



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:32 am BST

PDB ID : 6NLZ  
Title : Crystal structure of Mycobacterium tuberculosis dethiobiotin synthetase in complex with fragment degradation product B9D  
Authors : Thompson, A.P.; Polyak, S.W.; Wegener, K.L.; Bruning, J.B.  
Deposited on : 2019-01-10  
Resolution : 1.90 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.

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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 : 2.11  
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) : 2.11

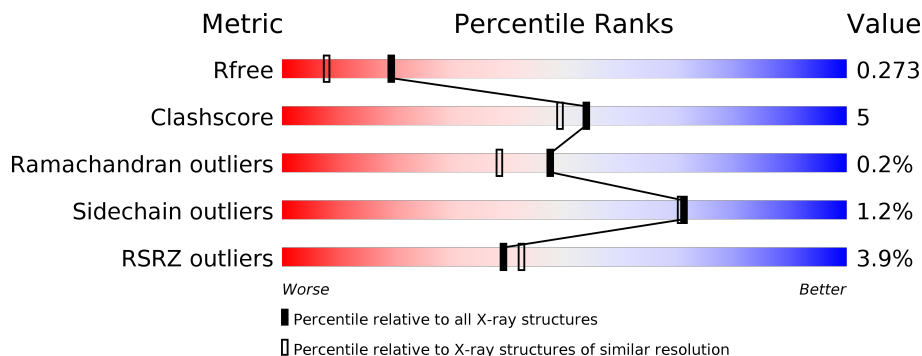
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	233	
1	B	233	
1	C	233	
1	D	233	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	304	-	-	X	-
4	SO4	B	304	-	-	X	-
4	SO4	C	304	-	-	X	-
4	SO4	D	304	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7171 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 ATP-dependent dethiobiotin synthetase BioD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	Total 1606	C 999	N 294	O 304	S 9	0	5	0
1	B	226	Total 1574	C 982	N 285	O 299	S 8	0	1	0
1	C	229	Total 1606	C 1002	N 291	O 305	S 8	0	3	0
1	D	227	Total 1584	C 988	N 287	O 301	S 8	0	2	0

There are 32 discrepancies between the modelled and reference sequences:

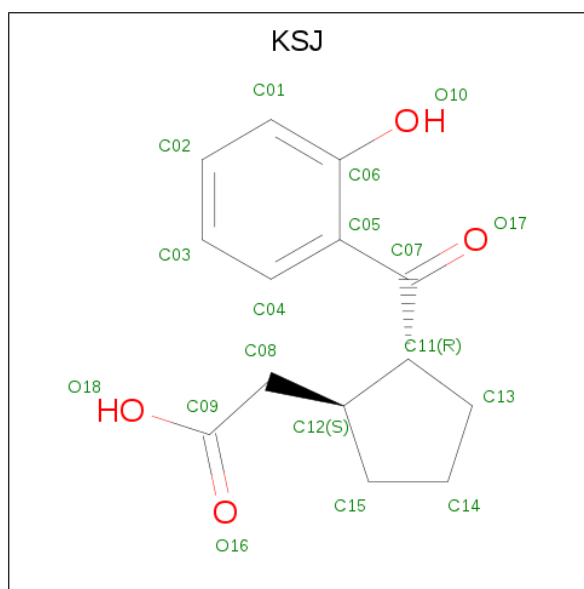
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP P9WPQ5
A	-5	HIS	-	expression tag	UNP P9WPQ5
A	-4	HIS	-	expression tag	UNP P9WPQ5
A	-3	HIS	-	expression tag	UNP P9WPQ5
A	-2	HIS	-	expression tag	UNP P9WPQ5
A	-1	HIS	-	expression tag	UNP P9WPQ5
A	0	GLY	-	expression tag	UNP P9WPQ5
A	1	GLY	-	expression tag	UNP P9WPQ5
B	-6	HIS	-	expression tag	UNP P9WPQ5
B	-5	HIS	-	expression tag	UNP P9WPQ5
B	-4	HIS	-	expression tag	UNP P9WPQ5
B	-3	HIS	-	expression tag	UNP P9WPQ5
B	-2	HIS	-	expression tag	UNP P9WPQ5
B	-1	HIS	-	expression tag	UNP P9WPQ5
B	0	GLY	-	expression tag	UNP P9WPQ5
B	1	GLY	-	expression tag	UNP P9WPQ5
C	-6	HIS	-	expression tag	UNP P9WPQ5
C	-5	HIS	-	expression tag	UNP P9WPQ5
C	-4	HIS	-	expression tag	UNP P9WPQ5
C	-3	HIS	-	expression tag	UNP P9WPQ5
C	-2	HIS	-	expression tag	UNP P9WPQ5

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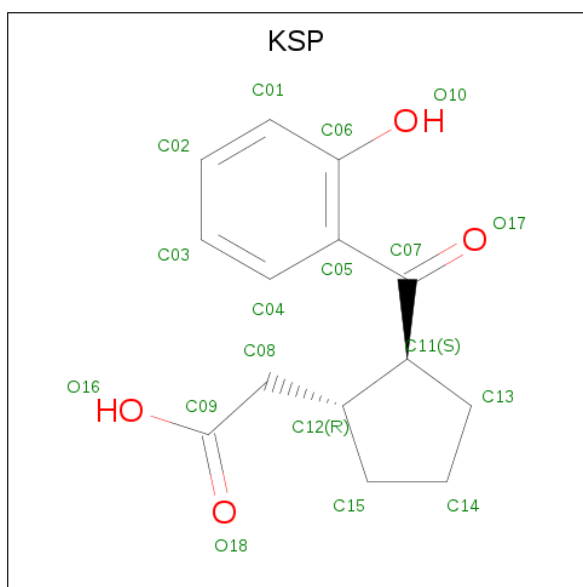
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP P9WPQ5
C	0	GLY	-	expression tag	UNP P9WPQ5
C	1	GLY	-	expression tag	UNP P9WPQ5
D	-6	HIS	-	expression tag	UNP P9WPQ5
D	-5	HIS	-	expression tag	UNP P9WPQ5
D	-4	HIS	-	expression tag	UNP P9WPQ5
D	-3	HIS	-	expression tag	UNP P9WPQ5
D	-2	HIS	-	expression tag	UNP P9WPQ5
D	-1	HIS	-	expression tag	UNP P9WPQ5
D	0	GLY	-	expression tag	UNP P9WPQ5
D	1	GLY	-	expression tag	UNP P9WPQ5

- Molecule 2 is [(1S,2R)-2-(2-hydroxybenzene-1-carbonyl)cyclopentyl]acetic acid (three-letter code: KSJ) (formula: C<sub>14</sub>H<sub>16</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



