



# Full wwPDB X-ray Structure Validation Report

Jan 14, 2024 – 11:32 am GMT


PDB ID : 6TQ6  
Title : Crystal structure of the Orexin-1 receptor in complex with Compound 14  
Authors : Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.  
Deposited on : 2019-12-16  
Resolution : 2.55 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

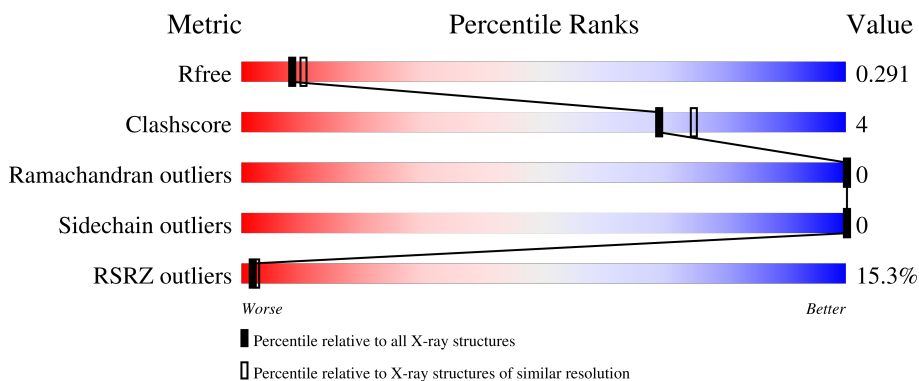
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NVH	B	401	-	-	-	X
5	SOG	A	405	-	-	-	X
5	SOG	B	408	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2358	1569	388	384	17	0	0	0
1	B	301	2386	1581	399	389	17	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

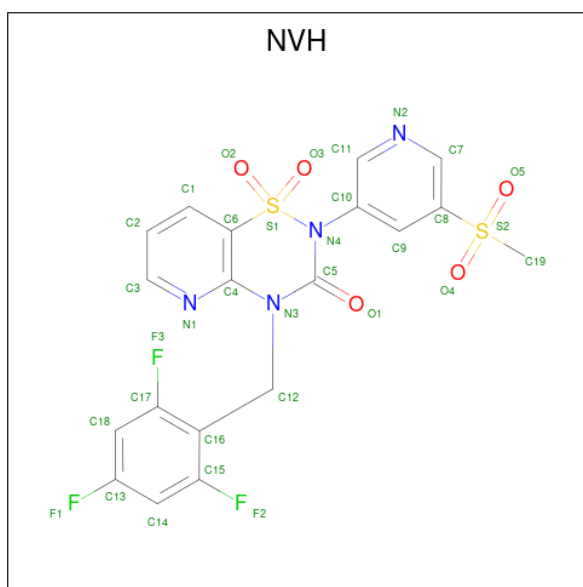
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU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

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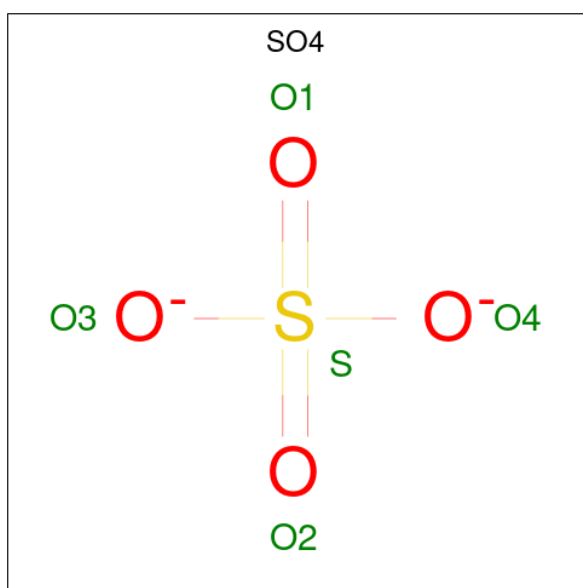
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered 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-(5-methylsulfonylpyridin-3-yl)-1,1-bis(oxidanylidene)-4-[[2,4,6-tris(fluoro-nyl)phenyl]methyl]pyrido[2,3-e][1,2,4]thiadiazin-3-one (three-letter code: NVH) (formula: C<sub>19</sub>H<sub>13</sub>F<sub>3</sub>N<sub>4</sub>O<sub>5</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	Total	33	19	3	4	5	2	0
2	B	1	Total	33	19	3	4	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



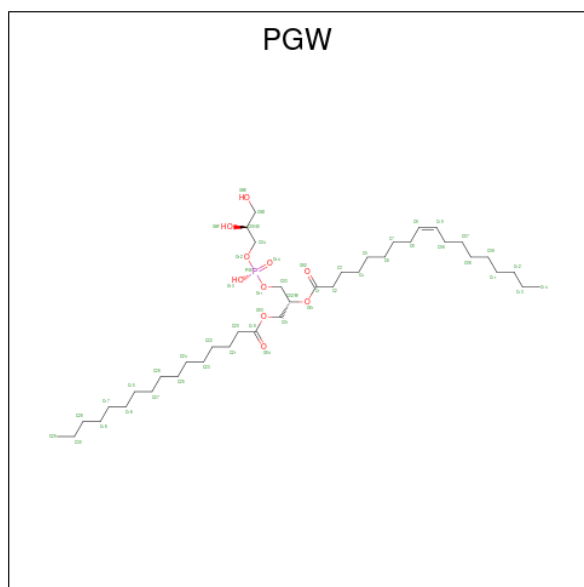
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	O	S			
3	A	1	Total	5	4	1	0	0
3	A	1	Total	5	4	1	0	0

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

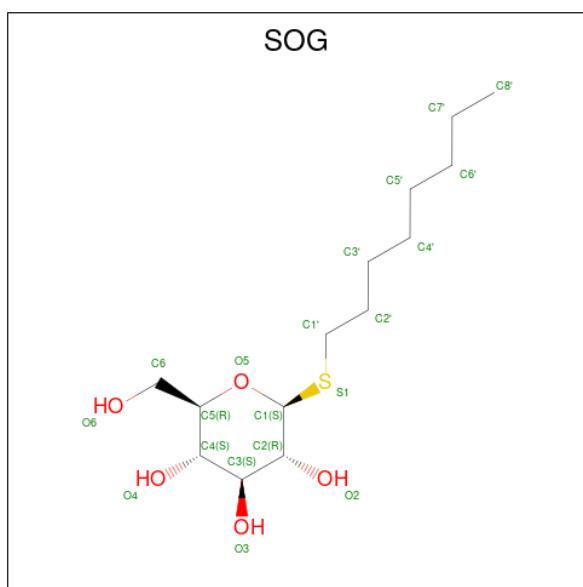
- Molecule 4 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



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

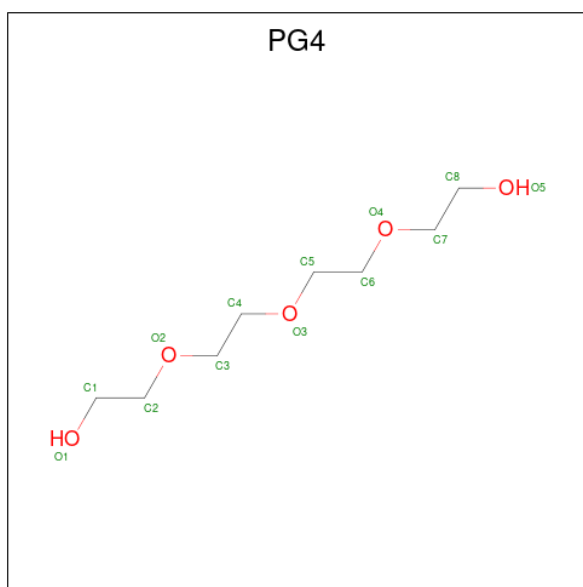
- Molecule 5 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>5</sub>S).





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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

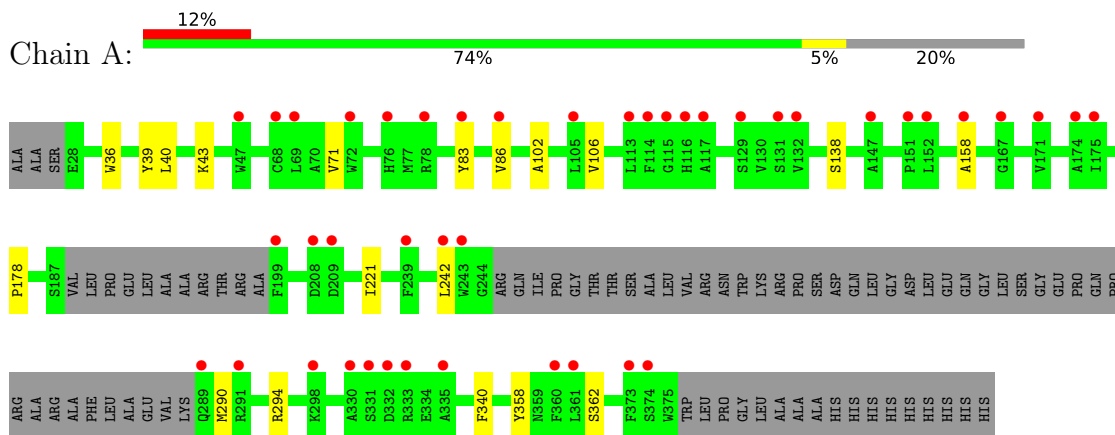
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	14	Total O 14 14	0	0
7	B	12	Total O 12 12	0	0

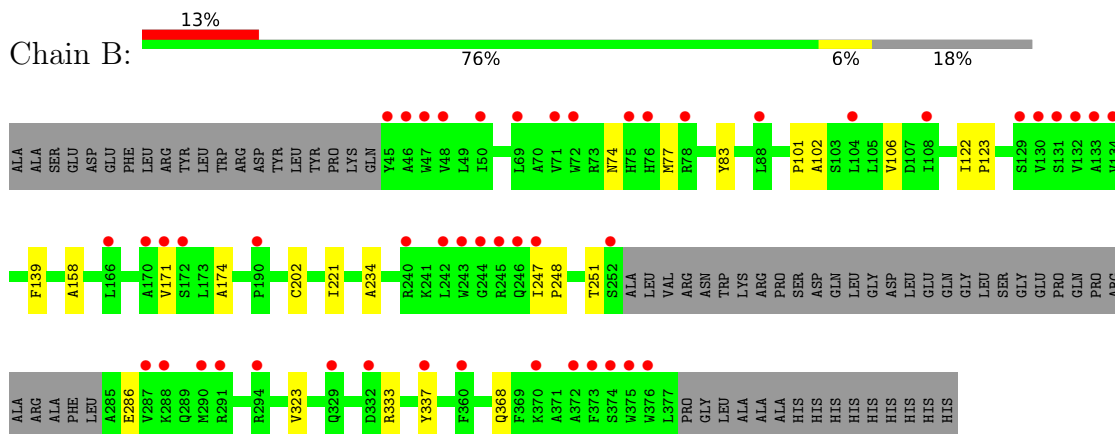
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.83Å 147.07Å 72.26Å 90.00° 111.56° 90.00°	Depositor
Resolution (Å)	34.06 – 2.55 34.06 – 2.55	Depositor EDS
% Data completeness (in resolution range)	78.7 (34.06-2.55) 83.9 (34.06-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.18 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.223 , 0.263 0.239 , 0.291	Depositor DCC
$R_{free}$ test set	1809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NVH, PG4, SOG, PGW, 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	0.41	0/2425	0.54	0/3303
1	B	0.39	0/2452	0.53	0/3345
All	All	0.40	0/4877	0.54	0/6648

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2358	0	2397	15	0
1	B	2386	0	2453	19	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	51	0	76	3	0
4	B	51	0	76	4	0
5	A	80	0	112	2	0
5	B	120	0	168	2	0
6	A	13	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	18	2	0
7	A	14	0	0	0	0
7	B	12	0	0	0	0
All	All	5184	0	5318	39	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 4.

