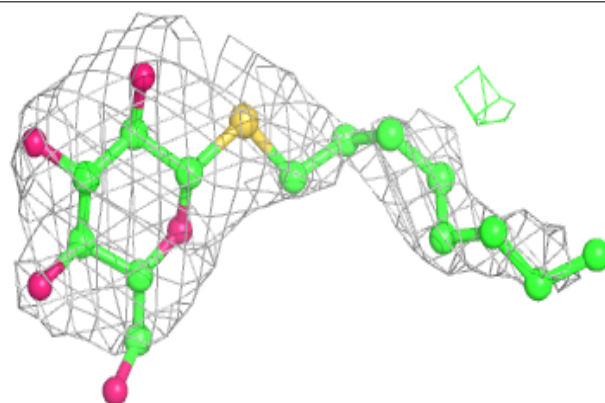


Electron density around SOG B 408:

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

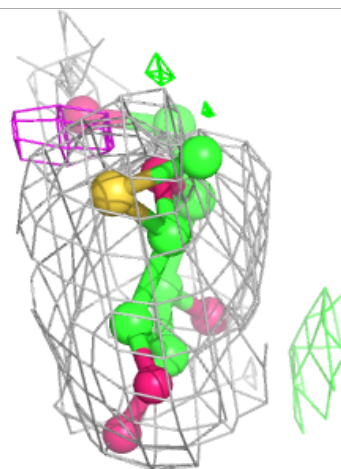
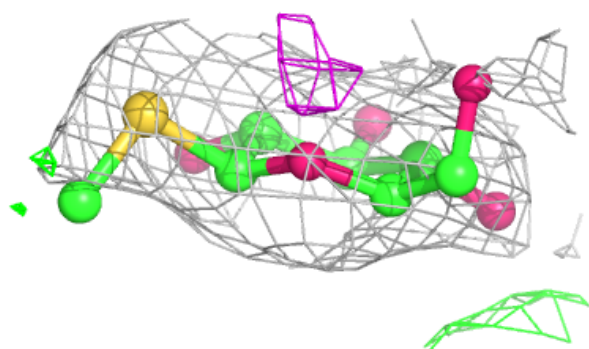
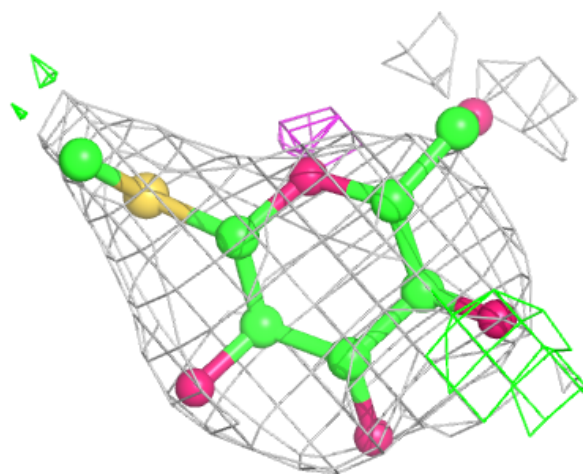
**Electron density around SOG B 404:**

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



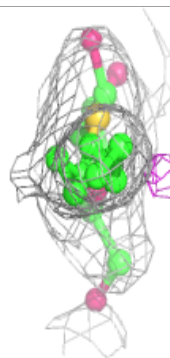
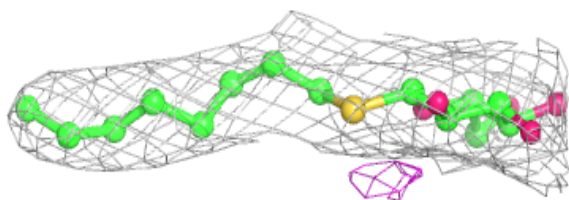
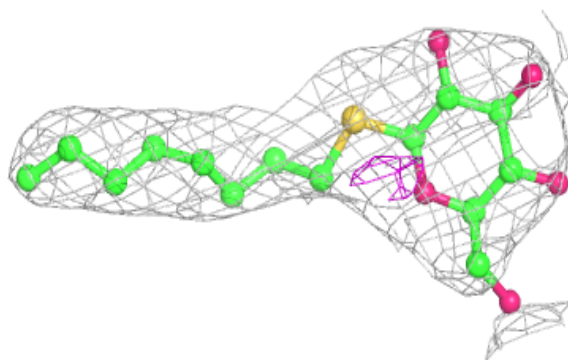
Electron density around SOG B 405:

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

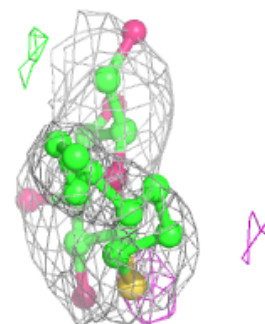
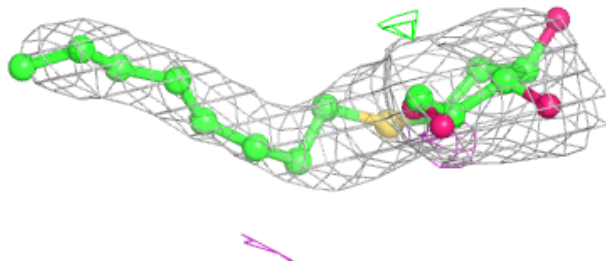
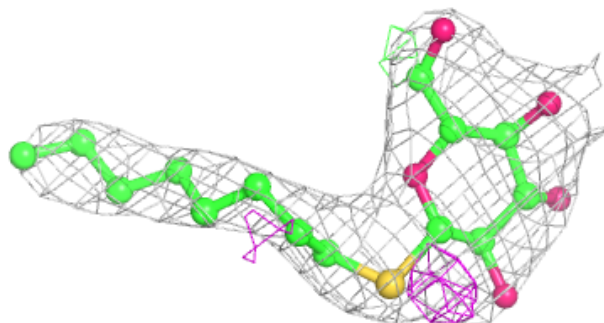


Electron density around SOG A 406:

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

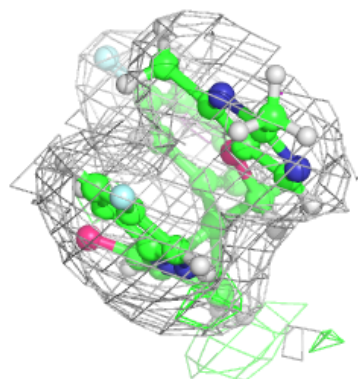
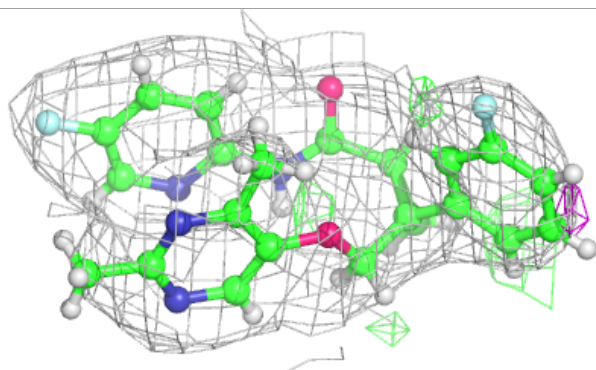
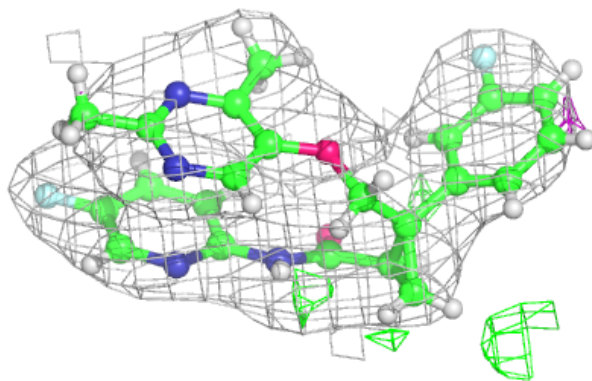
**Electron density around SOG B 406:**