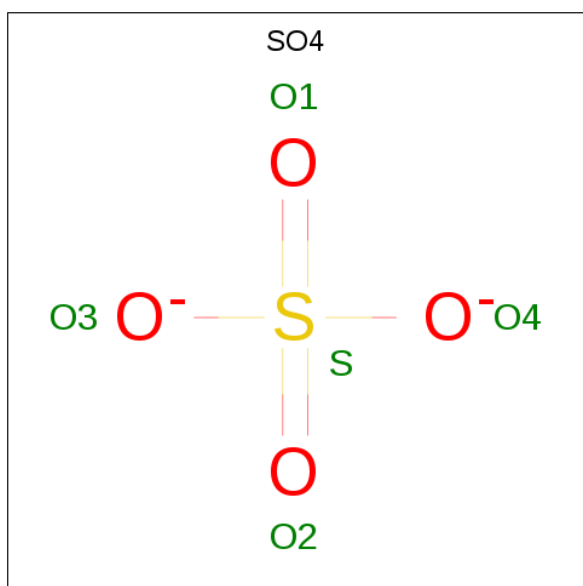
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			18	14	4		
2	B	1	Total	C	O	0	1
			18	14	4		
2	C	1	Total	C	O	0	1
			18	14	4		
2	D	1	Total	C	O	0	1
			18	14	4		

- Molecule 3 is [(1R,2S)-2-(2-hydroxybenzene-1-carbonyl)cyclopentyl]acetic acid (three-letter code: KSP) (formula: C<sub>14</sub>H<sub>16</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	1
			18	14 4		
3	B	1	Total	C O	0	1
			18	14 4		
3	C	1	Total	C O	0	1
			18	14 4		
3	D	1	Total	C O	0	1
			18	14 4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by author).



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

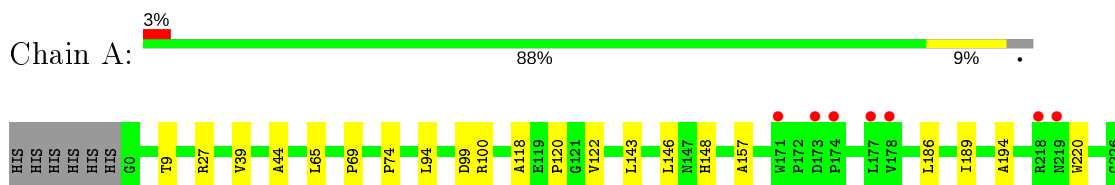
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	200	Total O 200 200	0	0
5	B	188	Total O 188 188	0	0
5	C	124	Total O 124 124	0	0
5	D	105	Total O 105 105	0	0

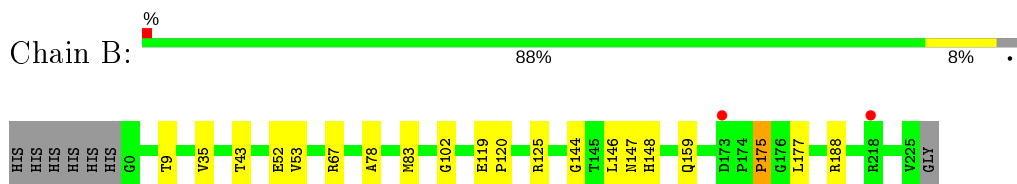
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

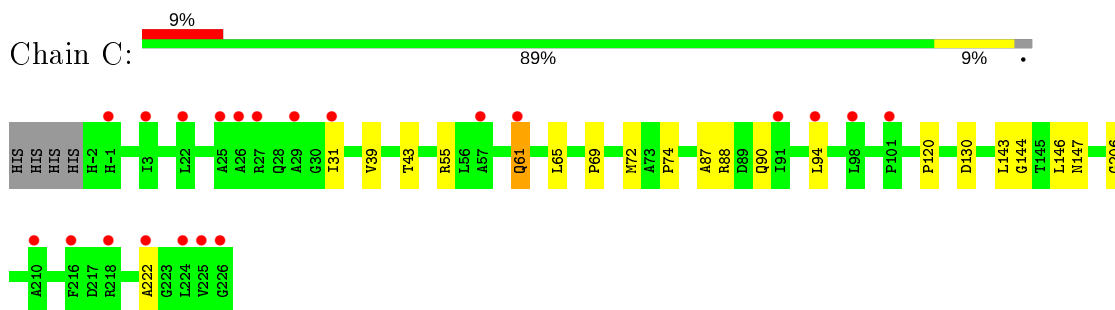
- Molecule 1: ATP-dependent dethiobiotin synthetase BioD



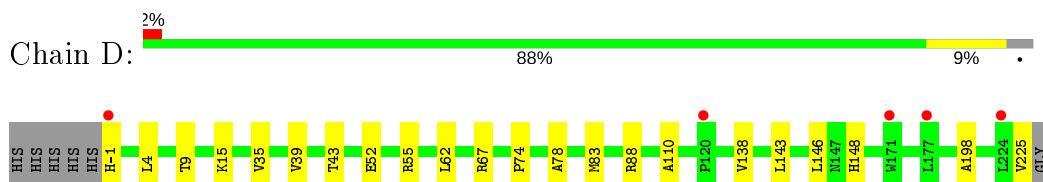
- Molecule 1: ATP-dependent dethiobiotin synthetase BioD



- Molecule 1: ATP-dependent dethiobiotin synthetase BioD



- Molecule 1: ATP-dependent dethiobiotin synthetase BioD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.61Å 105.72Å 154.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 1.90 46.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.31-1.90) 99.4 (46.31-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	38.78 (at 1.90Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.231 , 0.273 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	3490 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.589	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SO4, KSP, KSJ

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	0/1625	0.59	0/2221
1	B	0.37	0/1593	0.58	0/2179
1	C	0.31	0/1626	0.51	0/2225
1	D	0.32	0/1603	0.53	0/2193
All	All	0.36	0/6447	0.55	0/8818

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	1606	0	1650	14	0
1	B	1574	0	1624	15	0
1	C	1606	0	1646	17	0
1	D	1584	0	1627	16	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
2	C	18	0	0	1	0
2	D	18	0	0	2	0
3	A	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	2	0
3	C	18	0	0	2	0
3	D	18	0	0	3	0
4	A	10	0	0	2	0
4	B	10	0	0	3	0
4	C	10	0	0	6	0
4	D	10	0	0	2	0
5	A	200	0	0	4	0
5	B	188	0	0	6	0
5	C	124	0	0	6	0
5	D	105	0	0	3	0
All	All	7171	0	6547	69	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 5.