All (39) 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	2.11	0.86
1:A:71:VAL:HG21	1:A:86:VAL:HG21	1.69	0.75
1:A:290:MET:SD	1:A:294:ARG:NH2	2.61	0.74
1:B:101:PRO:HB2	5:B:405:SOG:H8'1	1.74	0.69
1:B:77:MET:HE1	1:B:368:GLN:HG3	1.78	0.65
5:A:406:SOG:H4'2	1:B:171:VAL:HG21	1.81	0.61
1:B:77:MET:CE	1:B:368:GLN:HG3	2.31	0.60
1:A:36:TRP:HA	1:A:40:LEU:HB2	1.84	0.60
1:A:39:TYR:CE1	1:A:43:LYS:CD	2.87	0.57
4:B:404:PGW:H01A	4:B:404:PGW:H04A	1.87	0.56
1:A:290:MET:O	1:A:294:ARG:HG3	2.06	0.55
1:B:122:ILE:HB	1:B:123:PRO:HD3	1.88	0.55
1:B:323:VAL:O	5:B:409:SOG:H1'2	2.06	0.55
4:A:404:PGW:H7A	1:B:234:ALA:HB2	1.89	0.54
1:A:242:LEU:O	1:A:294:ARG:NH2	2.42	0.53
6:A:409:PG4:H62	6:A:409:PG4:O5	2.09	0.53
1:B:102:ALA:O	1:B:106:VAL:HG23	2.10	0.52
1:A:102:ALA:O	1:A:106:VAL:HG23	2.11	0.51
1:B:251:THR:OG1	1:B:286:GLU:HG3	2.11	0.50
2:B:401:NVH:C17	2:B:401:NVH:N1	2.74	0.50
1:B:333:ARG:HE	1:B:337:TYR:HE2	1.61	0.49
1:B:83:TYR:CE2	1:B:158:ALA:HB1	2.48	0.49
1:A:83:TYR:CE2	1:A:158:ALA:HB1	2.47	0.49
1:A:221:ILE:HD12	1:B:221:ILE:HG13	1.95	0.48
2:A:401:NVH:N1	2:A:401:NVH:C17	2.77	0.47
1:A:340:PHE:CG	6:A:409:PG4:H82	2.49	0.47
1:A:138:SER:HB3	4:B:404:PGW:H07	1.95	0.47
1:B:247:ILE:HG13	1:B:248:PRO:HD2	1.95	0.47
5:A:406:SOG:H3'2	1:B:139:PHE:HZ	1.80	0.46
6:A:409:PG4:H52	6:A:409:PG4:H71	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:TYR:HE1	6:B:411:PG4:H32	1.83	0.42
1:B:174:ALA:HB1	4:B:404:PGW:H6A	2.02	0.42
1:A:71:VAL:CG2	1:A:86:VAL:HG21	2.45	0.42
1:A:178:PRO:HG3	4:A:404:PGW:O02	2.21	0.41
1:B:74:ASN:HB2	1:B:368:GLN:NE2	2.35	0.41
1:B:74:ASN:HD22	1:B:368:GLN:HE21	1.68	0.41
1:B:202:CYS:O	6:B:411:PG4:H81	2.22	0.40
1:A:358:TYR:O	1:A:362:SER:HB3	2.21	0.40
4:A:404:PGW:H14A	4:B:404:PGW:H13A	2.03	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	287/368 (78%)	283 (99%)	4 (1%)	0	100	100
1	B	299/368 (81%)	297 (99%)	2 (1%)	0	100	100
All	All	586/736 (80%)	580 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/305 (81%)	247 (100%)	0	100	100
1	B	250/305 (82%)	250 (100%)	0	100	100
All	All	497/610 (82%)	497 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SOG	A	407	-	20,20,20	0.97	2 (10%)	24,25,25	0.89	0
5	SOG	B	410	-	20,20,20	0.95	1 (5%)	24,25,25	1.24	3 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NVH	B	401	-	34,36,36	1.77	10 (29%)	46,56,56	3.12	17 (36%)
5	SOG	A	405	-	20,20,20	0.96	1 (5%)	24,25,25	0.75	1 (4%)
4	PGW	B	404	-	50,50,50	0.94	2 (4%)	53,56,56	0.95	2 (3%)
6	PG4	A	409	-	12,12,12	0.42	0	11,11,11	0.49	0
2	NVH	A	401	-	34,36,36	1.71	7 (20%)	46,56,56	2.63	19 (41%)
5	SOG	B	408	-	20,20,20	0.91	1 (5%)	24,25,25	1.19	2 (8%)
3	SO4	A	403	-	4,4,4	0.15	0	6,6,6	0.07	0
4	PGW	A	404	-	50,50,50	0.96	2 (4%)	53,56,56	0.93	3 (5%)
5	SOG	B	405	-	20,20,20	0.96	1 (5%)	24,25,25	0.73	0
3	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SOG	A	406	-	20,20,20	0.93	1 (5%)	24,25,25	0.99	1 (4%)
5	SOG	B	406	-	20,20,20	0.94	1 (5%)	24,25,25	0.91	1 (4%)
5	SOG	B	409	-	20,20,20	1.22	2 (10%)	24,25,25	1.13	2 (8%)
3	SO4	B	403	-	4,4,4	0.13	0	6,6,6	0.10	0
6	PG4	B	411	-	12,12,12	0.54	0	11,11,11	0.12	0
5	SOG	B	407	-	20,20,20	0.99	1 (5%)	24,25,25	0.65	0
5	SOG	A	408	-	20,20,20	0.92	1 (5%)	24,25,25	0.98	3 (12%)

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	407	-	-	10/11/31/31	0/1/1/1
2	NVH	A	401	-	-	4/14/38/38	0/3/4/4
5	SOG	B	406	-	-	7/11/31/31	0/1/1/1
4	PGW	A	404	-	-	24/55/55/55	-
5	SOG	B	408	-	-	3/11/31/31	0/1/1/1
5	SOG	B	409	-	-	6/11/31/31	0/1/1/1
6	PG4	A	409	-	-	4/10/10/10	-
5	SOG	B	407	-	-	11/11/31/31	0/1/1/1
5	SOG	B	405	-	-	7/11/31/31	0/1/1/1
5	SOG	A	405	-	-	8/11/31/31	0/1/1/1
4	PGW	B	404	-	-	24/55/55/55	-
6	PG4	B	411	-	-	7/10/10/10	-
5	SOG	A	406	-	-	7/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SOG	B	410	-	-	7/11/31/31	0/1/1/1
5	SOG	A	408	-	-	10/11/31/31	0/1/1/1
2	NVH	B	401	-	-	4/14/38/38	0/3/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NVH	C4-N3	4.78	1.45	1.39
4	A	404	PGW	O03-C19	4.38	1.46	1.33
2	A	401	NVH	C10-N4	-4.38	1.39	1.45
5	B	409	SOG	C1'-S1	-4.36	1.75	1.81
4	B	404	PGW	O03-C19	4.34	1.46	1.33
2	B	401	NVH	C4-N3	4.28	1.44	1.39
4	A	404	PGW	O01-C1	4.21	1.46	1.34
4	B	404	PGW	O01-C1	4.16	1.46	1.34
2	B	401	NVH	C10-N4	-3.62	1.40	1.45
5	B	407	SOG	C1'-S1	-3.61	1.76	1.81
5	B	406	SOG	C1'-S1	-3.56	1.76	1.81
5	B	410	SOG	C1'-S1	-3.53	1.76	1.81
5	B	405	SOG	C1'-S1	-3.50	1.76	1.81
5	A	407	SOG	C1'-S1	-3.46	1.77	1.81
5	A	405	SOG	C1'-S1	-3.45	1.77	1.81
5	A	408	SOG	C1'-S1	-3.38	1.77	1.81
5	A	406	SOG	C1'-S1	-3.33	1.77	1.81
2	B	401	NVH	O2-S1	3.18	1.47	1.43
2	B	401	NVH	O3-S1	3.17	1.47	1.43
5	B	408	SOG	C1'-S1	-3.16	1.77	1.81
5	B	409	SOG	C1-S1	-2.91	1.76	1.80
2	A	401	NVH	O2-S1	2.80	1.46	1.43
2	B	401	NVH	C16-C15	2.75	1.42	1.38
2	A	401	NVH	C16-C15	2.44	1.42	1.38
2	B	401	NVH	C12-C16	2.42	1.55	1.51
2	B	401	NVH	C16-C17	2.34	1.42	1.38
2	A	401	NVH	C6-S1	-2.20	1.72	1.75
2	B	401	NVH	C7-C8	2.19	1.40	1.38
2	B	401	NVH	C19-S2	2.15	1.83	1.75
5	A	407	SOG	C1-S1	-2.08	1.77	1.80
2	B	401	NVH	C11-C10	2.07	1.42	1.38
2	A	401	NVH	O3-S1	2.03	1.45	1.43
2	A	401	NVH	C19-S2	2.02	1.83	1.75

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NVH	C16-C12-N3	-12.50	97.01	114.01
2	B	401	NVH	C12-N3-C5	7.33	121.35	116.77
2	A	401	NVH	C16-C12-N3	-7.15	104.28	114.01
2	A	401	NVH	O5-S2-C8	-6.57	102.89	108.25
2	A	401	NVH	C14-C15-C16	-5.81	120.51	124.59
2	A	401	NVH	C18-C17-C16	-5.72	120.58	124.59
2	B	401	NVH	C6-S1-N4	-5.58	95.60	101.27
2	B	401	NVH	C14-C15-C16	-5.05	121.05	124.59
2	B	401	NVH	O3-S1-O2	4.95	124.66	118.59
2	B	401	NVH	C18-C17-C16	-4.89	121.16	124.59
2	A	401	NVH	C12-N3-C5	4.59	119.64	116.77
2	A	401	NVH	C4-N3-C5	4.48	126.43	122.22
2	B	401	NVH	O5-S2-C8	-4.33	104.71	108.25
2	A	401	NVH	O3-S1-O2	4.24	123.78	118.59
4	B	404	PGW	O01-C1-C2	3.98	120.08	111.50
4	A	404	PGW	O01-C1-C2	3.71	119.50	111.50
5	A	406	SOG	C1'-S1-C1	3.67	106.96	100.09
2	B	401	NVH	F2-C15-C16	3.54	121.85	117.63
2	B	401	NVH	C17-C18-C13	3.48	120.28	116.62
2	B	401	NVH	C15-C14-C13	3.42	120.21	116.62
5	B	410	SOG	C1'-S1-C1	3.32	106.31	100.09
2	B	401	NVH	C9-C10-N4	3.28	123.02	119.66
2	A	401	NVH	C17-C18-C13	3.24	120.02	116.62
2	A	401	NVH	C15-C14-C13	3.17	119.95	116.62
2	A	401	NVH	C17-C16-C15	3.08	118.80	114.51
5	B	408	SOG	O5-C1-C2	-2.99	106.56	110.31
5	A	408	SOG	C1'-S1-C1	2.98	105.66	100.09
2	B	401	NVH	C18-C13-C14	-2.97	119.76	123.52
2	B	401	NVH	C3-N1-C4	2.95	121.99	115.14
2	B	401	NVH	O4-S2-C8	2.86	110.58	108.25
5	B	408	SOG	C3-C4-C5	2.81	115.25	110.24
2	B	401	NVH	C4-N3-C5	2.73	124.79	122.22
2	A	401	NVH	O2-S1-N4	-2.71	105.41	107.89
2	A	401	NVH	F2-C15-C16	2.71	120.86	117.63
2	A	401	NVH	C18-C13-C14	-2.69	120.12	123.52
4	B	404	PGW	O03-C19-C20	2.59	120.05	111.91
2	B	401	NVH	F3-C17-C16	2.55	120.67	117.63
5	A	408	SOG	O5-C5-C6	2.48	112.61	106.44
5	B	406	SOG	C1'-S1-C1	2.47	104.71	100.09
4	A	404	PGW	O03-C19-C20	2.37	119.35	111.91
5	B	409	SOG	C1-O5-C5	-2.34	108.27	112.58
5	B	409	SOG	O5-C1-C2	-2.32	107.39	110.31
2	A	401	NVH	C19-S2-C8	2.26	107.25	104.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NVH	F3-C17-C16	2.23	120.30	117.63
2	A	401	NVH	C9-C8-S2	2.22	120.83	119.06
5	B	410	SOG	O5-C1-C2	-2.19	107.56	110.31
5	A	408	SOG	O5-C1-S1	2.15	114.95	109.82
2	A	401	NVH	C3-N1-C4	2.14	120.11	115.14
2	A	401	NVH	C9-C10-N4	2.13	121.84	119.66
2	B	401	NVH	C17-C16-C15	2.11	117.44	114.51
2	A	401	NVH	C10-C9-C8	-2.09	117.35	118.97
4	A	404	PGW	O03-C19-O04	-2.09	118.31	123.59
5	A	405	SOG	C1'-S1-C1	2.03	103.89	100.09
5	B	410	SOG	O5-C5-C4	2.01	113.34	109.69

