



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 07:17 PM EDT

PDB ID : 8V8F / pdb\_00008v8f  
Title : The co-crystal structure of anti-HIV scFv and Utag  
Authors : Chen, S.H.; Snow, C.D.  
Deposited on : 2023-12-05  
Resolution : 2.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

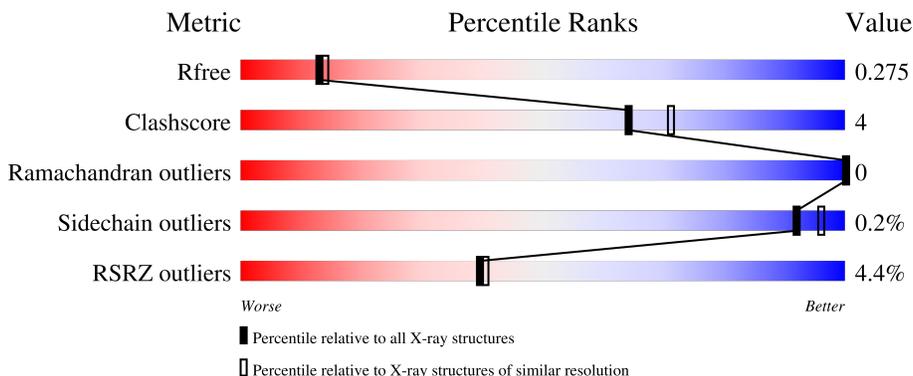
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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.



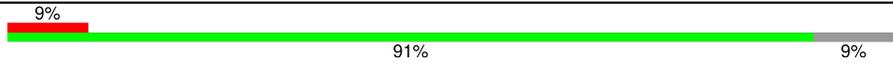
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	277	 4% 81% 5% 14%
1	B	277	 3% 75% 11% 14%
1	C	277	 5% 79% 7% 14%
1	D	277	 3% 78% 9% 13%
2	E	11	 82% 9% 9%

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Mol	Chain	Length	Quality of chain
2	F	11	
2	G	11	
2	H	11	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7865 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 anti-HIV scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	239	Total 1828	C 1152	N 308	O 360	S 8	1	1	0
1	A	239	Total 1813	C 1145	N 300	O 360	S 8	0	0	0
1	C	238	Total 1830	C 1156	N 307	O 359	S 8	1	3	0
1	D	240	Total 1841	C 1161	N 311	O 361	S 8	1	1	0

- Molecule 2 is a protein called Utag.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	10	Total 83	C 55	N 16	O 11	S 1	0	0	0
2	F	10	Total 83	C 55	N 16	O 11	S 1	0	0	0
2	G	10	Total 83	C 55	N 16	O 11	S 1	0	0	0
2	H	10	Total 83	C 55	N 16	O 11	S 1	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

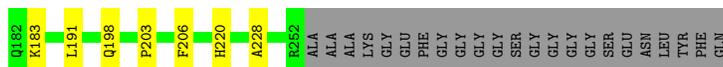
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	50	Total	O	0	0
			50	50		
4	A	38	Total	O	0	0
			38	38		
4	C	44	Total	O	0	0
			44	44		

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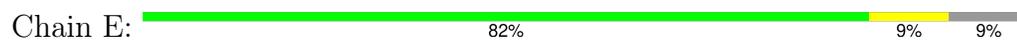
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	D	40	Total O 40 40	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	H	2	Total O 2 2	0	0

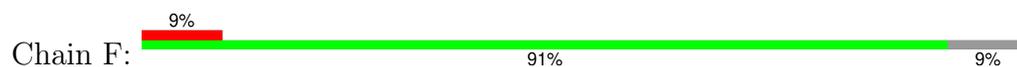




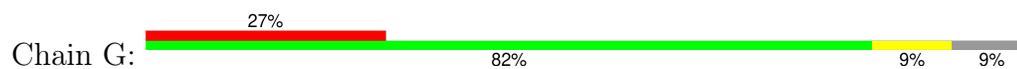
- Molecule 2: Utag



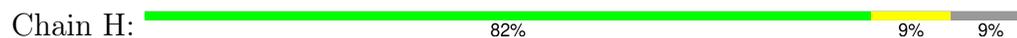
- Molecule 2: Utag



- Molecule 2: Utag



- Molecule 2: Utag



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.47Å 61.82Å 85.58Å 68.83° 77.90° 71.38°	Depositor
Resolution (Å)	45.71 – 2.27 45.71 – 2.27	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.71-2.27) 94.2 (45.71-2.27)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.27Å)	Xtrriage
Refinement program	PHENIX 1.21.2	Depositor
R, $R_{free}$	0.225 , 0.275 0.226 , 0.275	Depositor DCC
$R_{free}$ test set	43297 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.361	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0833e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.14	0/1856	0.35	0/2519
1	B	0.14	0/1870	0.32	0/2536
1	C	0.14	0/1876	0.34	0/2546
1	D	0.13	0/1883	0.33	0/2550
2	E	0.14	0/86	0.40	0/114
2	F	0.16	0/86	0.36	0/114
2	G	0.22	0/86	0.54	0/114
2	H	0.13	0/86	0.34	0/114
All	All	0.14	0/7829	0.34	0/10607

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	1813	0	1721	11	0
1	B	1828	0	1748	17	0
1	C	1830	0	1747	11	0
1	D	1841	0	1774	16	0
2	E	83	0	93	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	83	0	93	0	0
2	G	83	0	93	1	0
2	H	83	0	93	1	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	1	0
4	A	38	0	0	0	0
4	B	50	0	0	0	0
4	C	44	0	0	0	0
4	D	40	0	0	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	2	0	0	0	0
All	All	7865	0	7362	57	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.

The worst 5 of 57 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:D:87:ARG:NH2	4:D:401:HOH:O	2.27	0.65
1:D:91:THR:HG23	1:D:122:THR:HA	1.78	0.65
1:C:29:PHE:HB3	1:C:77:ASN:HD22	1.64	0.63
3:A:302:SO4:O1	2:H:-4:MET:N	2.34	0.60
1:B:205:ARG:NH1	1:B:226:ASP:OD2	2.35	0.60

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	235/277 (85%)	229 (97%)	6 (3%)	0	100	100
1	B	236/277 (85%)	229 (97%)	7 (3%)	0	100	100
1	C	237/277 (86%)	231 (98%)	6 (2%)	0	100	100
1	D	237/277 (86%)	232 (98%)	5 (2%)	0	100	100
2	E	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
2	F	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
2	G	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
2	H	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	977/1152 (85%)	948 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/212 (90%)	190 (100%)	1 (0%)	86	93
1	B	193/212 (91%)	192 (100%)	1 (0%)	86	93
1	C	193/212 (91%)	193 (100%)	0	100	100
1	D	195/212 (92%)	195 (100%)	0	100	100
2	E	9/10 (90%)	9 (100%)	0	100	100
2	F	9/10 (90%)	9 (100%)	0	100	100
2	G	9/10 (90%)	9 (100%)	0	100	100
2	H	9/10 (90%)	9 (100%)	0	100	100
All	All	808/888 (91%)	806 (100%)	2 (0%)	92	96

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

Mol	Chain	Res	Type
1	B	12	VAL
1	A	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	82	GLN
1	D	157	GLN
1	A	82	GLN
1	A	117	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

9 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	302	-	4,4,4	0.68	0	6,6,6	0.09	0
3	SO4	D	301	-	4,4,4	0.66	0	6,6,6	0.06	0
3	SO4	B	302	-	4,4,4	0.68	0	6,6,6	0.13	0
3	SO4	D	302	-	4,4,4	0.70	0	6,6,6	0.10	0
3	SO4	C	301	-	4,4,4	0.66	0	6,6,6	0.14	0
3	SO4	A	301	-	4,4,4	0.67	0	6,6,6	0.07	0
3	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	303	-	4,4,4	0.69	0	6,6,6	0.09	0
3	SO4	E	101	-	4,4,4	0.67	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