All (69) 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:C:147:ASN:N	4:C:304:SO4:O4	2.06	0.88
1:B:147:ASN:N	4:B:304:SO4:O1	2.09	0.84
1:B:175:PRO:O	5:B:401:HOH:O	2.01	0.79
1:D:146:LEU:N	4:D:304:SO4:O2	2.18	0.77
1:C:94:LEU:O	5:C:401:HOH:O	2.04	0.73
4:C:304:SO4:O2	5:C:402:HOH:O	2.07	0.73
1:C:55:ARG:NH1	5:C:403:HOH:O	2.14	0.66
1:C:31:ILE:HD11	1:C:222:ALA:HA	1.78	0.64
1:C:65:LEU:HB2	1:C:94:LEU:HD22	1.79	0.63
1:B:120:PRO:O	5:B:402:HOH:O	2.16	0.61
1:A:65:LEU:HB2	1:A:94:LEU:HD22	1.83	0.60
1:A:27[A]:ARG:NH2	5:A:408:HOH:O	2.35	0.59
1:A:220:TRP:O	5:A:401:HOH:O	2.17	0.59
1:B:102:GLY:O	5:B:403:HOH:O	2.17	0.58
1:B:144:GLY:HA2	4:B:304:SO4:O3	2.03	0.58
4:C:304:SO4:O3	5:C:404:HOH:O	2.16	0.58
1:B:119:GLU:OE2	5:B:404:HOH:O	2.17	0.58
1:D:146:LEU:HB2	4:D:304:SO4:O4	2.04	0.57
3:D:302[B]:KSP:O10	3:D:302[B]:KSP:O17	2.17	0.57
1:A:146:LEU:N	4:A:304:SO4:O1	2.35	0.57
1:B:52:GLU:OE1	5:B:405:HOH:O	2.18	0.57
1:C:88:ARG:NH2	1:C:130:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302[B]:KSP:O17	3:A:302[B]:KSP:O10	2.19	0.56
1:B:188:ARG:NH2	5:B:412:HOH:O	2.40	0.55
1:B:35:VAL:HG21	1:B:53:VAL:HG11	1.87	0.55
1:B:43:THR:HG21	1:B:67:ARG:HB3	1.89	0.54
1:A:157:ALA:HB1	1:C:120:PRO:HG3	1.91	0.53
1:D:52:GLU:HG3	1:D:55:ARG:HH11	1.75	0.52
1:A:146:LEU:HB2	4:A:304:SO4:O1	2.10	0.52
1:D:52:GLU:HG3	1:D:55:ARG:NH1	2.25	0.51
1:C:146:LEU:HB2	4:C:304:SO4:O4	2.11	0.51
1:D:9:THR:HB	1:D:148:HIS:HB3	1.94	0.50
1:B:146:LEU:HB2	4:B:304:SO4:O1	2.11	0.50
4:C:304:SO4:O1	5:C:405:HOH:O	2.18	0.50
3:C:302[B]:KSP:O10	3:C:302[B]:KSP:O17	2.30	0.49
1:D:43:THR:HG21	1:D:67:ARG:HB3	1.95	0.49
3:B:302[B]:KSP:O10	3:B:302[B]:KSP:O17	2.25	0.49
1:A:186:LEU:O	1:A:189:ILE:HG12	2.12	0.49
1:D:198:ALA:O	5:D:401:HOH:O	2.19	0.48
1:A:143:LEU:HG	3:B:302[B]:KSP:C03	2.45	0.47
1:C:74:PRO:HD3	3:C:302[B]:KSP:O10	2.15	0.47
1:D:88[A]:ARG:NH2	5:D:411:HOH:O	2.47	0.46
1:C:143:LEU:HG	3:D:302[B]:KSP:C03	2.45	0.46
1:C:206:GLY:HA3	5:C:508:HOH:O	2.16	0.45
1:C:61:GLN:H	1:C:61:GLN:HG2	1.58	0.45
1:C:87:ALA:HB3	1:C:90:GLN:HG3	1.98	0.45
1:B:9:THR:HB	1:B:148:HIS:HB3	2.00	0.44
1:C:43:THR:OG1	1:C:69:PRO:HA	2.18	0.44
1:D:15:LYS:HA	1:D:138:VAL:HG21	1.99	0.44
1:C:74:PRO:HD3	2:C:301[A]:KSJ:O10	2.17	0.43
2:D:301[A]:KSJ:O10	2:D:301[A]:KSJ:O17	2.36	0.43
1:A:99:ASP:HA	5:A:434:HOH:O	2.19	0.42
1:A:9:THR:HB	1:A:148:HIS:HB3	2.01	0.42
1:D:74:PRO:HD3	3:D:302[B]:KSP:O10	2.19	0.42
1:D:78:ALA:HB1	1:D:83:MET:O	2.19	0.42
1:D:35:VAL:HB	1:D:62:LEU:HD23	2.02	0.42
1:C:39:VAL:HG11	1:C:74:PRO:HB3	2.00	0.42
1:A:39:VAL:HG11	1:A:74:PRO:HB3	2.02	0.42
1:C:144:GLY:HA2	4:C:304:SO4:O2	2.20	0.41
1:D:15:LYS:HB2	1:D:15:LYS:HE2	1.85	0.41
1:A:44:ALA:HB2	1:A:69:PRO:HB3	2.02	0.41
1:D:39:VAL:HG11	1:D:74:PRO:HB3	2.03	0.41
1:A:118:ALA:HB3	1:A:122:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:HIS:N	5:D:416:HOH:O	2.54	0.41
1:B:119:GLU:HA	1:B:120:PRO:HA	1.79	0.40
1:B:125:ARG:HD2	1:B:159:GLN:HG3	2.03	0.40
1:D:110:ALA:HB1	2:D:301[A]:KSJ:O10	2.22	0.40
1:A:194:ALA:HA	5:A:470:HOH:O	2.22	0.40
1:B:78:ALA:HB1	1:B:83:MET:O	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	230/233 (99%)	223 (97%)	6 (3%)	1 (0%)	34	24
1	B	225/233 (97%)	221 (98%)	3 (1%)	1 (0%)	34	24
1	C	230/233 (99%)	227 (99%)	3 (1%)	0	100	100
1	D	227/233 (97%)	225 (99%)	2 (1%)	0	100	100
All	All	912/932 (98%)	896 (98%)	14 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	PRO
1	A	120	PRO