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	PGW	C04-O12-P-O14
5	A	405	SOG	C2-C1-S1-C1'
5	A	405	SOG	O5-C1-S1-C1'
5	A	407	SOG	C2-C1-S1-C1'
5	A	407	SOG	O5-C1-S1-C1'
5	A	408	SOG	C2-C1-S1-C1'
5	A	408	SOG	O5-C1-S1-C1'
5	A	408	SOG	C2'-C1'-S1-C1
5	B	405	SOG	C2'-C1'-S1-C1
5	B	407	SOG	C2-C1-S1-C1'
5	B	407	SOG	O5-C1-S1-C1'
5	B	407	SOG	C2'-C1'-S1-C1
5	B	409	SOG	O5-C1-S1-C1'
5	B	410	SOG	O5-C1-S1-C1'
4	A	404	PGW	O04-C19-O03-C01
4	A	404	PGW	C20-C19-O03-C01
4	B	404	PGW	C20-C19-O03-C01
5	A	405	SOG	S1-C1'-C2'-C3'
5	A	408	SOG	S1-C1'-C2'-C3'
4	B	404	PGW	O04-C19-O03-C01
5	B	406	SOG	O5-C5-C6-O6
5	A	405	SOG	O5-C5-C6-O6
5	A	407	SOG	S1-C1'-C2'-C3'
5	B	405	SOG	O5-C5-C6-O6
5	A	407	SOG	O5-C5-C6-O6
5	B	407	SOG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	408	SOG	O5-C5-C6-O6
2	A	401	NVH	C7-C8-S2-C19
2	B	401	NVH	C7-C8-S2-C19
4	B	404	PGW	C1-C2-C3-C4
5	B	406	SOG	C4-C5-C6-O6
5	A	407	SOG	C4-C5-C6-O6
5	A	405	SOG	C1'-C2'-C3'-C4'
5	A	406	SOG	C1'-C2'-C3'-C4'
6	B	411	PG4	O1-C1-C2-O2
2	A	401	NVH	C9-C8-S2-C19
2	B	401	NVH	C9-C8-S2-C19
5	A	406	SOG	O5-C5-C6-O6
5	B	407	SOG	O5-C5-C6-O6
4	A	404	PGW	C04-O12-P-O11
5	B	407	SOG	C1'-C2'-C3'-C4'
5	B	410	SOG	C1'-C2'-C3'-C4'
2	B	401	NVH	C7-C8-S2-O5
4	B	404	PGW	C10-C06-C07-C08
5	A	407	SOG	C1'-C2'-C3'-C4'
5	B	405	SOG	C1'-C2'-C3'-C4'
4	B	404	PGW	C3-C4-C5-C6
4	B	404	PGW	C5-C6-C7-C8
4	B	404	PGW	C20-C21-C22-C23
5	A	408	SOG	C3'-C4'-C5'-C6'
4	B	404	PGW	C27-C15-C16-C17
4	A	404	PGW	C24-C25-C26-C27
2	A	401	NVH	C7-C8-S2-O5
4	A	404	PGW	C15-C16-C17-C18
5	B	406	SOG	C2'-C3'-C4'-C5'
6	A	409	PG4	C5-C6-O4-C7
2	B	401	NVH	C9-C8-S2-O5
5	A	405	SOG	C4-C5-C6-O6
4	A	404	PGW	C1-C2-C3-C4
4	B	404	PGW	C2-C3-C4-C5
4	B	404	PGW	C25-C26-C27-C15
5	B	406	SOG	C4'-C5'-C6'-C7'
5	B	409	SOG	O5-C5-C6-O6
5	B	407	SOG	C3'-C4'-C5'-C6'
4	B	404	PGW	C09-C11-C12-C13
5	A	406	SOG	C4'-C5'-C6'-C7'
5	B	407	SOG	C4'-C5'-C6'-C7'
4	A	404	PGW	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	401	NVH	C9-C8-S2-O5
4	A	404	PGW	C20-C21-C22-C23
4	A	404	PGW	C17-C18-C28-C30
4	A	404	PGW	C16-C15-C27-C26
5	B	407	SOG	C2'-C3'-C4'-C5'
5	B	407	SOG	S1-C1'-C2'-C3'
4	B	404	PGW	C07-C08-C09-C11
4	B	404	PGW	C23-C24-C25-C26
5	A	408	SOG	C4'-C5'-C6'-C7'
4	A	404	PGW	O02-C1-O01-C02
5	B	405	SOG	C4'-C5'-C6'-C7'
5	A	408	SOG	C2'-C3'-C4'-C5'
5	B	410	SOG	C2'-C3'-C4'-C5'
4	A	404	PGW	C5-C6-C7-C8
5	B	406	SOG	C3'-C4'-C5'-C6'
4	A	404	PGW	C2-C1-O01-C02
5	B	406	SOG	S1-C1'-C2'-C3'
4	B	404	PGW	C21-C22-C23-C24
5	B	405	SOG	C4-C5-C6-O6
6	B	411	PG4	O4-C7-C8-O5
5	B	408	SOG	C1'-C2'-C3'-C4'
5	B	406	SOG	C5'-C6'-C7'-C8'
5	B	408	SOG	C5'-C6'-C7'-C8'
5	B	407	SOG	C5'-C6'-C7'-C8'
4	A	404	PGW	C3-C4-C5-C6
5	A	405	SOG	C3'-C4'-C5'-C6'
5	B	405	SOG	C5'-C6'-C7'-C8'
4	B	404	PGW	C11-C12-C13-C14
6	B	411	PG4	O3-C5-C6-O4
4	B	404	PGW	O03-C01-C02-C03
5	A	406	SOG	C2'-C3'-C4'-C5'
4	A	404	PGW	C25-C26-C27-C15
5	A	408	SOG	C5'-C6'-C7'-C8'
4	B	404	PGW	O03-C01-C02-O01
5	B	409	SOG	S1-C1'-C2'-C3'
5	A	406	SOG	C5'-C6'-C7'-C8'
5	A	407	SOG	C2'-C1'-S1-C1
4	B	404	PGW	C22-C23-C24-C25
5	A	406	SOG	S1-C1'-C2'-C3'
5	B	405	SOG	C3'-C4'-C5'-C6'
6	B	411	PG4	C1-C2-O2-C3
4	A	404	PGW	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	B	404	PGW	C16-C15-C27-C26
4	A	404	PGW	O12-C04-C05-CAD
6	B	411	PG4	C5-C6-O4-C7
4	A	404	PGW	C06-C07-C08-C09
5	A	408	SOG	C4-C5-C6-O6
4	A	404	PGW	C04-O12-P-O13
5	A	407	SOG	C4'-C5'-C6'-C7'
5	A	405	SOG	C2'-C3'-C4'-C5'
6	B	411	PG4	C6-C5-O3-C4
5	B	409	SOG	C2-C1-S1-C1'
5	B	410	SOG	C2-C1-S1-C1'
5	B	408	SOG	S1-C1'-C2'-C3'
5	B	410	SOG	C4'-C5'-C6'-C7'
5	B	410	SOG	S1-C1'-C2'-C3'
6	A	409	PG4	O1-C1-C2-O2
4	B	404	PGW	C16-C17-C18-C28
5	A	407	SOG	C2'-C3'-C4'-C5'
4	B	404	PGW	C19-C20-C21-C22
5	A	406	SOG	C3'-C4'-C5'-C6'
5	B	409	SOG	C1'-C2'-C3'-C4'
5	B	410	SOG	C5'-C6'-C7'-C8'
6	B	411	PG4	C4-C3-O2-C2
4	A	404	PGW	C04-C05-CAD-OAE
4	A	404	PGW	C7-C8-C9-C10
4	B	404	PGW	O01-C02-C03-O11
5	A	407	SOG	C3'-C4'-C5'-C6'
5	B	409	SOG	C2'-C1'-S1-C1
6	A	409	PG4	O3-C5-C6-O4
4	B	404	PGW	C18-C28-C30-C29
4	B	404	PGW	C24-C25-C26-C27
6	A	409	PG4	O4-C7-C8-O5
4	A	404	PGW	C22-C23-C24-C25
4	A	404	PGW	C07-C06-C10-C9

There are no ring outliers.

9 monomers are involved in 17 short contacts:

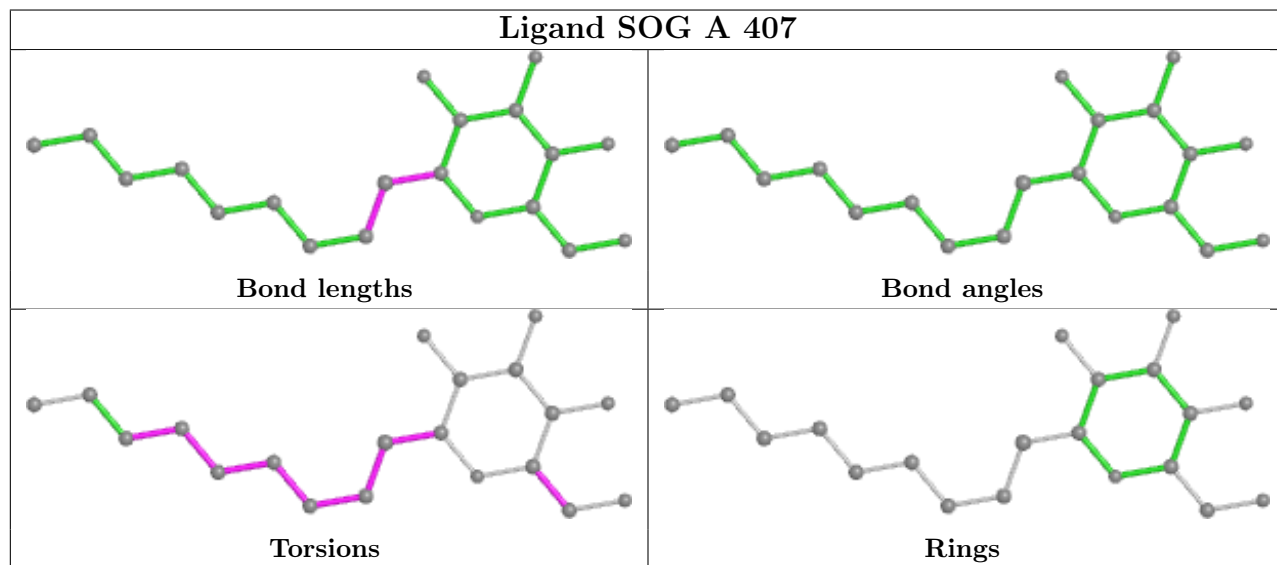
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NVH	1	0
4	B	404	PGW	4	0
6	A	409	PG4	3	0
2	A	401	NVH	1	0