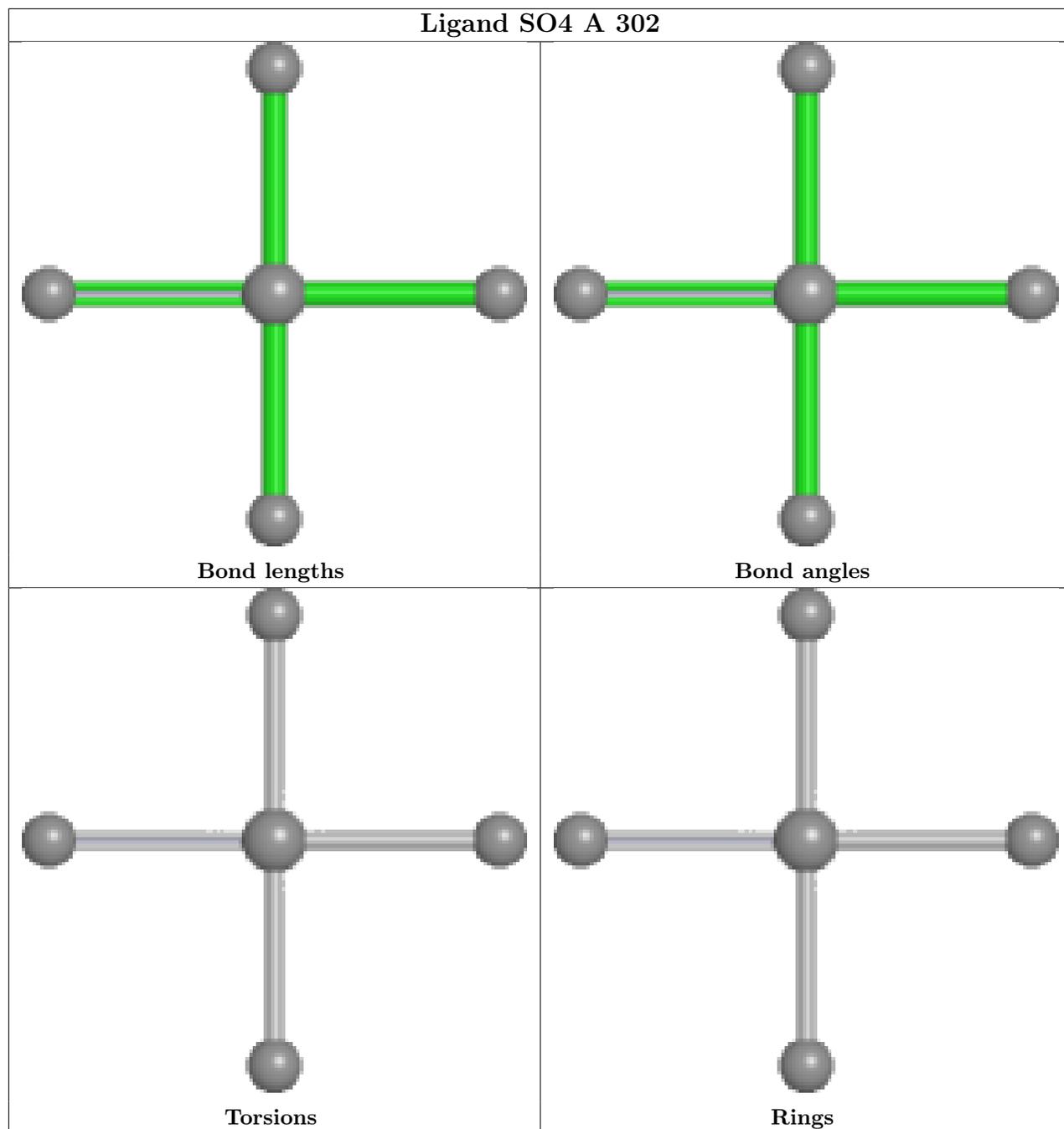
There are no torsion outliers.

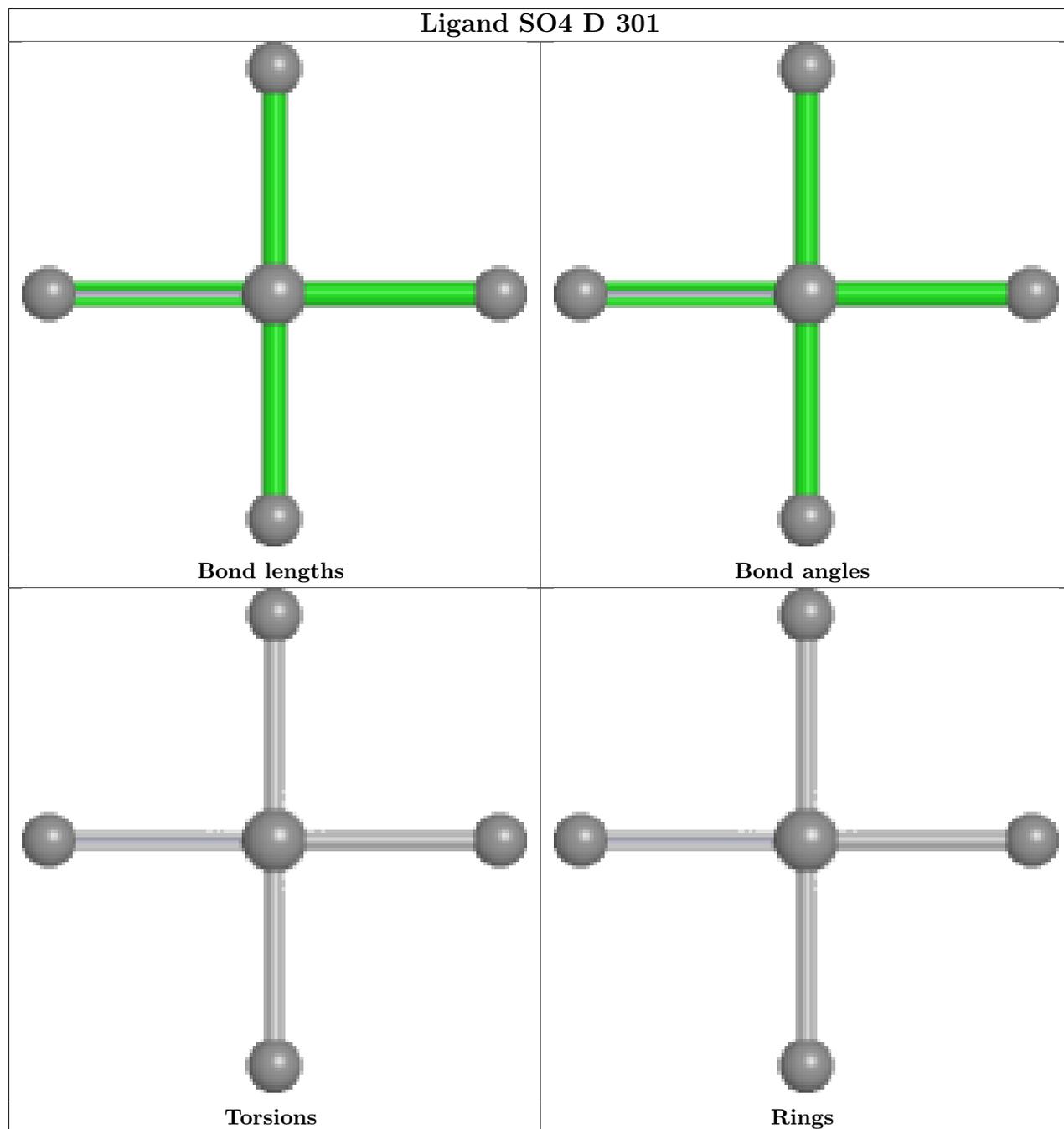
There are no ring outliers.