### 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	155/157 (99%)	154 (99%)	1 (1%)	86	87
1	B	152/157 (97%)	151 (99%)	1 (1%)	84	84
1	C	154/157 (98%)	152 (99%)	2 (1%)	69	68
1	D	152/157 (97%)	149 (98%)	3 (2%)	55	51
All	All	613/628 (98%)	606 (99%)	7 (1%)	71	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	B	177	LEU
1	C	61	GLN
1	C	72	MET
1	D	4	LEU
1	D	143	LEU
1	D	225	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 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	D	304	-	4,4,4	0.15	0	6,6,6	0.49	0
4	SO4	B	304	-	4,4,4	0.27	0	6,6,6	1.05	0
4	SO4	B	303	-	4,4,4	0.22	0	6,6,6	0.26	0
2	KSJ	D	301[A]	-	16,19,19	1.28	1 (6%)	19,26,26	1.92	7 (36%)
2	KSJ	B	301[A]	-	16,19,19	1.40	4 (25%)	19,26,26	1.49	3 (15%)
3	KSP	B	302[B]	-	16,19,19	1.87	5 (31%)	19,26,26	2.75	8 (42%)
4	SO4	A	304	-	4,4,4	0.37	0	6,6,6	1.02	1 (16%)
3	KSP	A	302[B]	-	16,19,19	1.72	4 (25%)	19,26,26	3.25	8 (42%)
4	SO4	A	303	-	4,4,4	0.30	0	6,6,6	0.31	0
3	KSP	C	302[B]	-	16,19,19	1.65	3 (18%)	19,26,26	2.71	8 (42%)
4	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.46	0
2	KSJ	C	301[A]	-	16,19,19	1.34	3 (18%)	19,26,26	1.50	3 (15%)
2	KSJ	A	301[A]	-	16,19,19	1.34	3 (18%)	19,26,26	1.32	3 (15%)
4	SO4	D	303	-	4,4,4	0.12	0	6,6,6	0.26	0
3	KSP	D	302[B]	-	16,19,19	1.60	3 (18%)	19,26,26	3.12	9 (47%)
4	SO4	C	304	-	4,4,4	0.36	0	6,6,6	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KSJ	D	301[A]	-	-	0/10/22/22	0/2/2/2
2	KSJ	B	301[A]	-	-	0/10/22/22	0/2/2/2
3	KSP	B	302[B]	-	-	1/10/22/22	0/2/2/2
3	KSP	A	302[B]	-	-	2/10/22/22	0/2/2/2
3	KSP	C	302[B]	-	-	0/10/22/22	0/2/2/2
2	KSJ	C	301[A]	-	-	0/10/22/22	0/2/2/2
2	KSJ	A	301[A]	-	-	0/10/22/22	0/2/2/2
3	KSP	D	302[B]	-	-	4/10/22/22	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[B]	KSP	C11-C07	4.18	1.57	1.52
3	C	302[B]	KSP	C11-C07	3.51	1.56	1.52
3	A	302[B]	KSP	C05-C07	3.28	1.54	1.49
3	A	302[B]	KSP	C11-C07	3.25	1.56	1.52
3	B	302[B]	KSP	O17-C07	-3.20	1.17	1.22
3	D	302[B]	KSP	C11-C07	3.19	1.56	1.52
3	B	302[B]	KSP	C05-C07	3.13	1.54	1.49
3	A	302[B]	KSP	O17-C07	-2.91	1.18	1.22
3	C	302[B]	KSP	C05-C07	2.84	1.54	1.49
3	B	302[B]	KSP	O10-C06	2.59	1.41	1.36
3	D	302[B]	KSP	C05-C07	2.55	1.53	1.49
2	A	301[A]	KSJ	O17-C07	-2.51	1.18	1.22
3	C	302[B]	KSP	O10-C06	2.51	1.41	1.36
2	C	301[A]	KSJ	O10-C06	2.49	1.41	1.36
2	B	301[A]	KSJ	O17-C07	-2.47	1.18	1.22
2	D	301[A]	KSJ	O10-C06	2.33	1.41	1.36
2	B	301[A]	KSJ	O10-C06	2.28	1.41	1.36
2	A	301[A]	KSJ	C05-C07	2.20	1.53	1.49
2	A	301[A]	KSJ	O10-C06	2.19	1.40	1.36
2	B	301[A]	KSJ	C11-C07	2.18	1.55	1.52
3	A	302[B]	KSP	O10-C06	2.17	1.40	1.36
2	B	301[A]	KSJ	C05-C07	2.16	1.52	1.49
2	C	301[A]	KSJ	O17-C07	-2.10	1.19	1.22
2	C	301[A]	KSJ	C05-C07	2.09	1.52	1.49
3	B	302[B]	KSP	C14-C15	2.07	1.60	1.51
3	D	302[B]	KSP	O10-C06	2.00	1.40	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[B]	KSP	C06-C05-C07	-11.50	113.40	119.57
3	D	302[B]	KSP	C06-C05-C07	-10.95	113.69	119.57
3	C	302[B]	KSP	C06-C05-C07	-8.56	114.98	119.57
3	B	302[B]	KSP	C06-C05-C07	-8.51	115.01	119.57
2	D	301[A]	KSJ	C06-C05-C07	-5.01	116.88	119.57
3	B	302[B]	KSP	O17-C07-C05	-4.81	113.40	120.62
2	C	301[A]	KSJ	C15-C12-C11	4.44	109.73	103.34
3	A	302[B]	KSP	O17-C07-C05	-4.08	114.49	120.62
3	C	302[B]	KSP	C15-C12-C08	-3.94	106.62	113.67
3	A	302[B]	KSP	O17-C07-C11	-3.77	115.48	120.28
3	C	302[B]	KSP	O17-C07-C11	-3.71	115.56	120.28
3	D	302[B]	KSP	O17-C07-C05	-3.57	115.26	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[A]	KSJ	C15-C12-C11	3.46	108.32	103.34
2	B	301[A]	KSJ	C15-C12-C11	3.30	108.09	103.34
3	B	302[B]	KSP	O17-C07-C11	-3.15	116.28	120.28
3	A	302[B]	KSP	C04-C05-C07	3.03	127.15	119.49
3	C	302[B]	KSP	O17-C07-C05	-2.85	116.34	120.62
3	B	302[B]	KSP	C14-C13-C11	-2.84	98.92	104.78
3	D	302[B]	KSP	C08-C12-C11	-2.84	108.17	114.74
2	C	301[A]	KSJ	C08-C12-C11	-2.83	108.18	114.74
3	D	302[B]	KSP	C04-C05-C07	2.77	126.48	119.49
2	C	301[A]	KSJ	C13-C11-C12	2.76	109.11	103.66
3	C	302[B]	KSP	C14-C13-C11	-2.75	99.12	104.78
2	D	301[A]	KSJ	C13-C11-C12	2.74	109.06	103.66
3	D	302[B]	KSP	O17-C07-C11	-2.73	116.80	120.28
3	B	302[B]	KSP	C01-C06-C05	2.68	122.77	119.89
3	B	302[B]	KSP	C15-C12-C08	-2.64	108.93	113.67
2	A	301[A]	KSJ	C13-C11-C12	2.62	108.83	103.66
2	B	301[A]	KSJ	C13-C11-C12	2.60	108.79	103.66
3	B	302[B]	KSP	C04-C05-C07	2.48	125.77	119.49
3	A	302[B]	KSP	C15-C12-C08	-2.48	109.23	113.67
2	B	301[A]	KSJ	C06-C05-C07	-2.46	118.25	119.57
3	A	302[B]	KSP	C01-C06-C05	2.45	122.53	119.89
3	C	302[B]	KSP	C04-C05-C07	2.45	125.68	119.49
3	D	302[B]	KSP	O10-C06-C05	-2.41	117.26	121.70
2	D	301[A]	KSJ	C08-C12-C11	-2.38	109.24	114.74
3	D	302[B]	KSP	C01-C06-C05	2.36	122.43	119.89
3	B	302[B]	KSP	C02-C01-C06	-2.35	117.08	120.05
2	D	301[A]	KSJ	O17-C07-C11	-2.33	117.32	120.28
3	D	302[B]	KSP	C13-C11-C12	2.33	108.25	103.66
2	A	301[A]	KSJ	C06-C05-C07	-2.33	118.32	119.57
2	A	301[A]	KSJ	C15-C12-C11	2.26	106.59	103.34
3	C	302[B]	KSP	C01-C06-C05	2.21	122.27	119.89
2	D	301[A]	KSJ	O10-C06-C05	-2.21	117.64	121.70
3	A	302[B]	KSP	C14-C13-C11	-2.18	100.29	104.78
2	D	301[A]	KSJ	C04-C05-C06	2.14	120.83	118.15
4	A	304	SO4	O4-S-O1	-2.12	98.22	109.31
3	D	302[B]	KSP	C15-C12-C11	2.12	106.40	103.34
3	A	302[B]	KSP	O10-C06-C05	-2.11	117.81	121.70
3	C	302[B]	KSP	O10-C06-C05	-2.04	117.95	121.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