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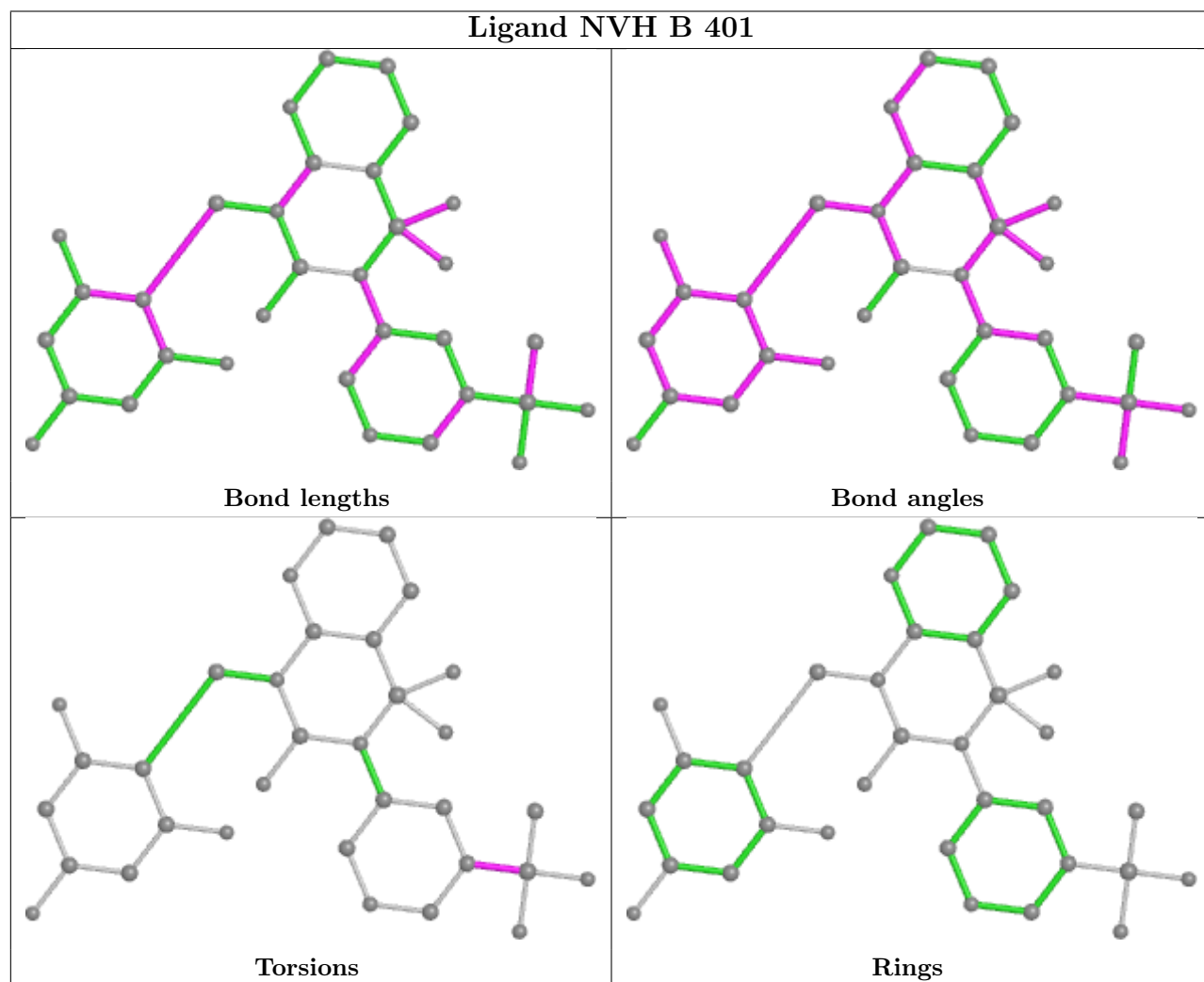
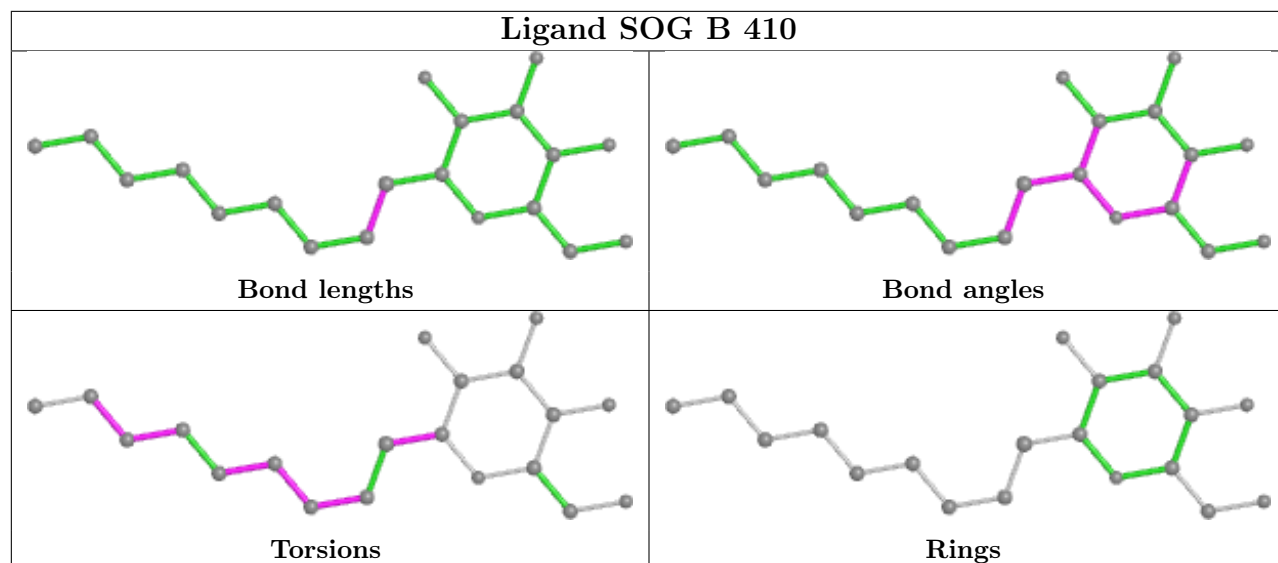
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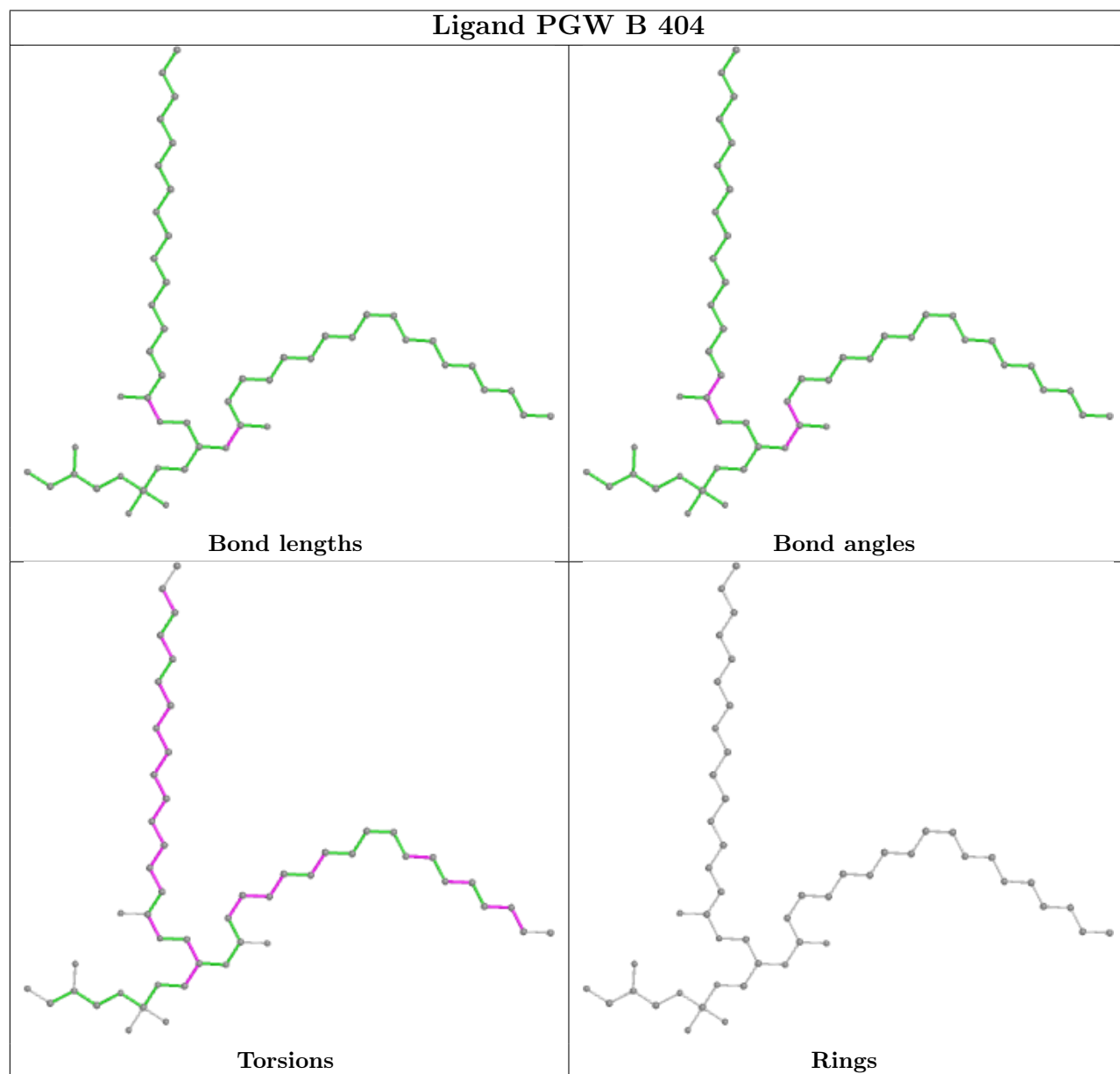
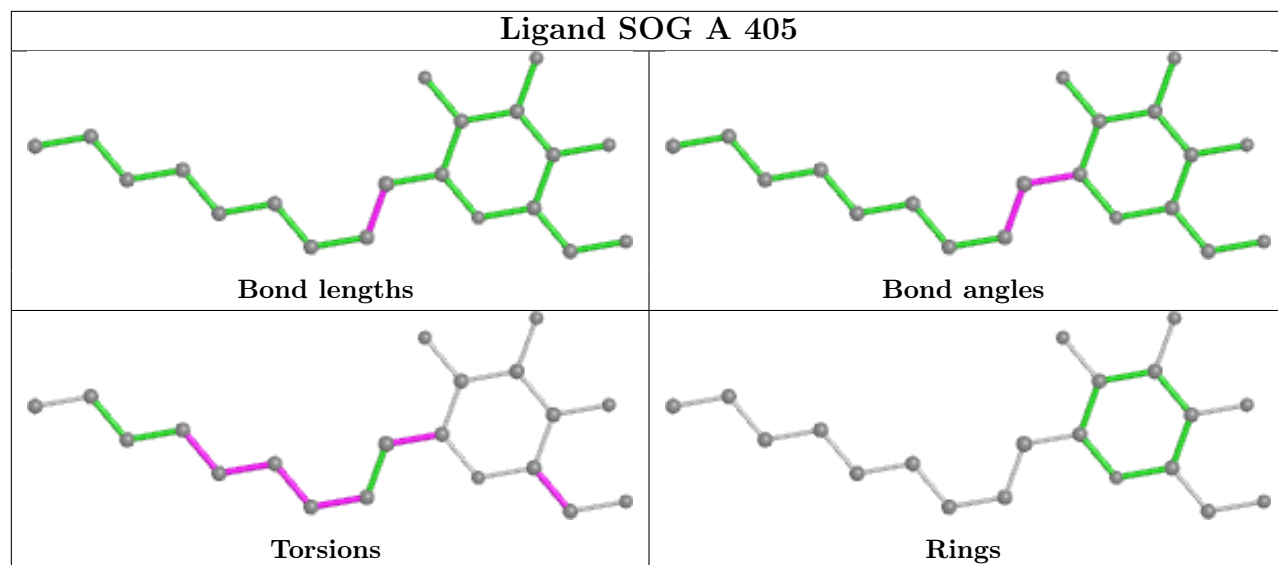
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	PGW	3	0
5	B	405	SOG	1	0
5	A	406	SOG	2	0
5	B	409	SOG	1	0
6	B	411	PG4	2	0