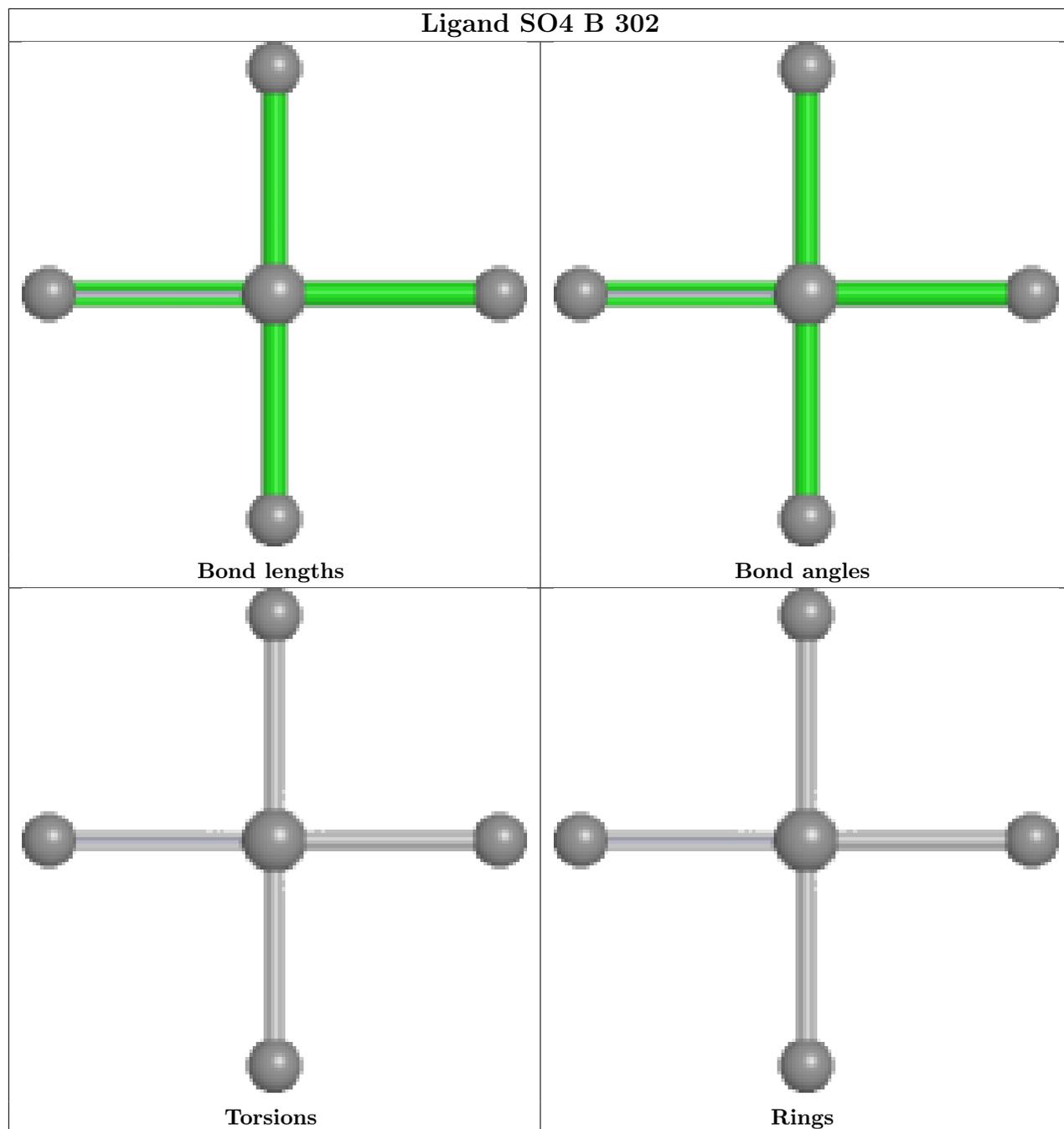
3 monomers are involved in 3 short contacts:

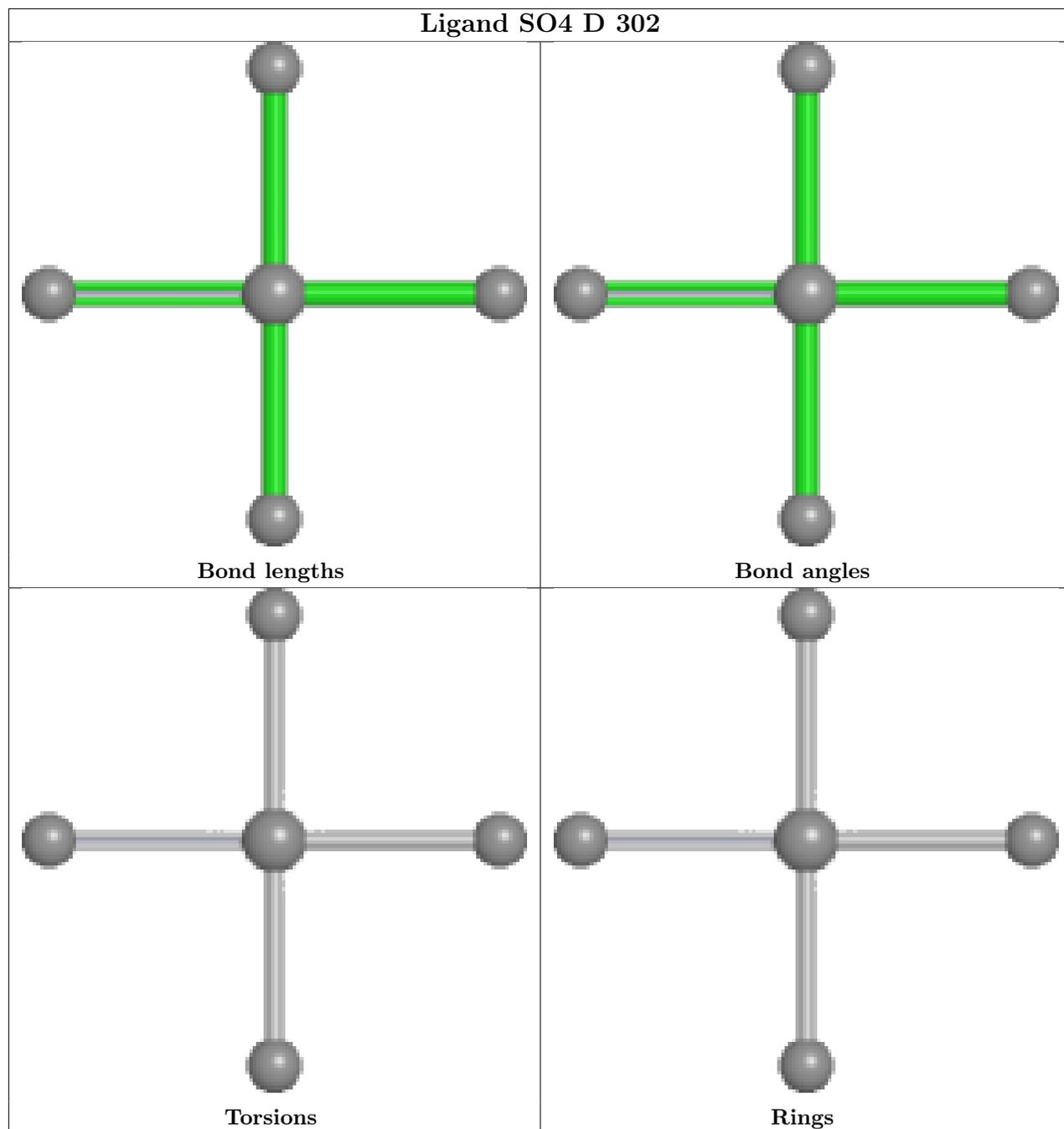
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SO4	1	0
3	A	303	SO4	1	0
3	E	101	SO4	1	0

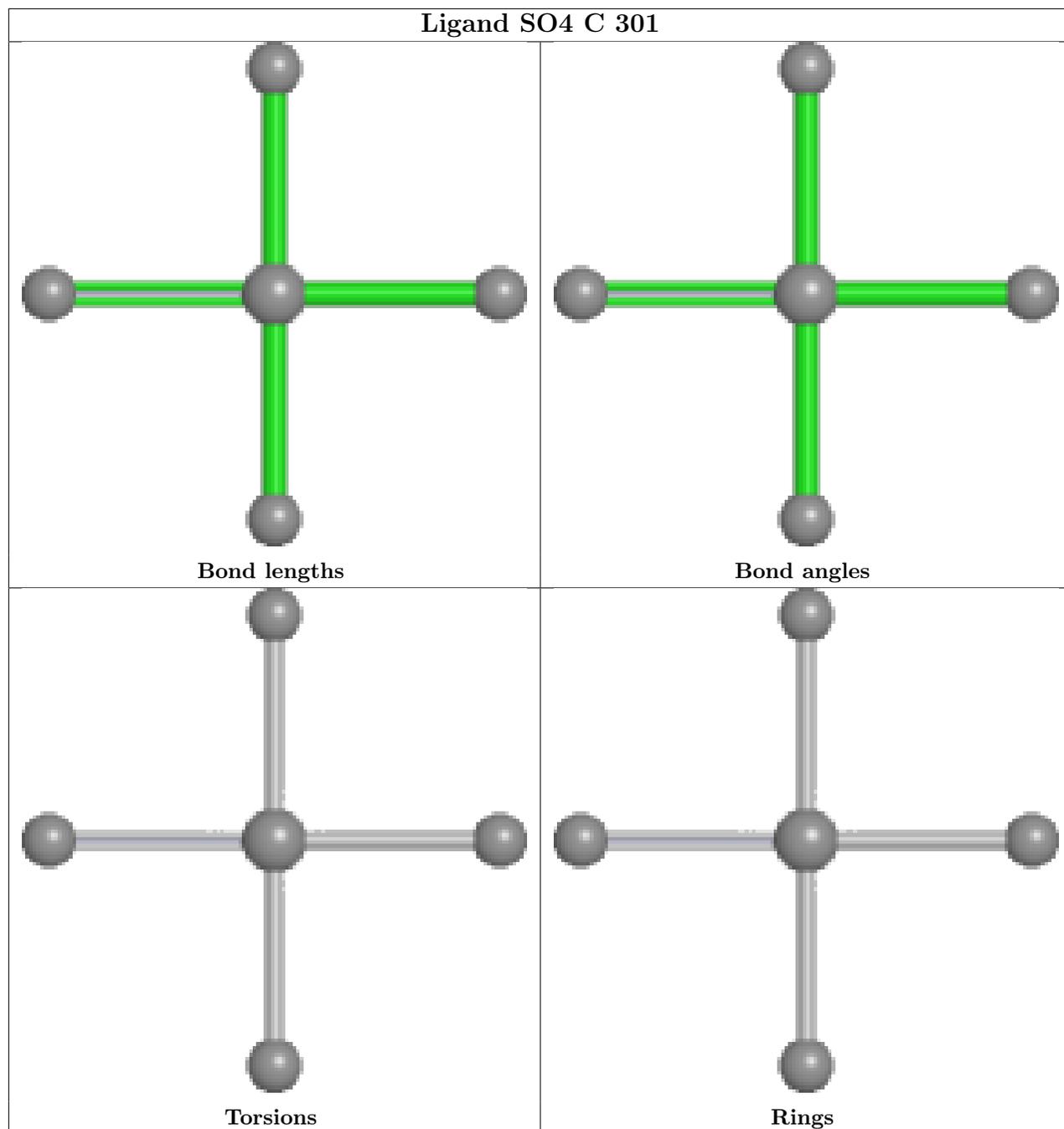
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