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

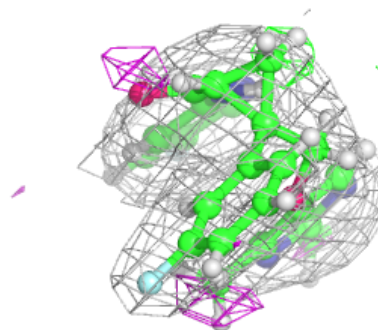
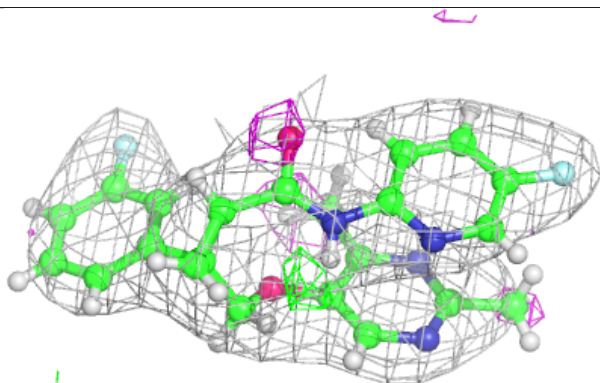
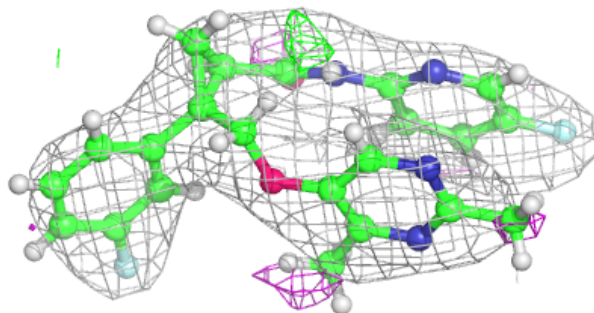


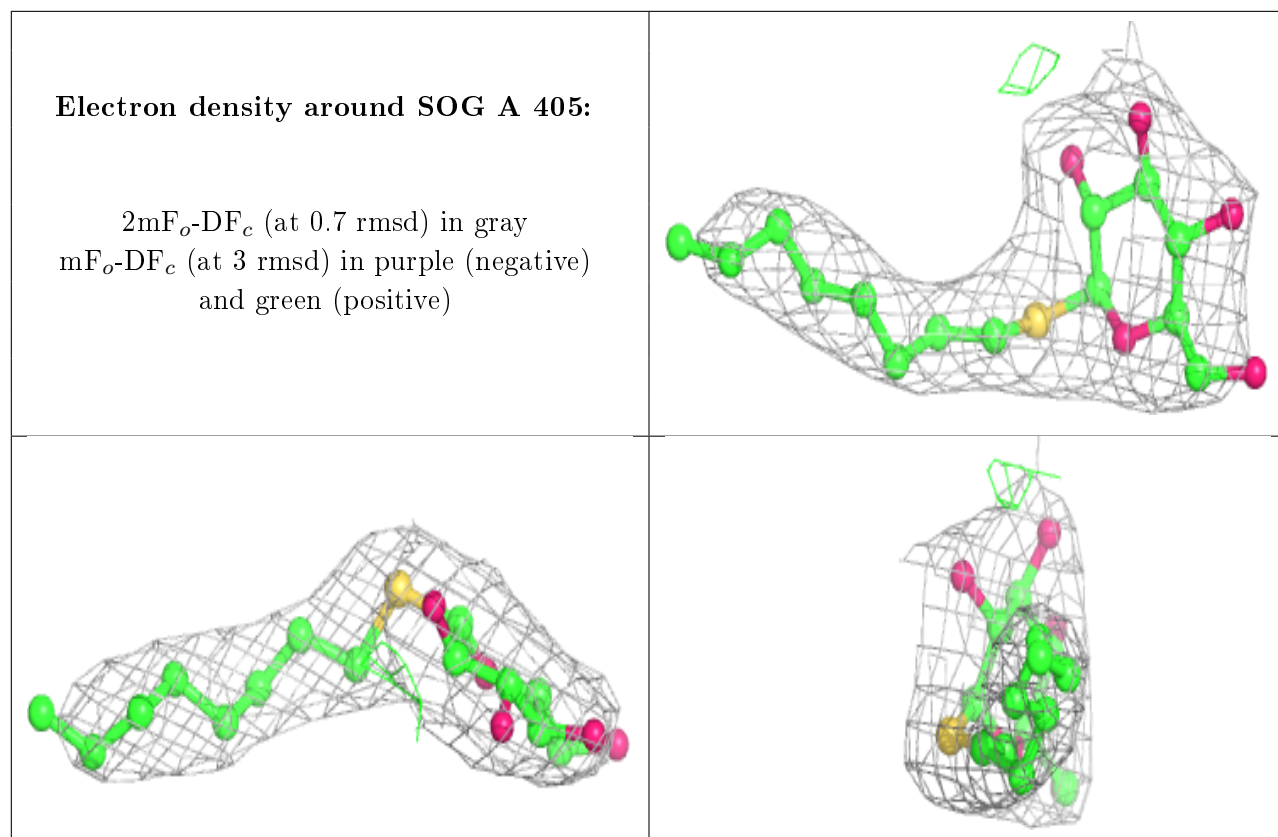
Electron density around NRK A 401:

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

**Electron density around NRK 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.