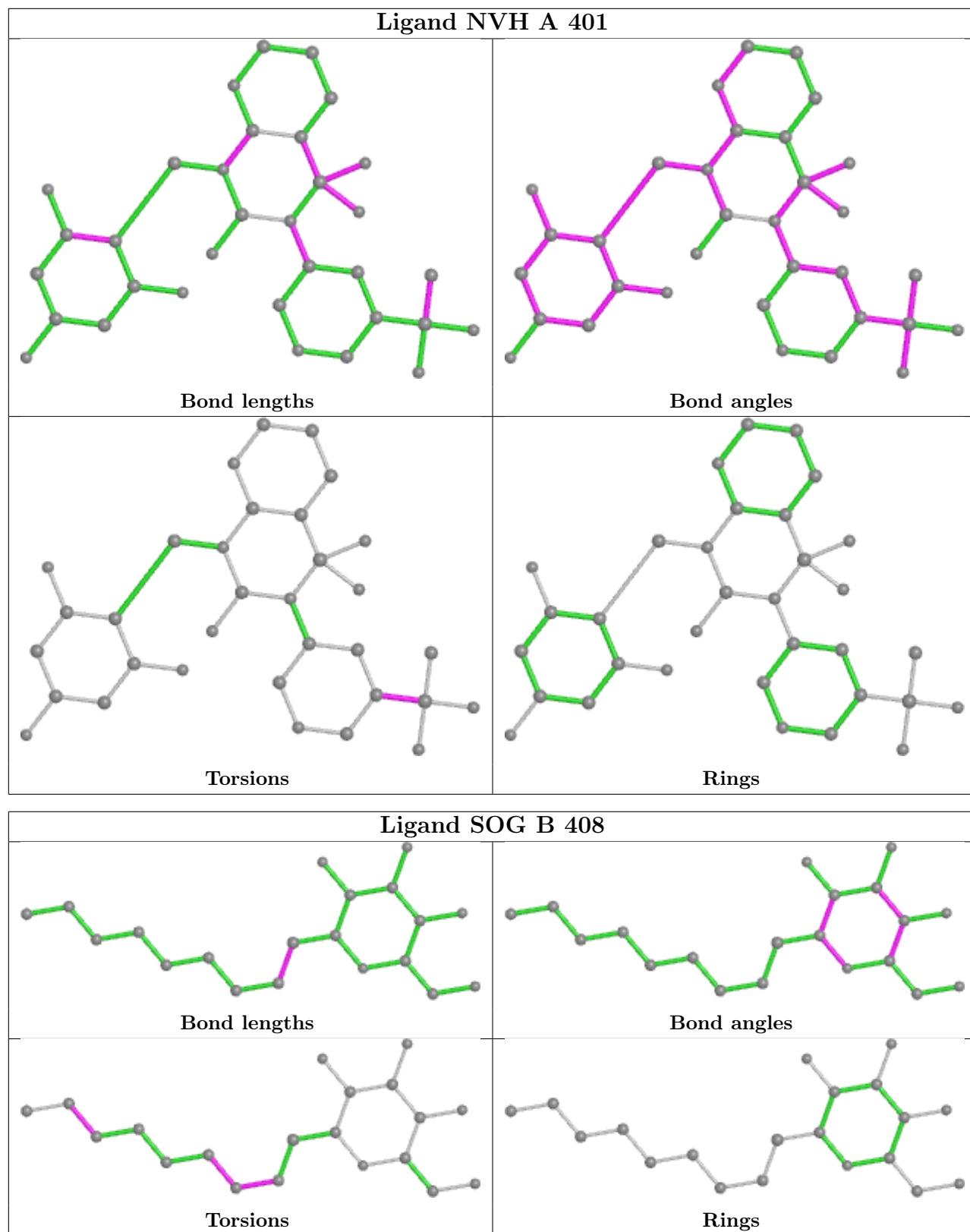
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

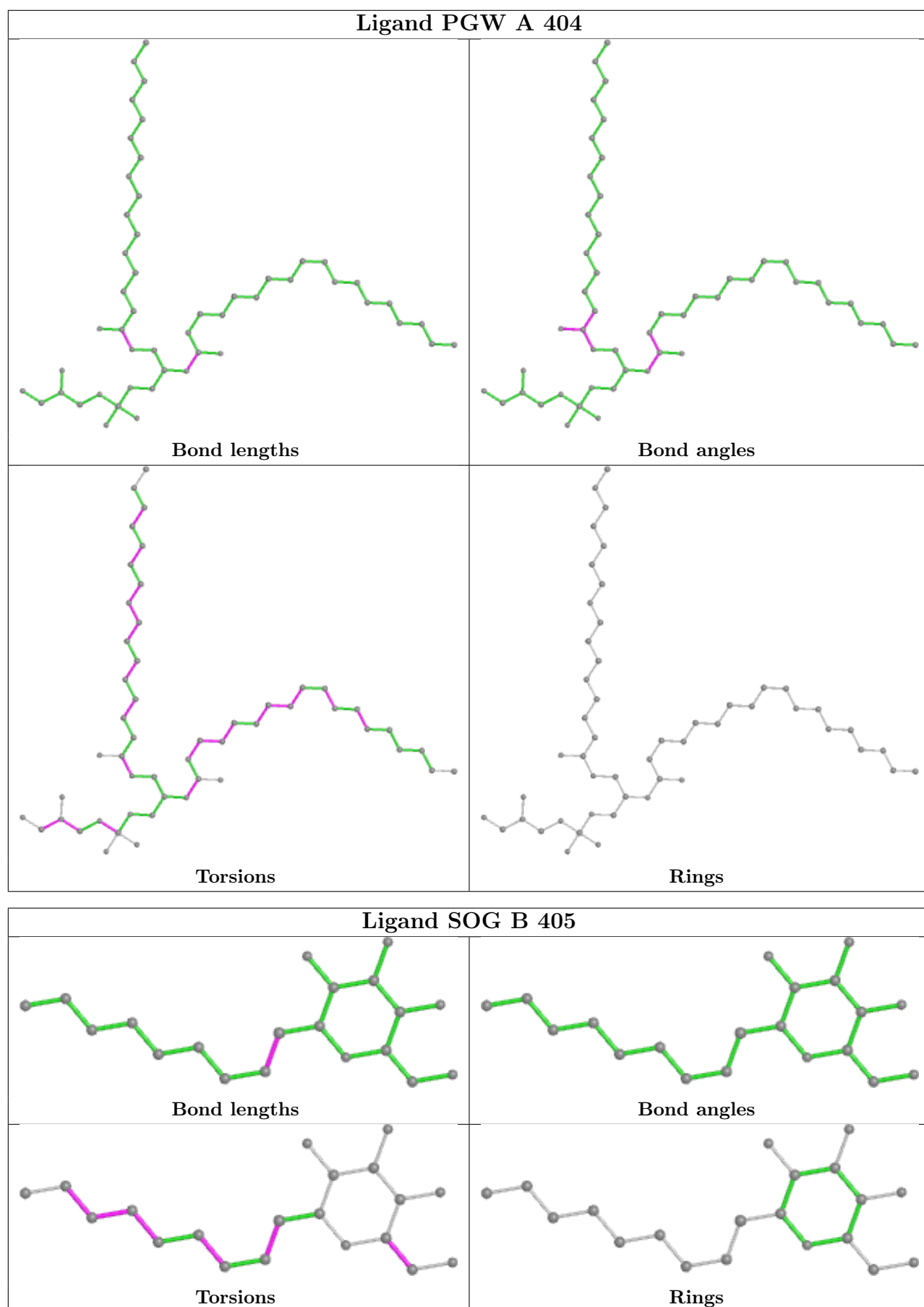


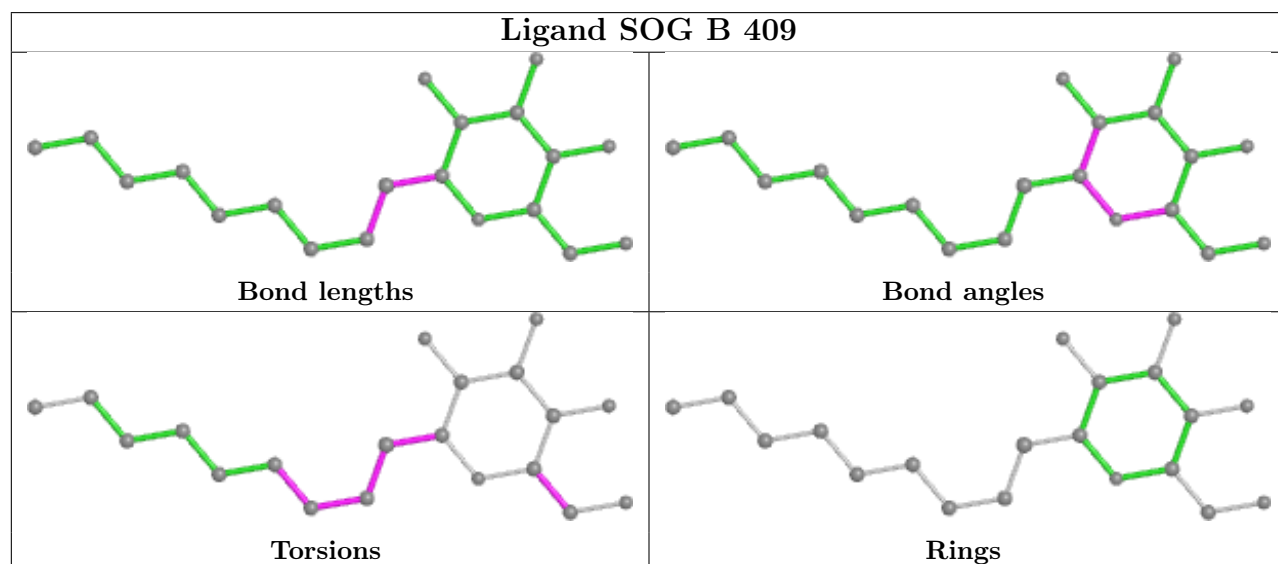
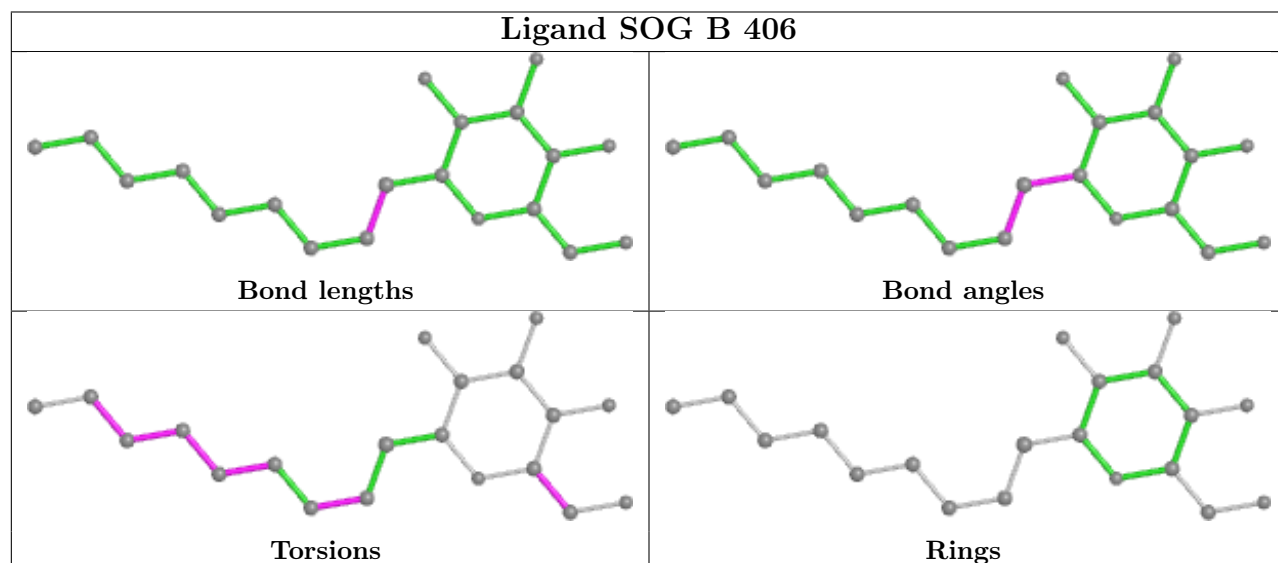
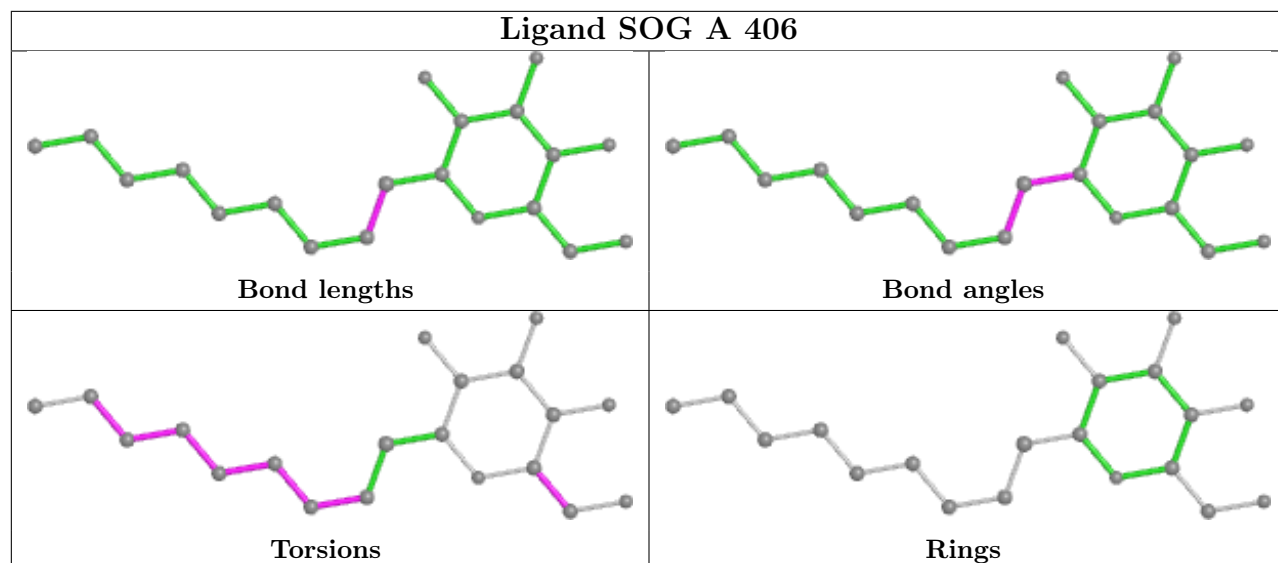