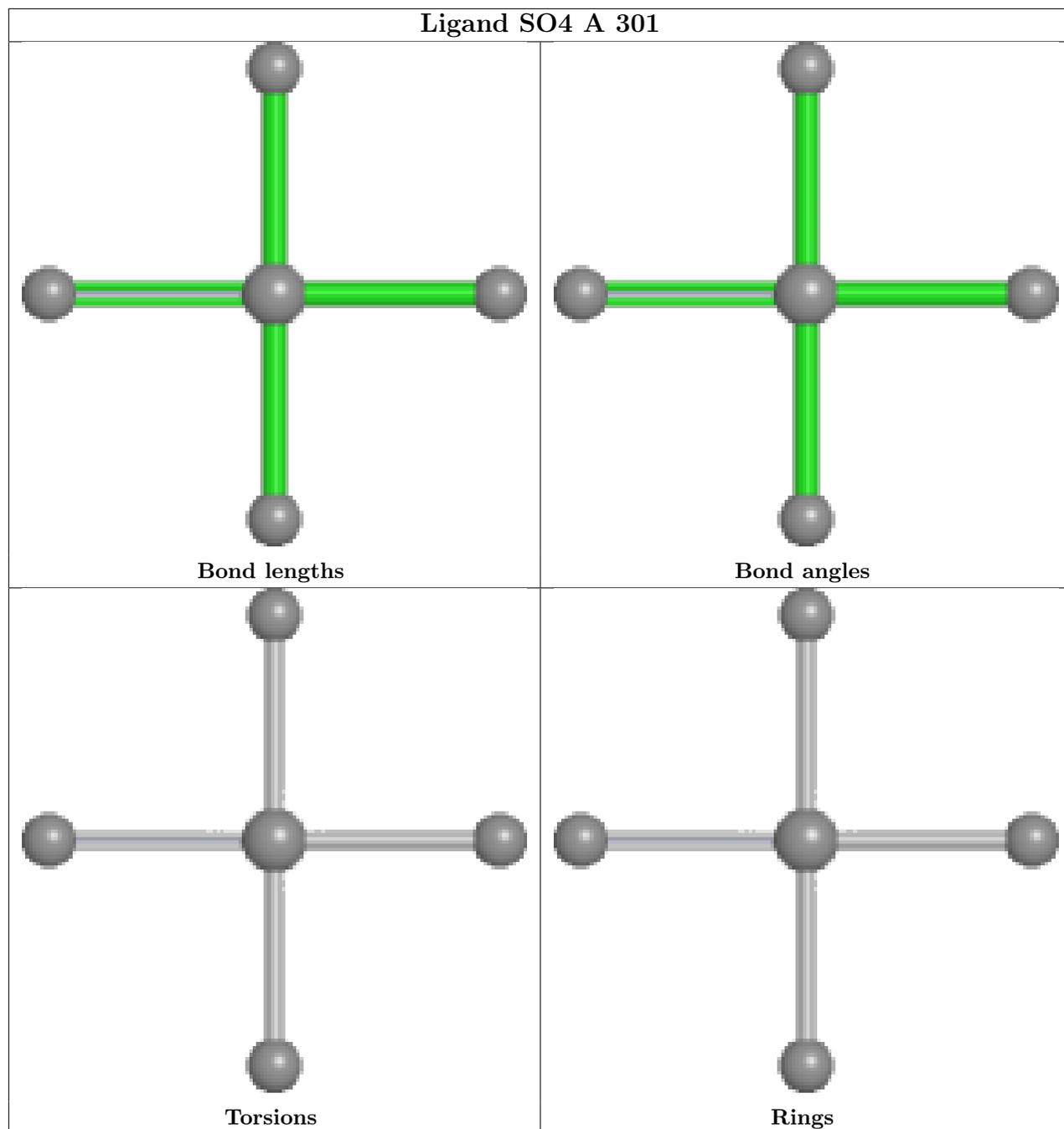


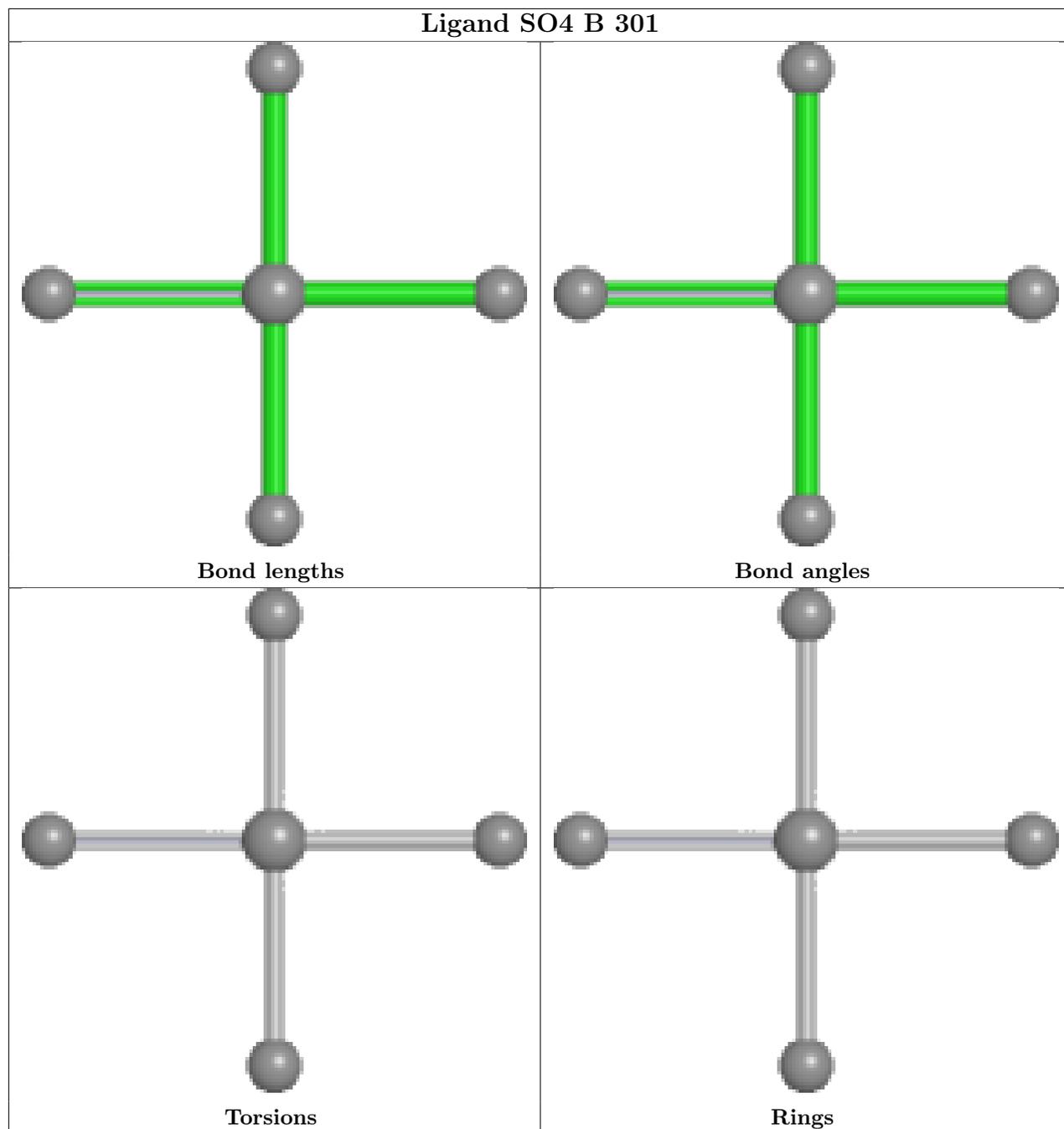


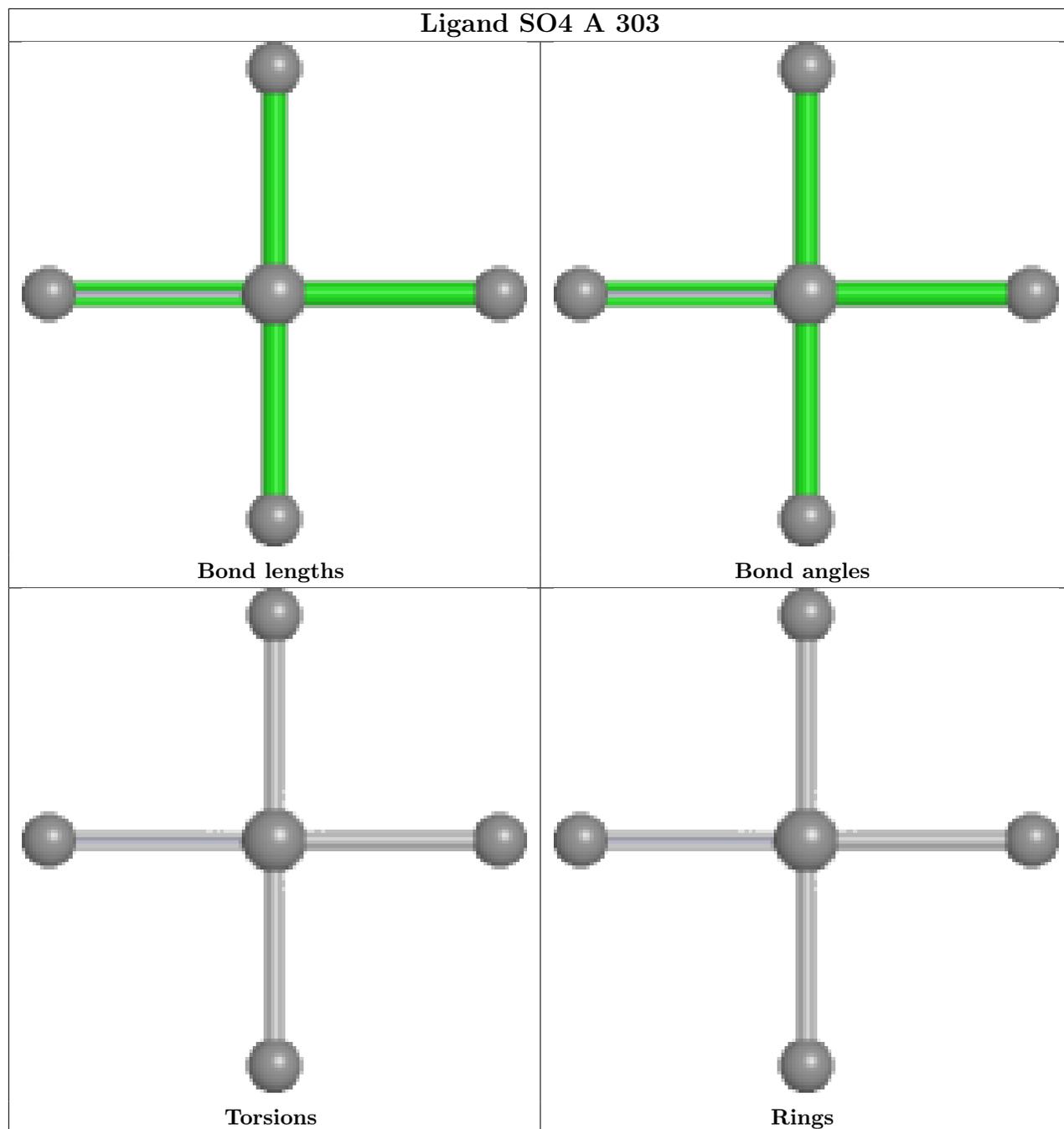


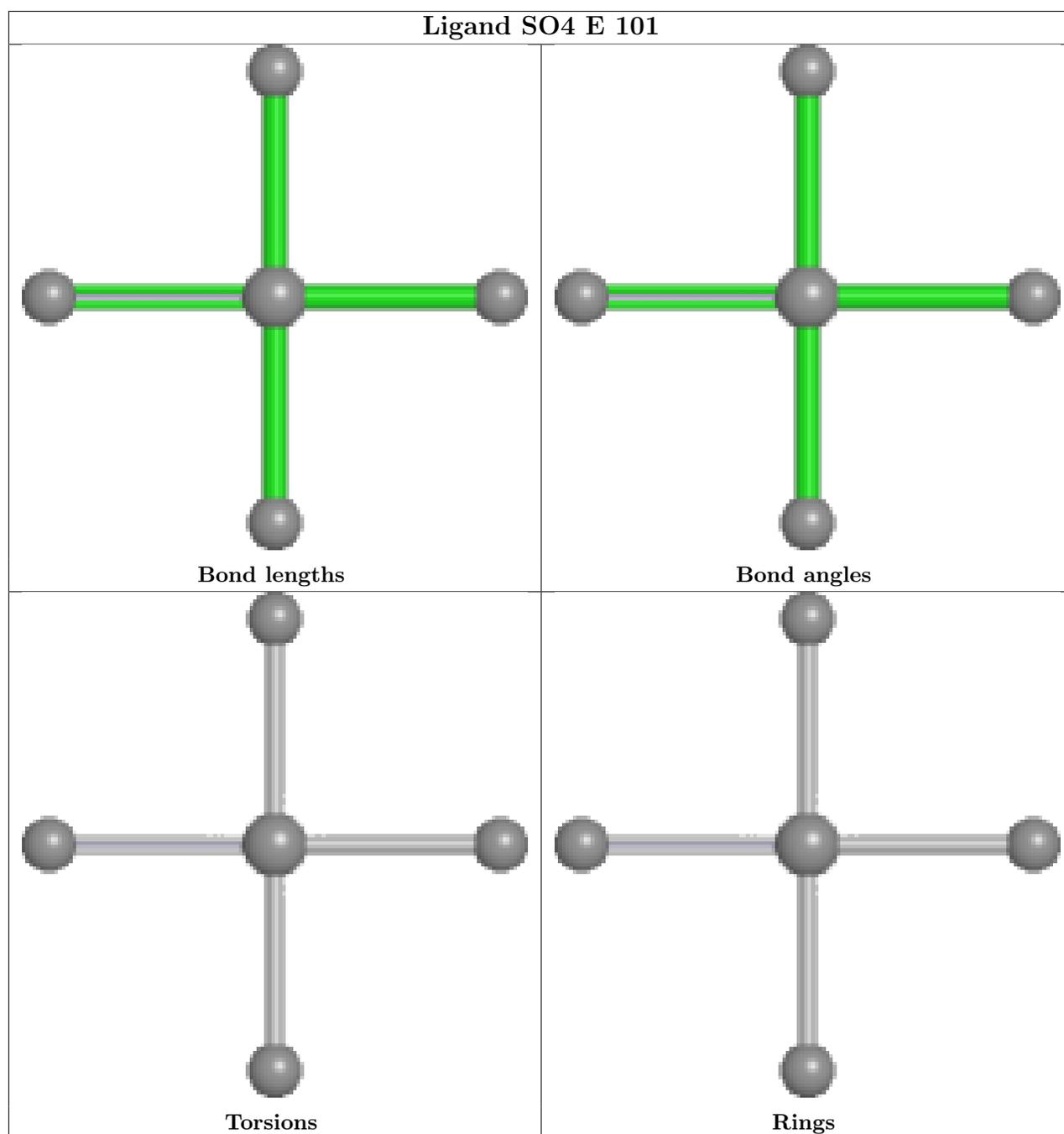












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	239/277 (86%)	0.58	12 (5%) 35 36	28, 40, 67, 92	0
1	B	239/277 (86%)	0.35	7 (2%) 54 55	16, 35, 56, 94	2 (0%)
1	C	238/277 (85%)	0.47	14 (5%) 29 31	18, 37, 61, 97	4 (1%)
1	D	240/277 (86%)	0.51	7 (2%) 54 55	20, 38, 62, 84	2 (0%)
2	E	10/11 (90%)	0.52	0 100 100	35, 40, 49, 66	0
2	F	10/11 (90%)	0.78	1 (10%) 14 15	33, 40, 52, 60	0
2	G	10/11 (90%)	1.25	3 (30%) 1 1	40, 48, 60, 94	0
2	H	10/11 (90%)	0.83	0 100 100	39, 52, 58, 70	0
All	All	996/1152 (86%)	0.49	44 (4%) 39 40	16, 38, 62, 97	8 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	ALA	4.4
1	D	9	GLY	4.3
1	A	251	LYS	4.3
1	D	124	SER	4.0
1	B	9	GLY	3.9