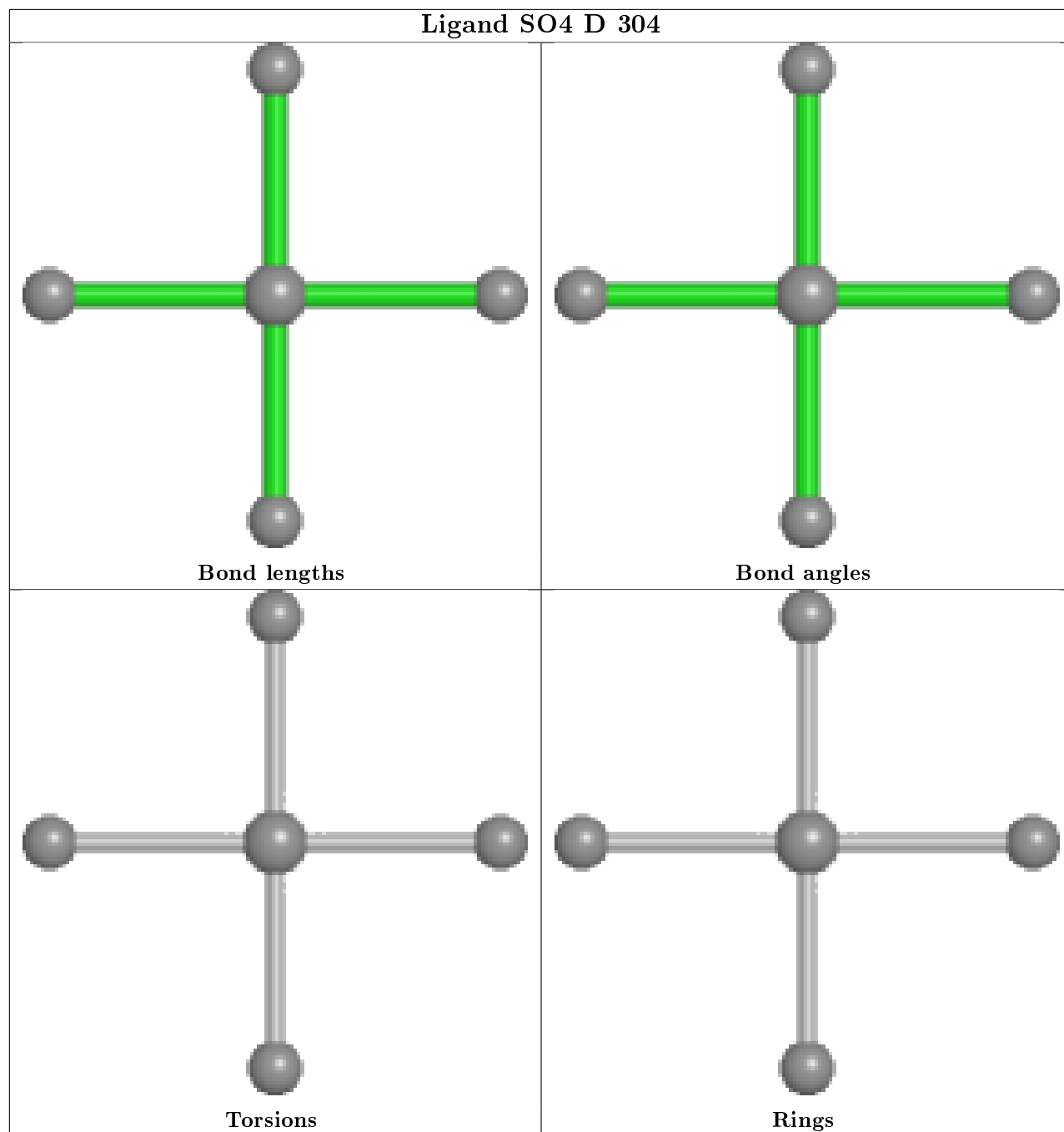
Mol	Chain	Res	Type	Atoms
3	D	302[B]	KSP	C09-C08-C12-C11
3	D	302[B]	KSP	C09-C08-C12-C15
3	B	302[B]	KSP	C05-C07-C11-C13
3	A	302[B]	KSP	C05-C07-C11-C13
3	A	302[B]	KSP	C09-C08-C12-C11
3	D	302[B]	KSP	C05-C07-C11-C13
3	D	302[B]	KSP	O17-C07-C11-C13