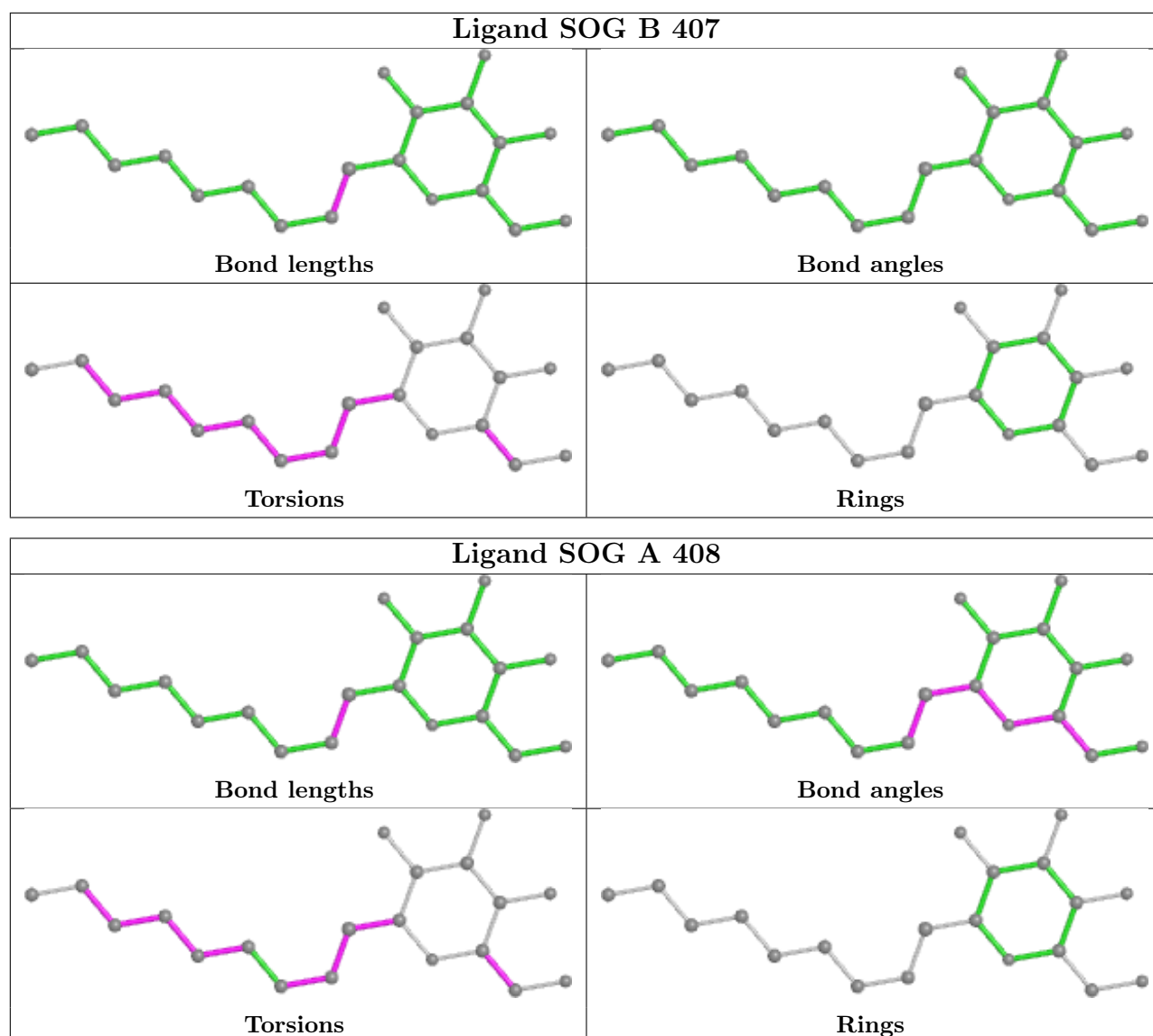












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	293/368 (79%)	0.76	43 (14%) <b>2</b>   <b>3</b>	33, 69, 127, 152	0
1	B	301/368 (81%)	0.85	48 (15%) <b>1</b>   <b>2</b>	39, 71, 137, 186	0
All	All	594/736 (80%)	0.81	91 (15%) <b>2</b>   <b>2</b>	33, 70, 134, 186	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	TRP	12.3
1	B	245	ARG	9.7
1	B	287	VAL	8.0
1	B	288	LYS	7.5
1	B	45	TYR	7.1
1	A	361	LEU	6.7
1	B	242	LEU	6.7
1	A	332	ASP	6.5
1	B	72	TRP	6.3
1	A	335	ALA	6.3
1	A	374	SER	6.1
1	A	291	ARG	5.7
1	B	332	ASP	5.7
1	A	243	TRP	5.6
1	B	46	ALA	5.1
1	A	331	SER	5.0
1	A	239	PHE	4.9
1	A	113	LEU	4.8
1	B	252	SER	4.7
1	B	329	GLN	4.7
1	B	291	ARG	4.6
1	A	83	TYR	4.6
1	A	330	ALA	4.5
1	A	114	PHE	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	48	VAL	4.3
1	A	76	HIS	4.2
1	A	47	TRP	4.1
1	A	115	GLY	4.1
1	A	298	LYS	4.0
1	B	290	MET	3.9
1	B	376	TRP	3.8
1	B	246	GLN	3.7
1	A	242	LEU	3.6
1	B	373	PHE	3.6
1	B	75	HIS	3.5
1	A	289	GLN	3.4
1	A	68	CYS	3.4
1	A	78	ARG	3.3
1	B	130	VAL	3.3
1	B	244	GLY	3.3
1	A	72	TRP	3.3
1	A	151	PRO	3.2
1	A	360	PHE	3.1
1	A	69	LEU	3.1
1	A	105	LEU	3.1
1	A	333	ARG	3.0
1	A	175	ILE	2.9
1	B	132	VAL	2.9
1	A	199	PHE	2.9
1	B	129	SER	2.8
1	A	373	PHE	2.8
1	B	133	ALA	2.8
1	A	152	LEU	2.8
1	B	134	VAL	2.8
1	B	243	TRP	2.8
1	B	50	ILE	2.7
1	B	104	LEU	2.7
1	B	375	TRP	2.7
1	B	337	TYR	2.7
1	B	372	ALA	2.6
1	A	117	ALA	2.6
1	B	172	SER	2.6
1	A	208	ASP	2.6
1	B	71	VAL	2.5
1	B	190	PRO	2.5
1	B	171	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	374	SER	2.5
1	A	132	VAL	2.4
1	A	158	ALA	2.4
1	B	78	ARG	2.4
1	B	247	ILE	2.4
1	B	131	SER	2.4
1	B	88	LEU	2.4
1	B	69	LEU	2.3
1	B	360	PHE	2.3
1	B	108	ILE	2.3
1	A	147	ALA	2.2
1	A	129	SER	2.2
1	A	116	HIS	2.2
1	A	174	ALA	2.2
1	B	76	HIS	2.2
1	A	167	GLY	2.2
1	B	170	ALA	2.2
1	B	166	LEU	2.1
1	A	209	ASP	2.1
1	A	86	VAL	2.1
1	A	131	SER	2.1
1	B	240	ARG	2.1
1	B	294	ARG	2.1
1	A	171	VAL	2.0
1	B	370	LYS	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](#)

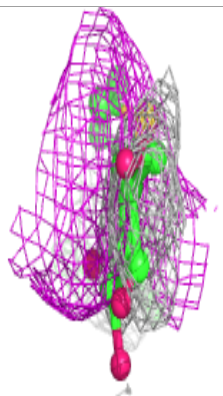
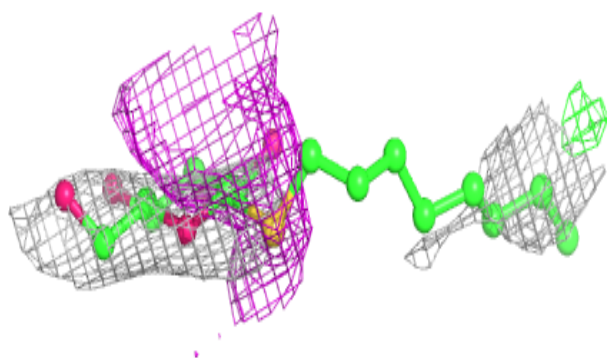
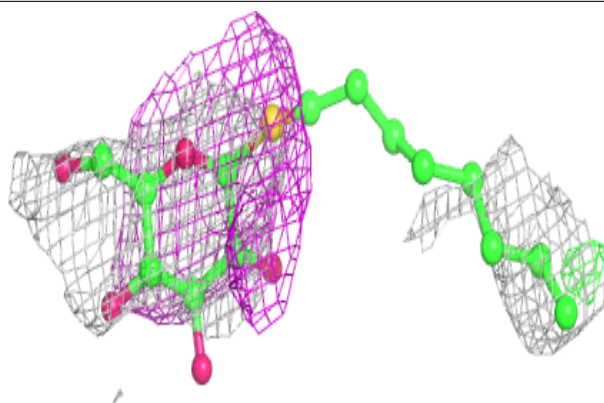
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SOG	A	405	20/20	0.40	0.75	122,126,129,131	0
6	PG4	A	409	13/13	0.59	0.30	98,102,105,107	0
5	SOG	B	408	20/20	0.62	0.41	81,106,114,117	0
2	NVH	B	401	33/33	0.69	0.45	129,135,137,138	33
4	PGW	A	404	51/51	0.75	0.32	41,82,120,121	0
5	SOG	A	408	20/20	0.78	0.25	86,97,110,111	0
5	SOG	B	409	20/20	0.80	0.24	66,88,104,104	0
5	SOG	A	407	20/20	0.80	0.28	147,149,151,152	0
6	PG4	B	411	13/13	0.81	0.56	91,104,113,114	0
2	NVH	A	401	33/33	0.82	0.24	96,110,120,124	4
3	SO4	A	403	5/5	0.83	0.25	152,152,152,153	0
5	SOG	A	406	20/20	0.83	0.37	111,119,124,125	0
3	SO4	B	403	5/5	0.84	0.12	131,134,134,135	0
5	SOG	B	405	20/20	0.85	0.35	88,97,100,102	0
3	SO4	B	402	5/5	0.86	0.14	100,100,104,104	0
5	SOG	B	410	20/20	0.86	0.17	113,121,125,125	0
5	SOG	B	407	20/20	0.87	0.48	109,121,124,127	0
4	PGW	B	404	51/51	0.88	0.21	51,77,117,118	0
3	SO4	A	402	5/5	0.88	0.17	112,113,115,121	0
5	SOG	B	406	20/20	0.96	0.20	55,69,83,88	0