### 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](#)

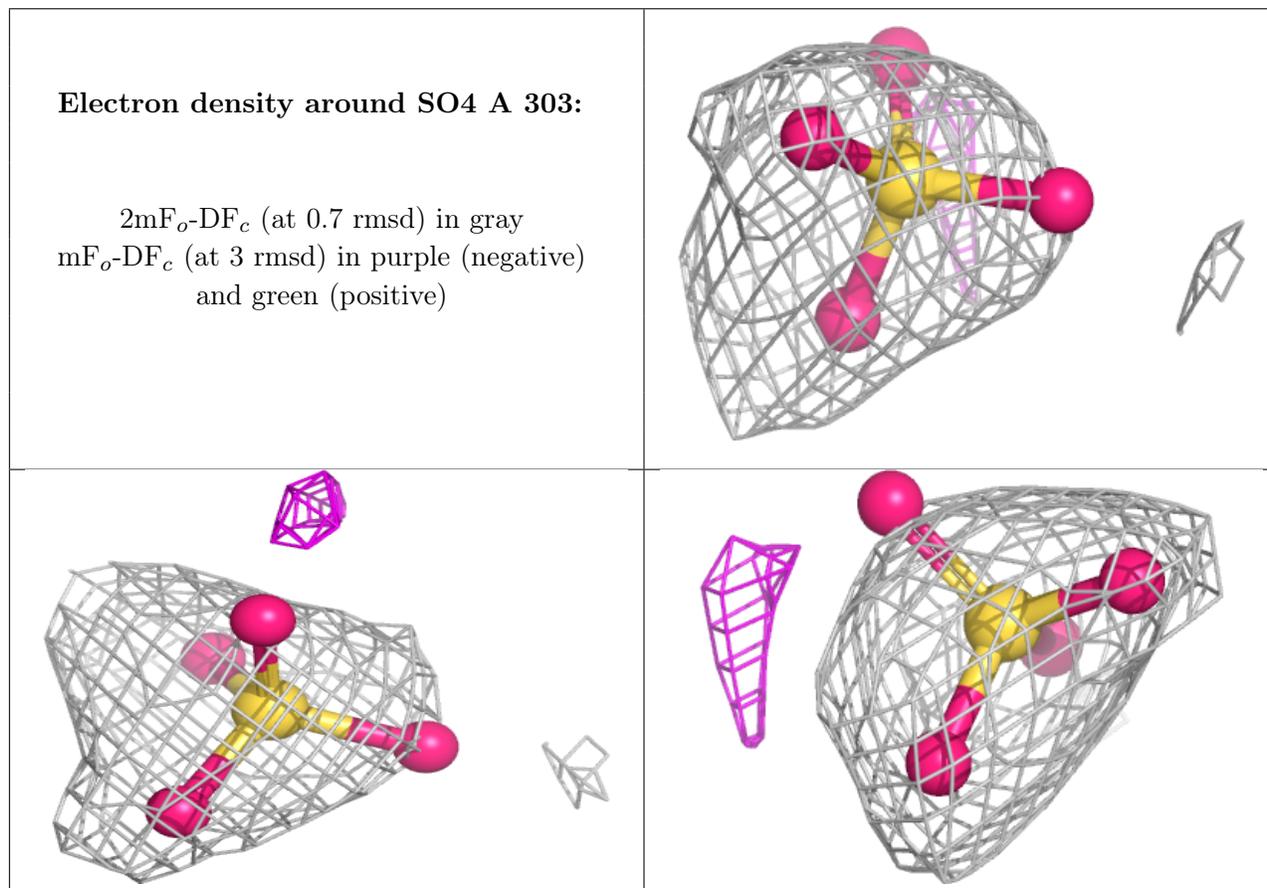
There are no monosaccharides in this entry.

## 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.

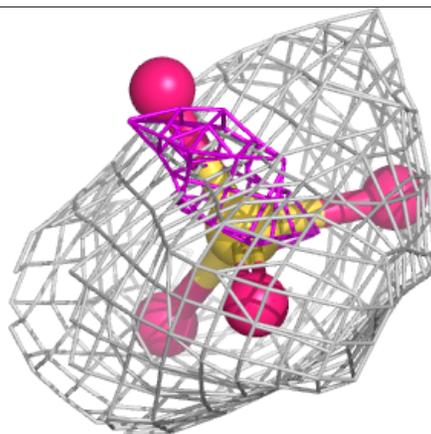
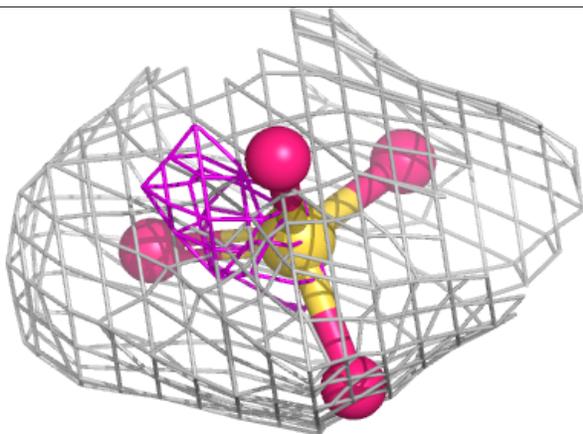
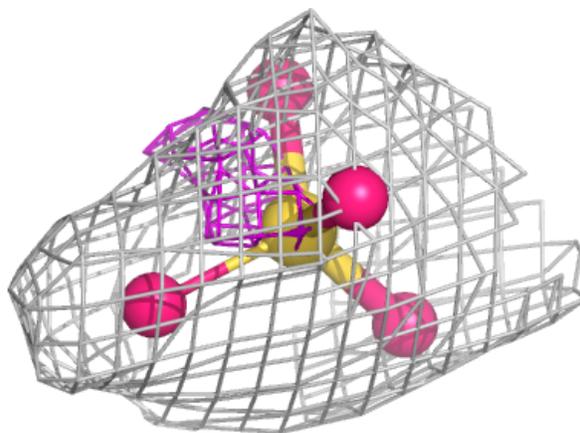
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	303	5/5	0.64	0.15	70,73,77,81	0
3	SO4	A	302	5/5	0.66	0.15	73,74,92,95	0
3	SO4	B	302	5/5	0.87	0.16	51,60,64,68	0
3	SO4	D	302	5/5	0.87	0.17	65,68,73,74	0
3	SO4	E	101	5/5	0.88	0.12	52,52,58,66	0
3	SO4	C	301	5/5	0.93	0.13	36,39,42,48	0
3	SO4	D	301	5/5	0.96	0.08	36,38,41,43	0
3	SO4	B	301	5/5	0.97	0.06	34,34,37,38	0
3	SO4	A	301	5/5	0.97	0.09	36,40,45,45	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.



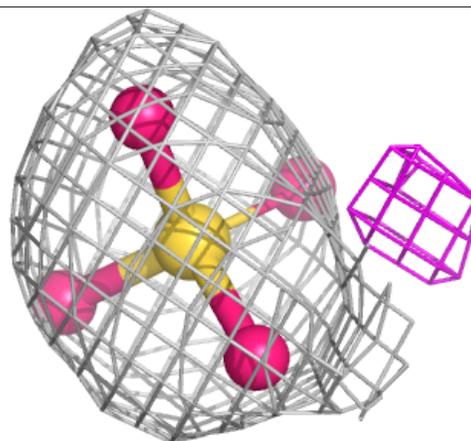
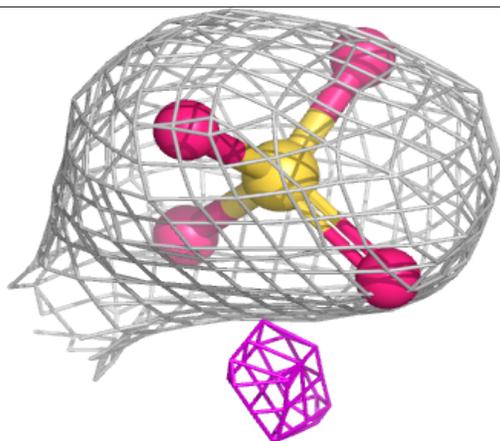
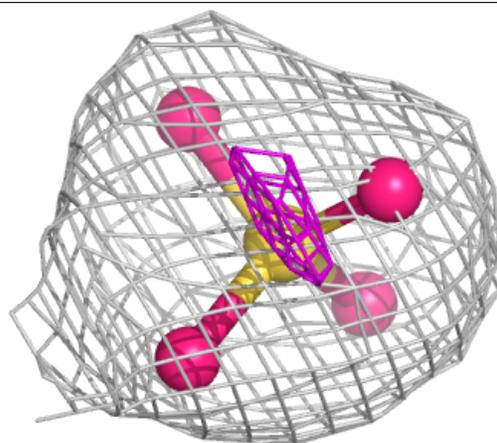
**Electron density around SO4 A 302:**