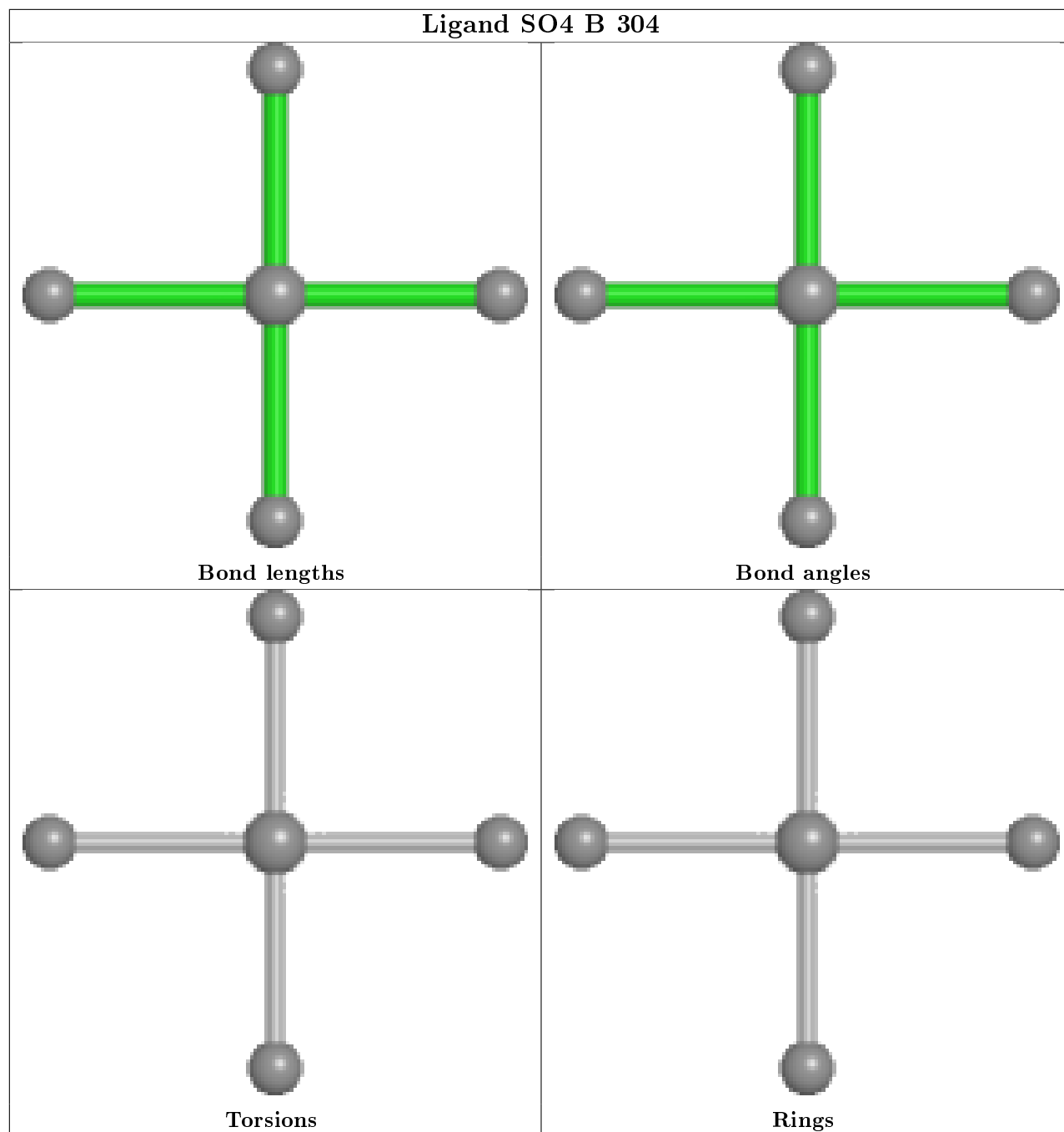
There are no ring outliers.

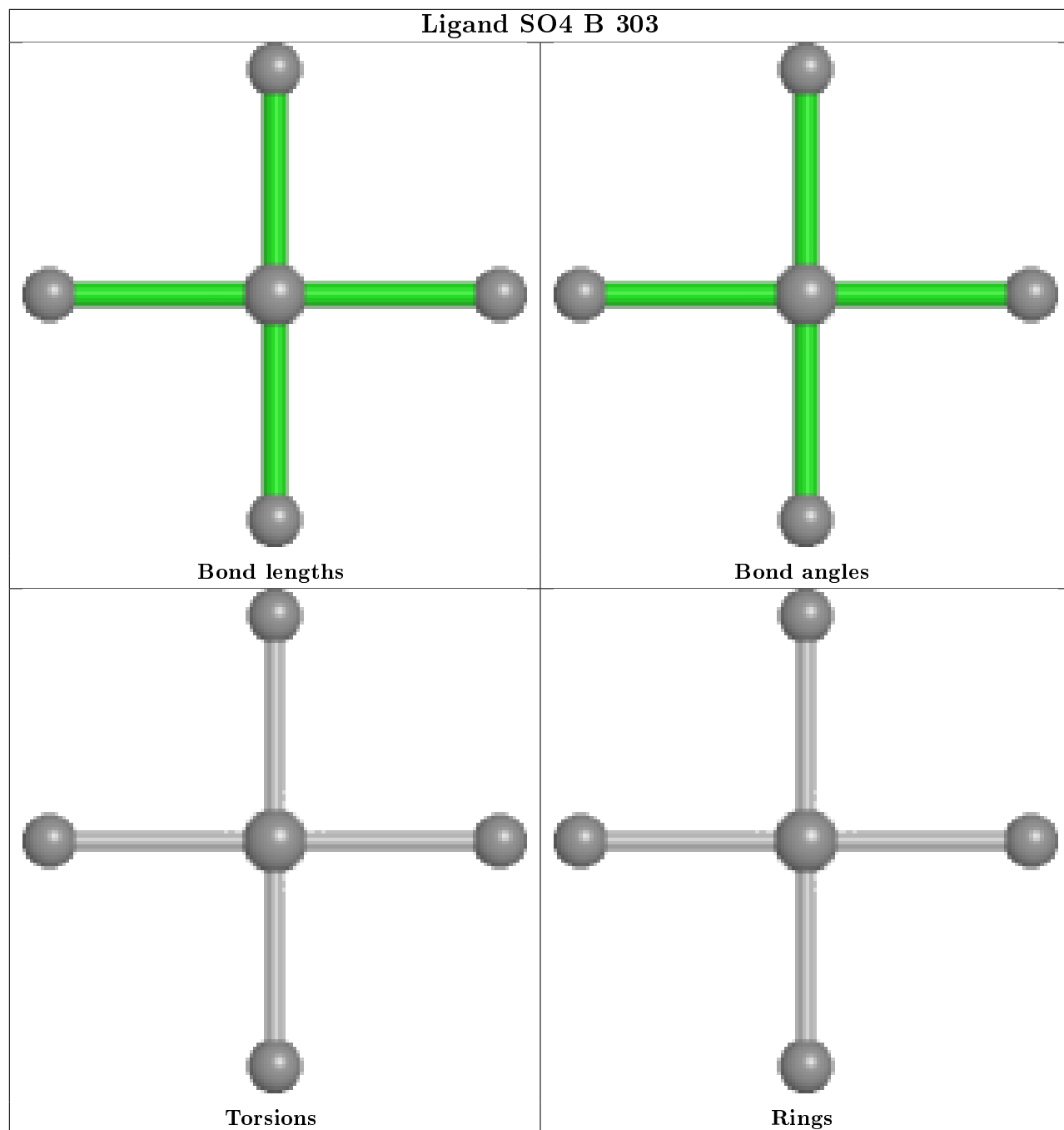
10 monomers are involved in 24 short contacts:

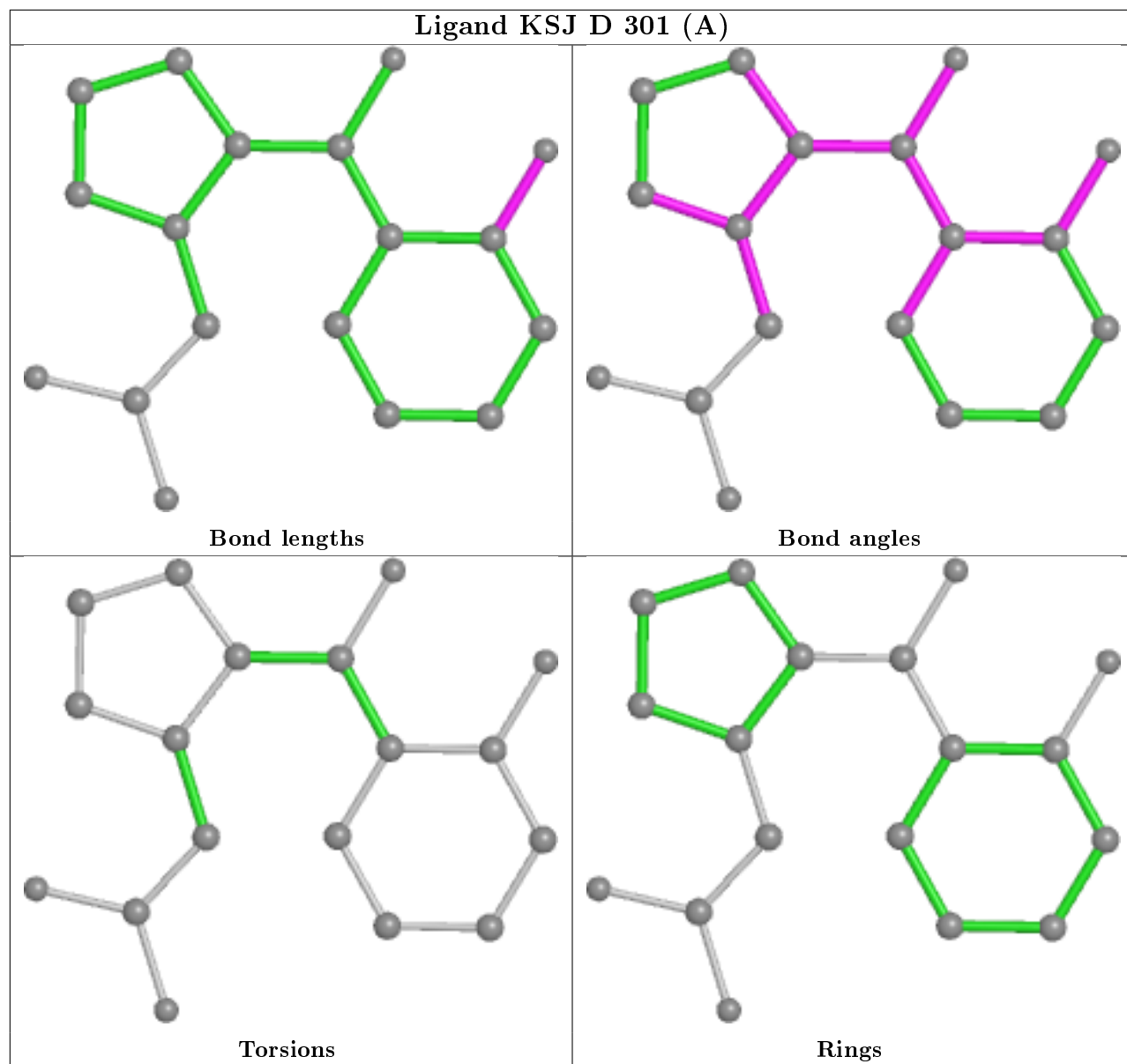
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	304	SO4	2	0
4	B	304	SO4	3	0
2	D	301[A]	KSJ	2	0
3	B	302[B]	KSP	2	0
4	A	304	SO4	2	0
3	A	302[B]	KSP	1	0
3	C	302[B]	KSP	2	0
2	C	301[A]	KSJ	1	0
3	D	302[B]	KSP	3	0
4	C	304	SO4	6	0