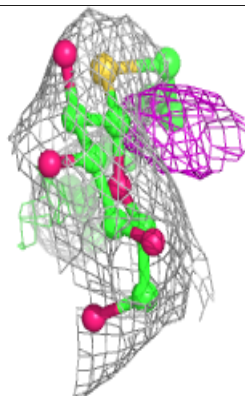
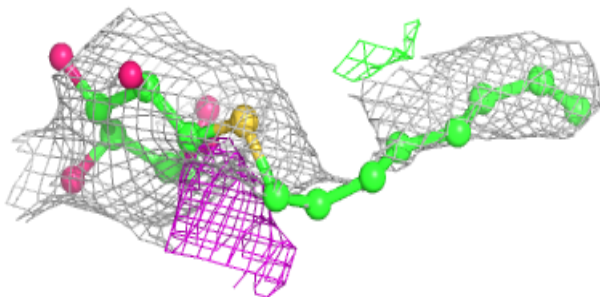
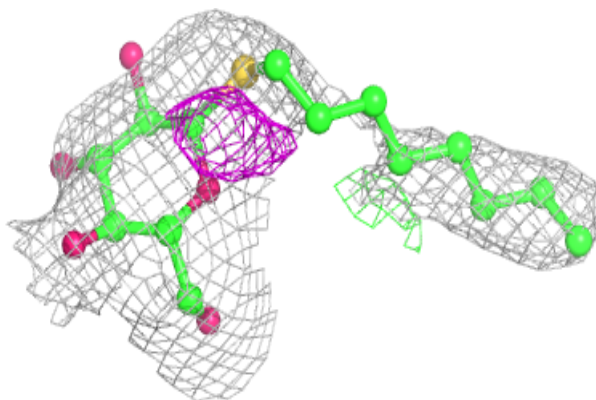
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SOG A 405:**

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

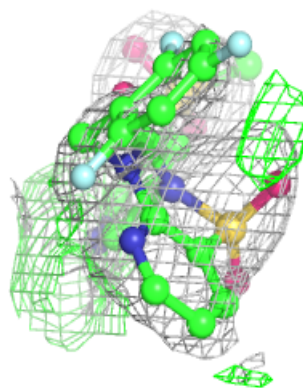
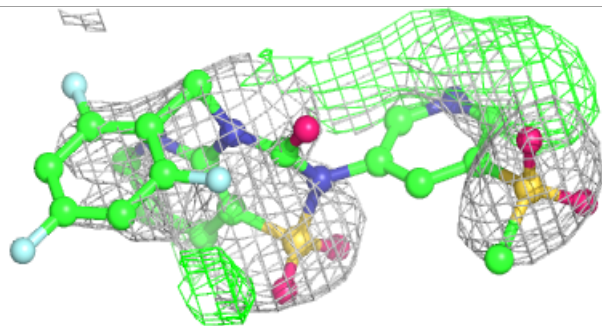
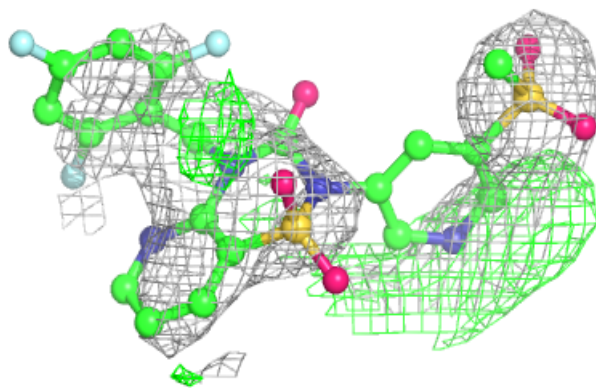
**Electron density around SOG B 408:**

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

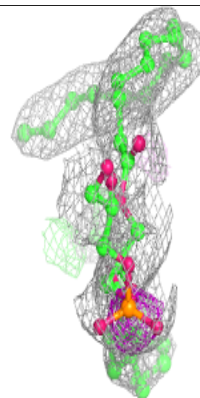
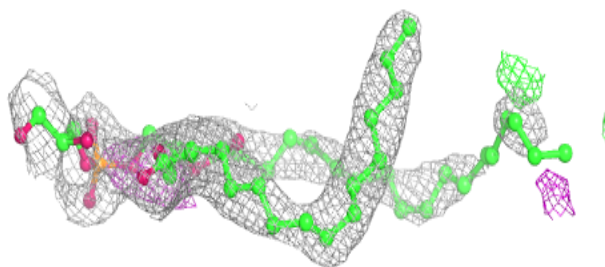
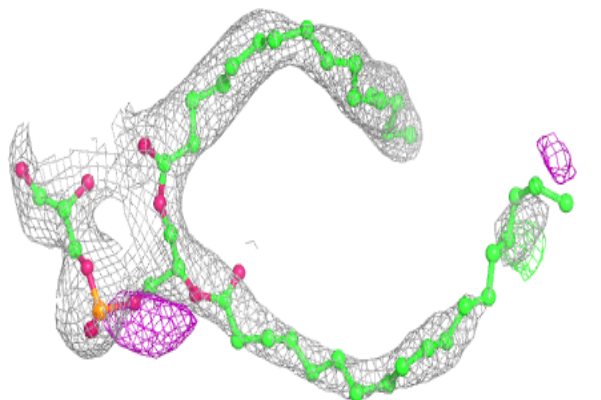


**Electron density around NVH B 401:**

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

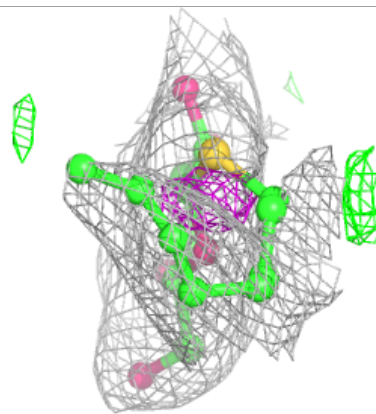
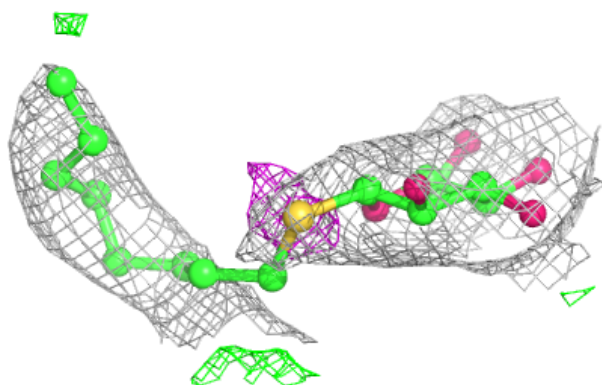
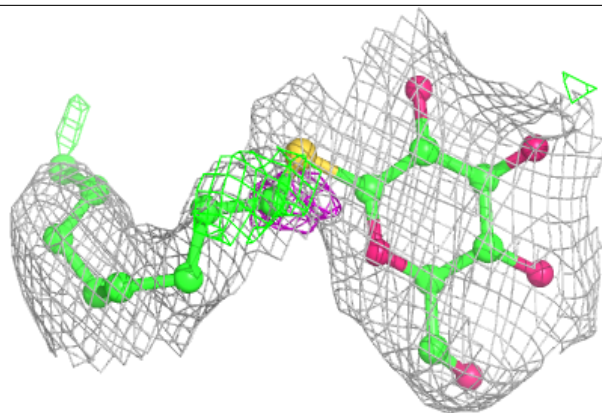
**Electron density around PGW A 404:**

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

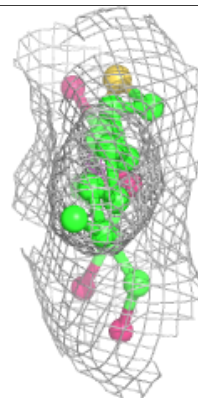
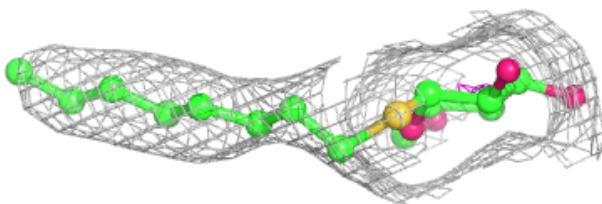
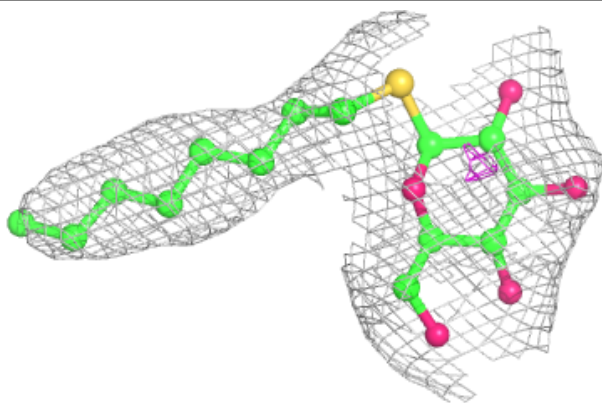


**Electron density around SOG A 408:**

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

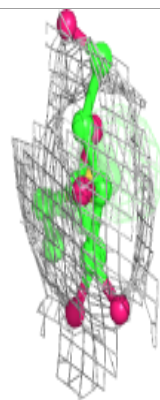
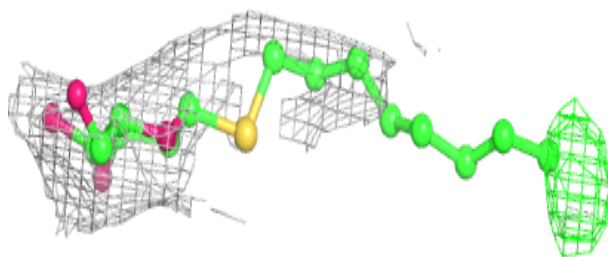
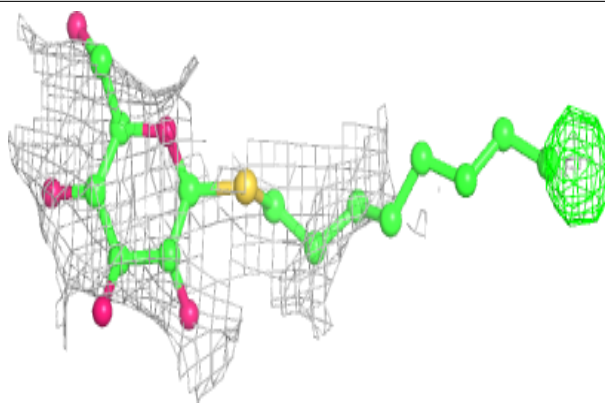
**Electron density around SOG B 409:**