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



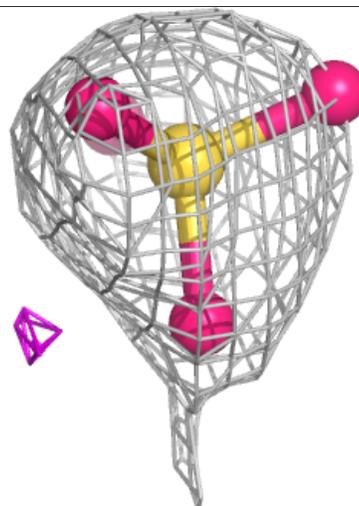
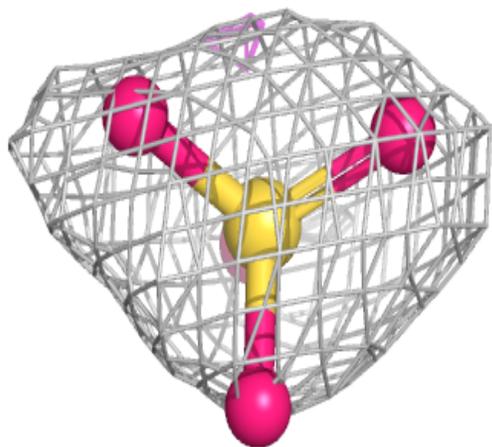
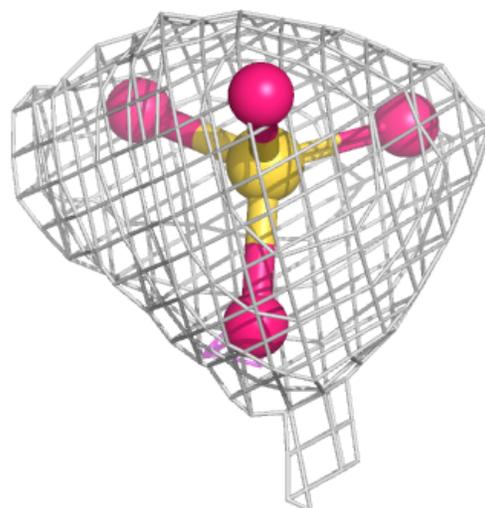
**Electron density around SO4 B 302:**

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



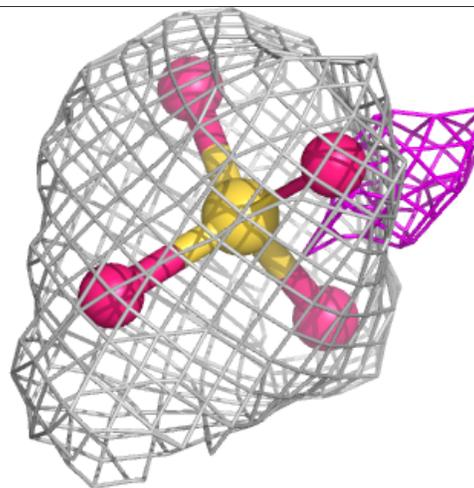
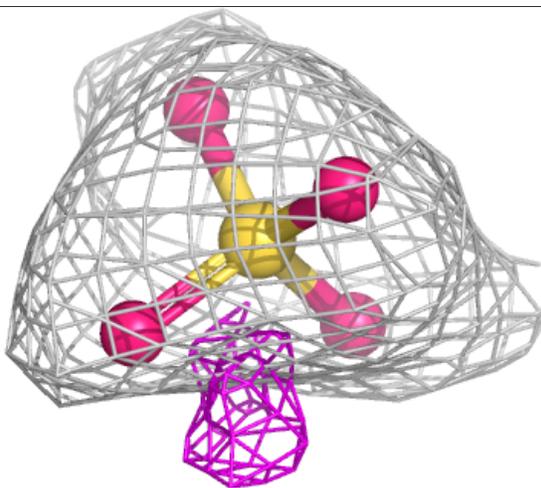
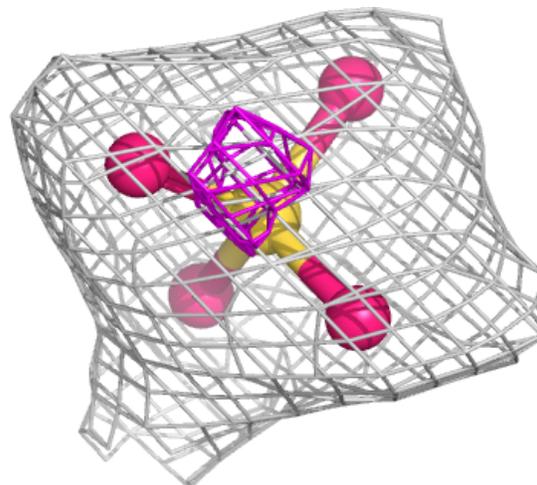
**Electron density around SO4 D 302:**

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



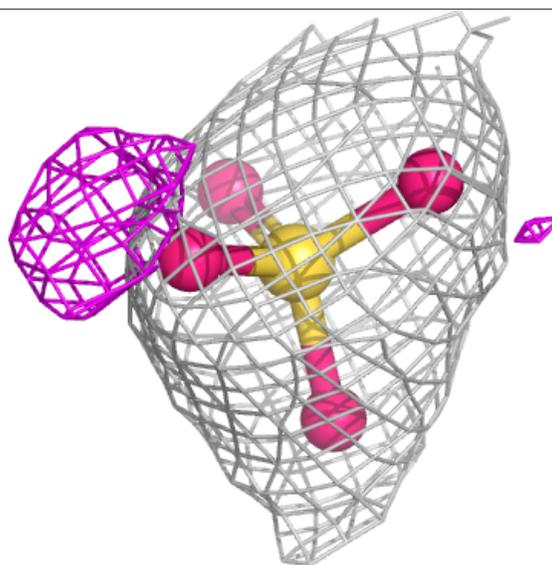
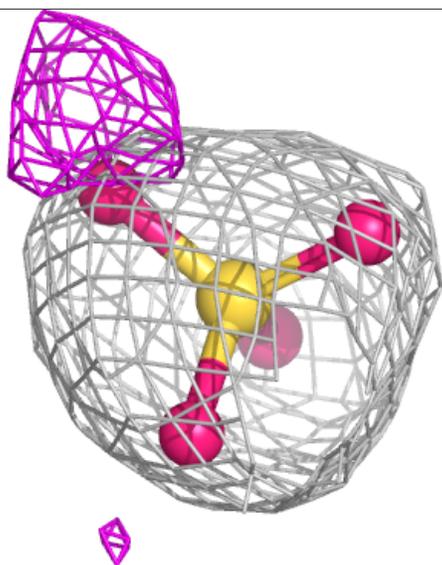
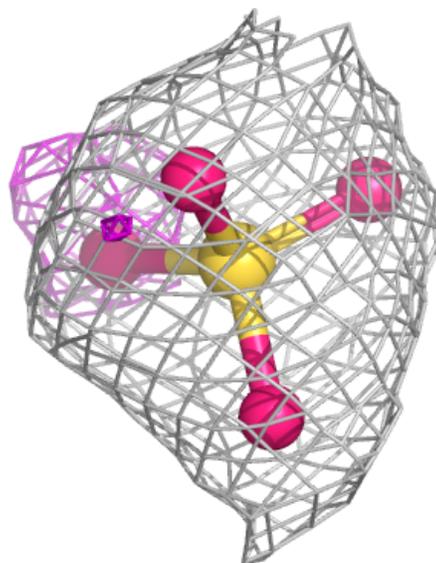
**Electron density around SO4 E 101:**