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

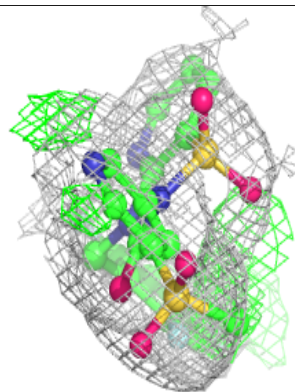
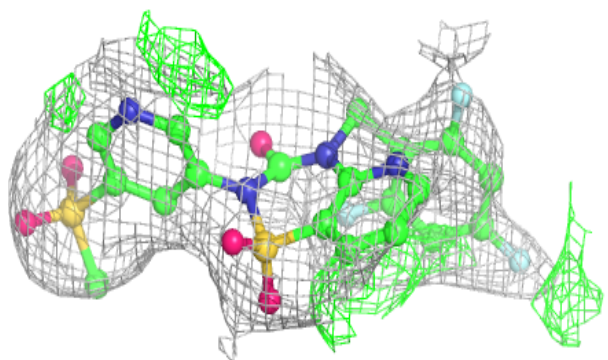
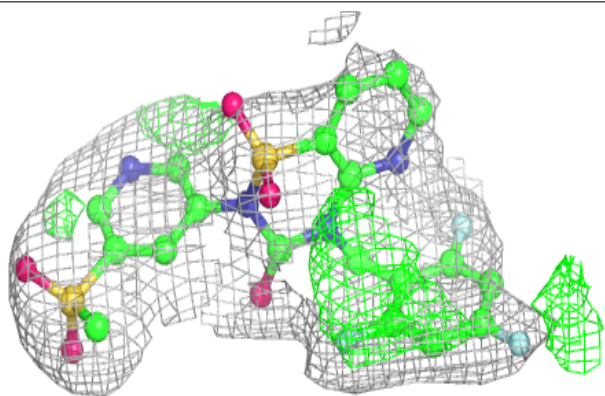


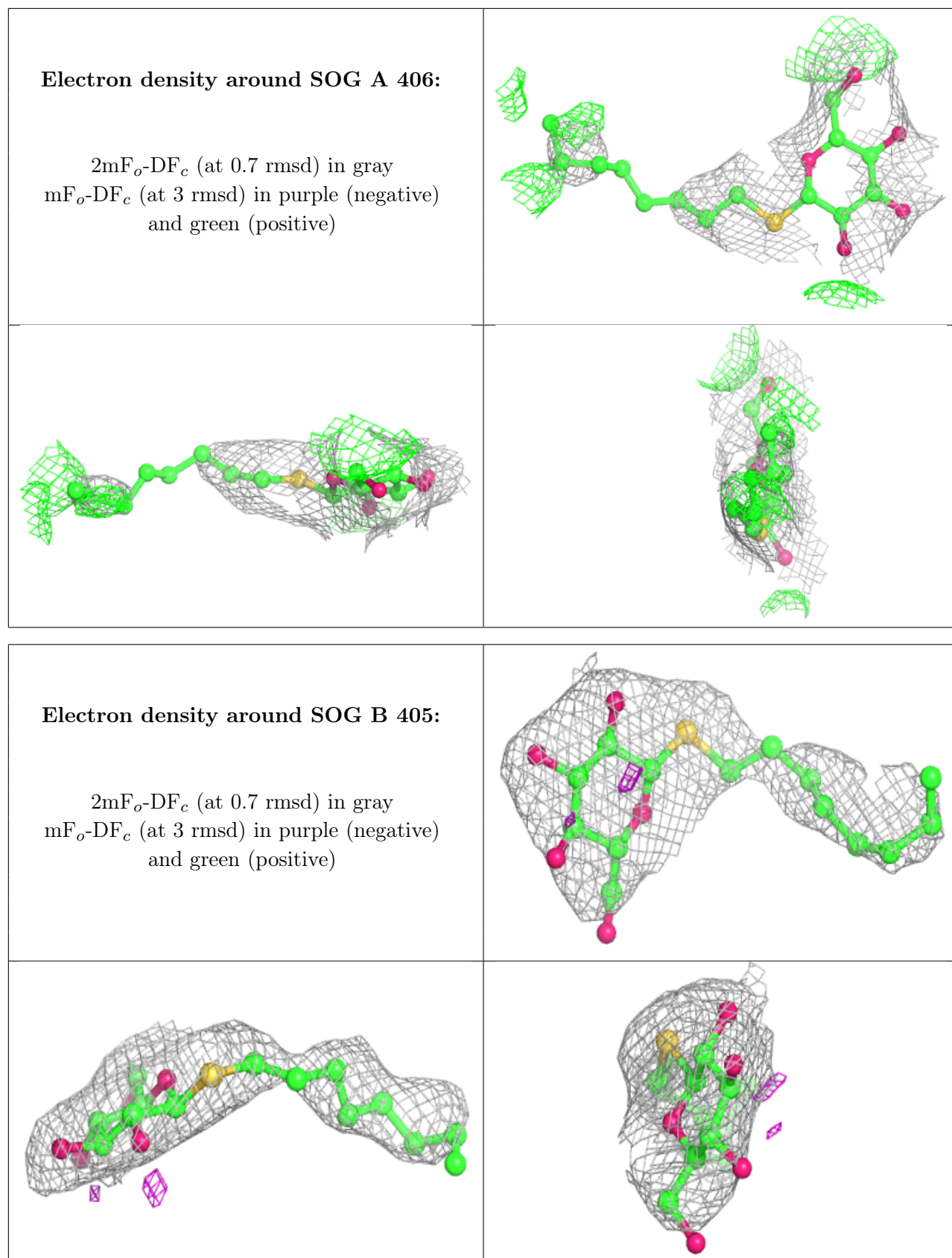
**Electron density around SOG A 407:**

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

**Electron density around NVH A 401:**

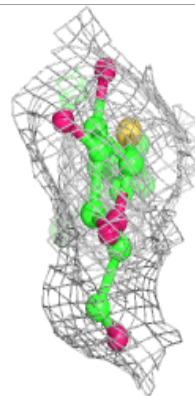
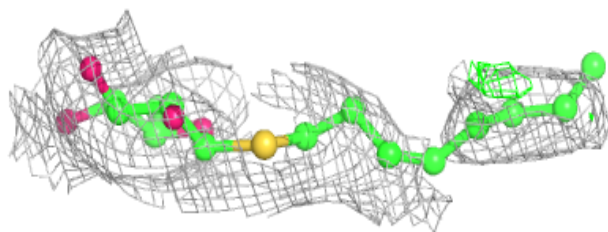
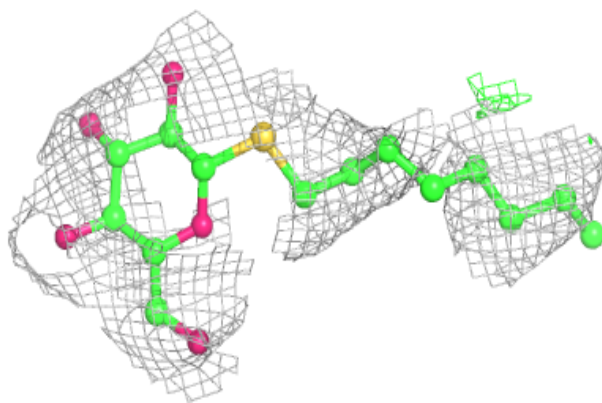
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



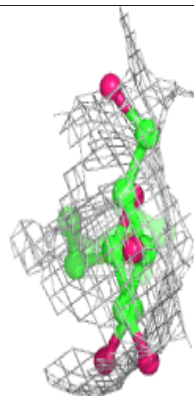
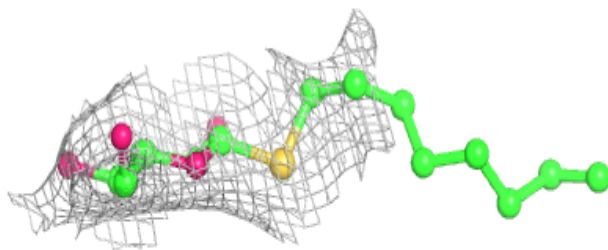
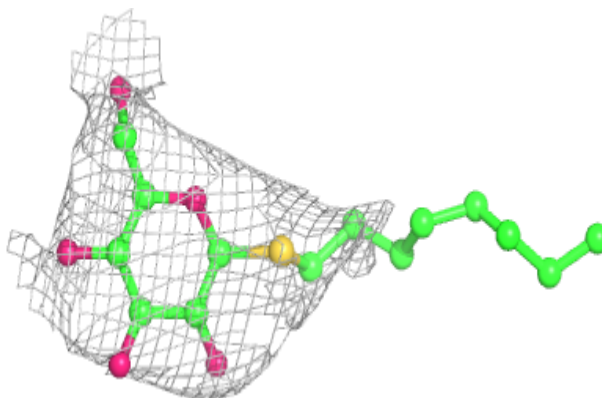


**Electron density around SOG B 410:**

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

**Electron density around SOG B 407:**

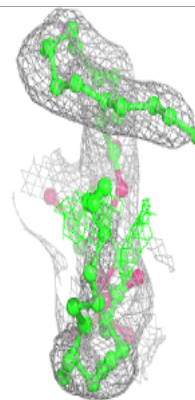
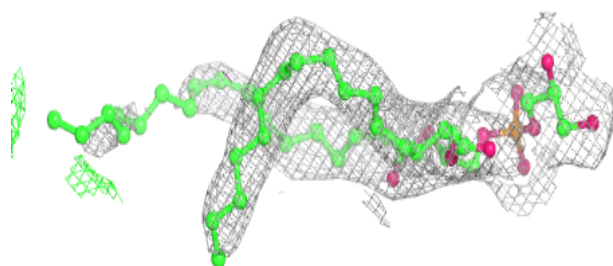
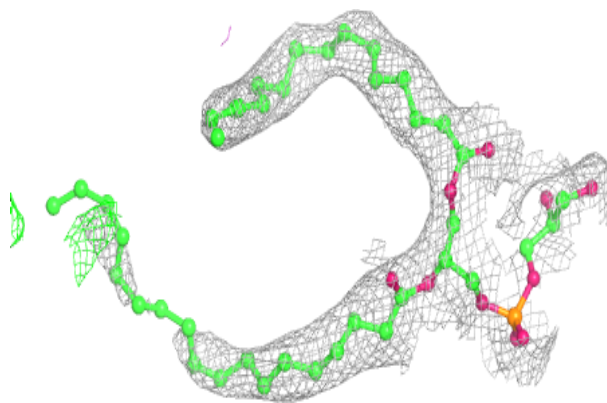
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



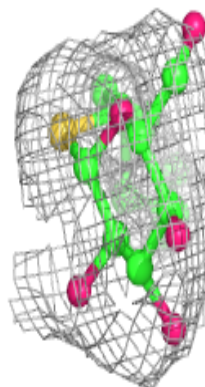
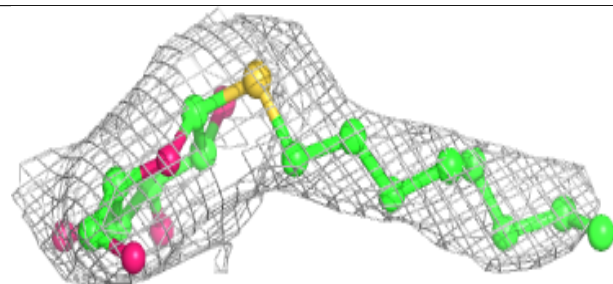
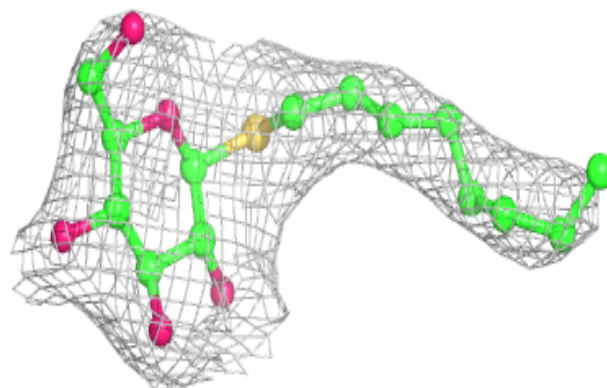


**Electron density around PGW B 404:**

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

**Electron density around SOG 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.