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



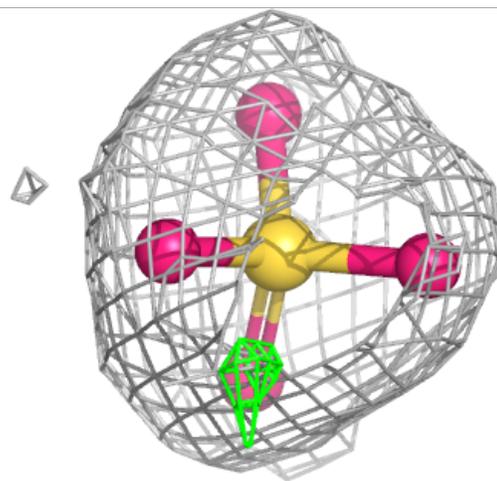
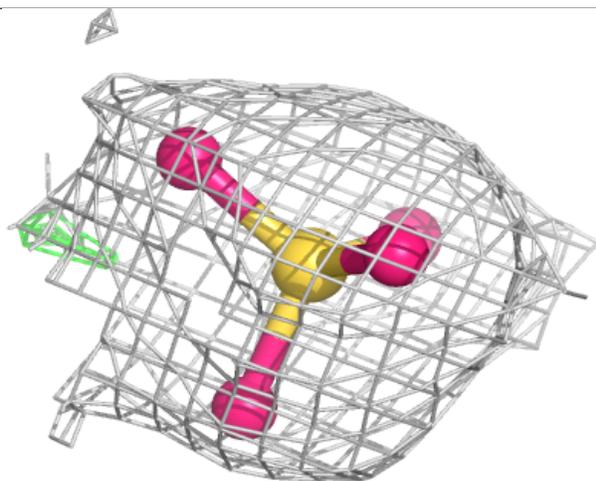
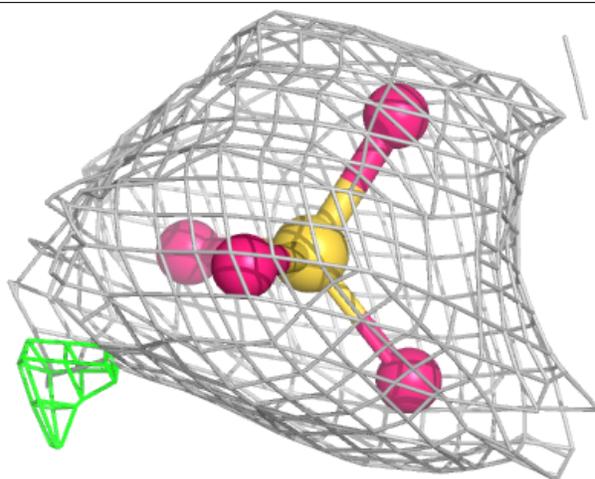
**Electron density around SO4 C 301:**

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



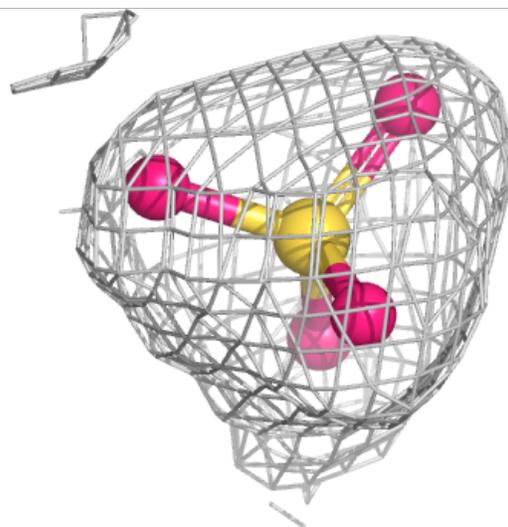
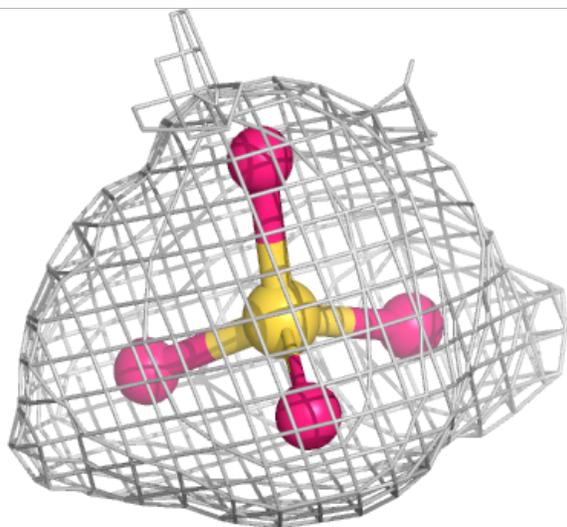
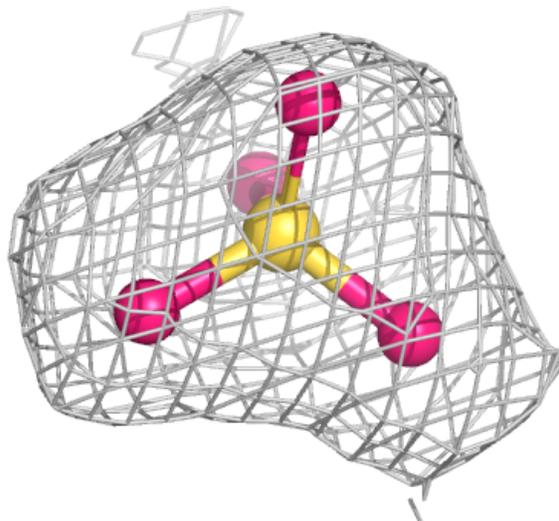
**Electron density around SO4 D 301:**

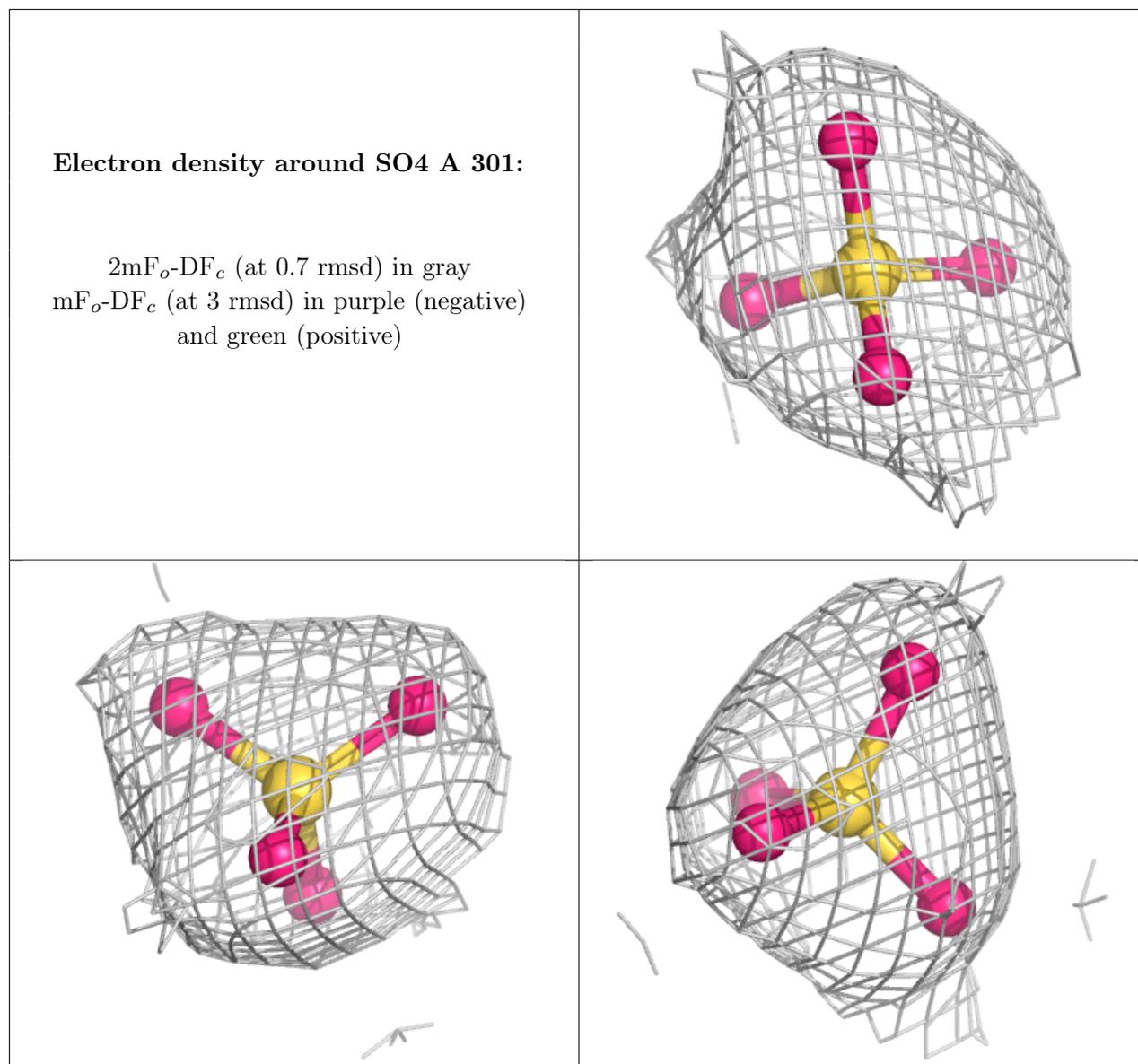
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 B 301:**

$2mF_o-DF_c$  (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.