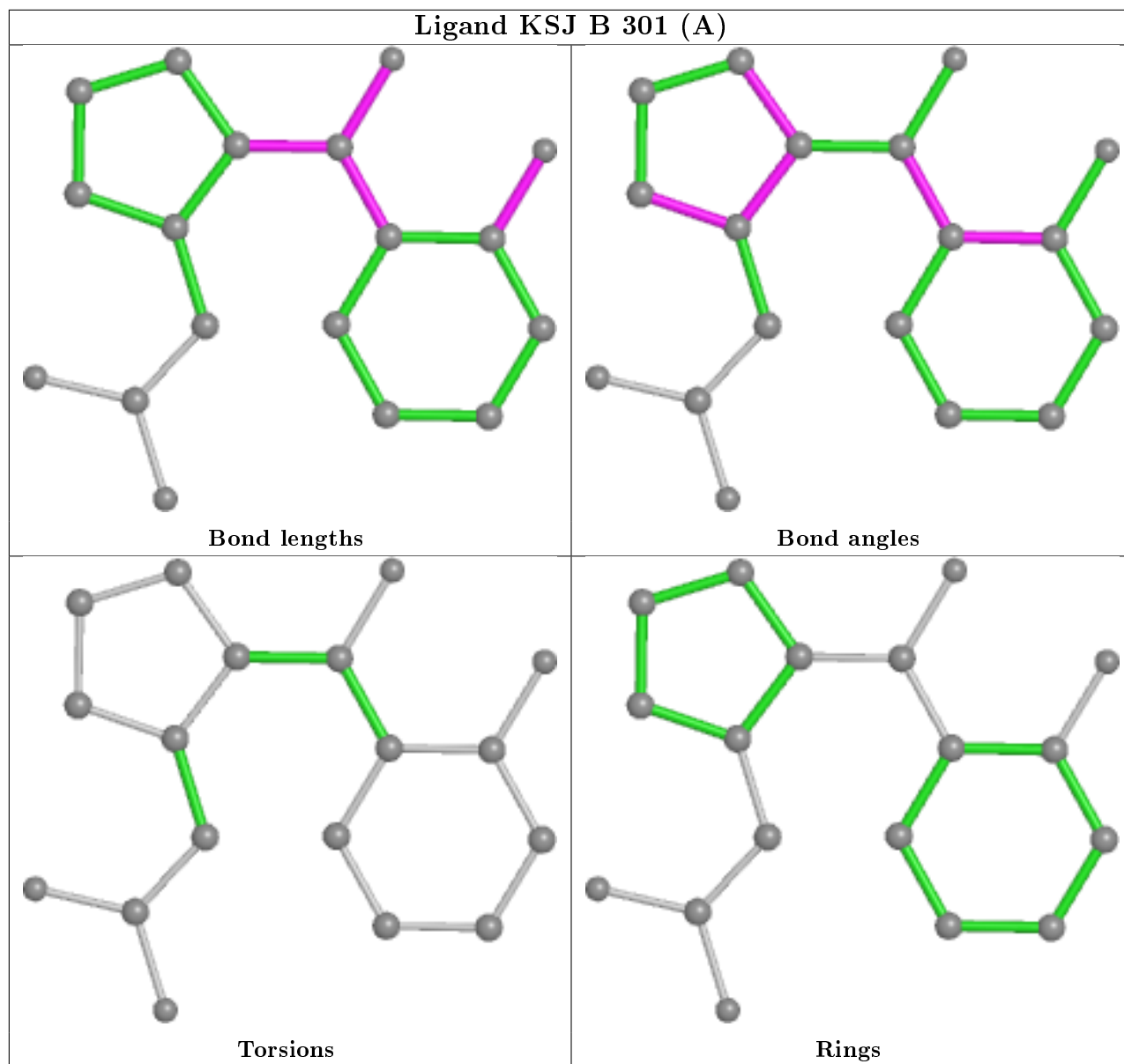
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

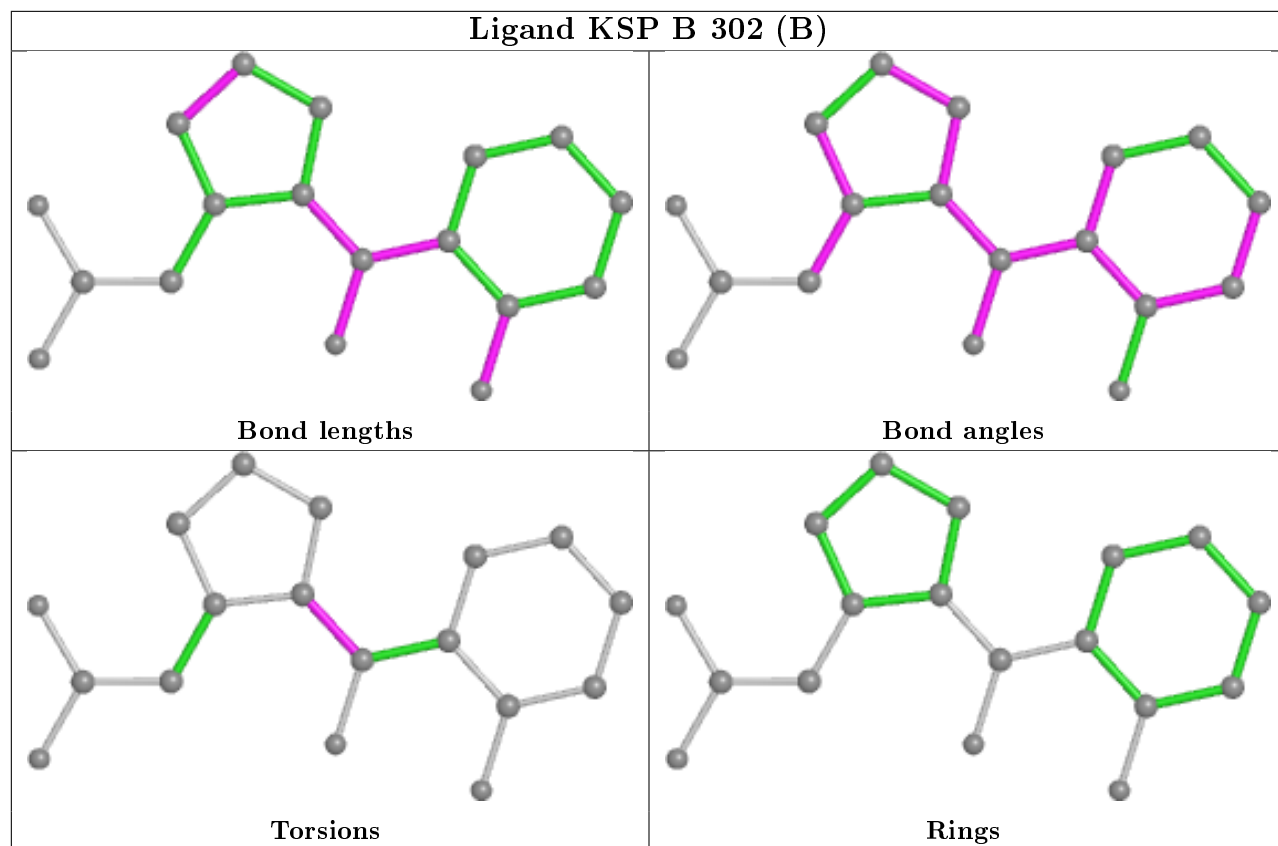




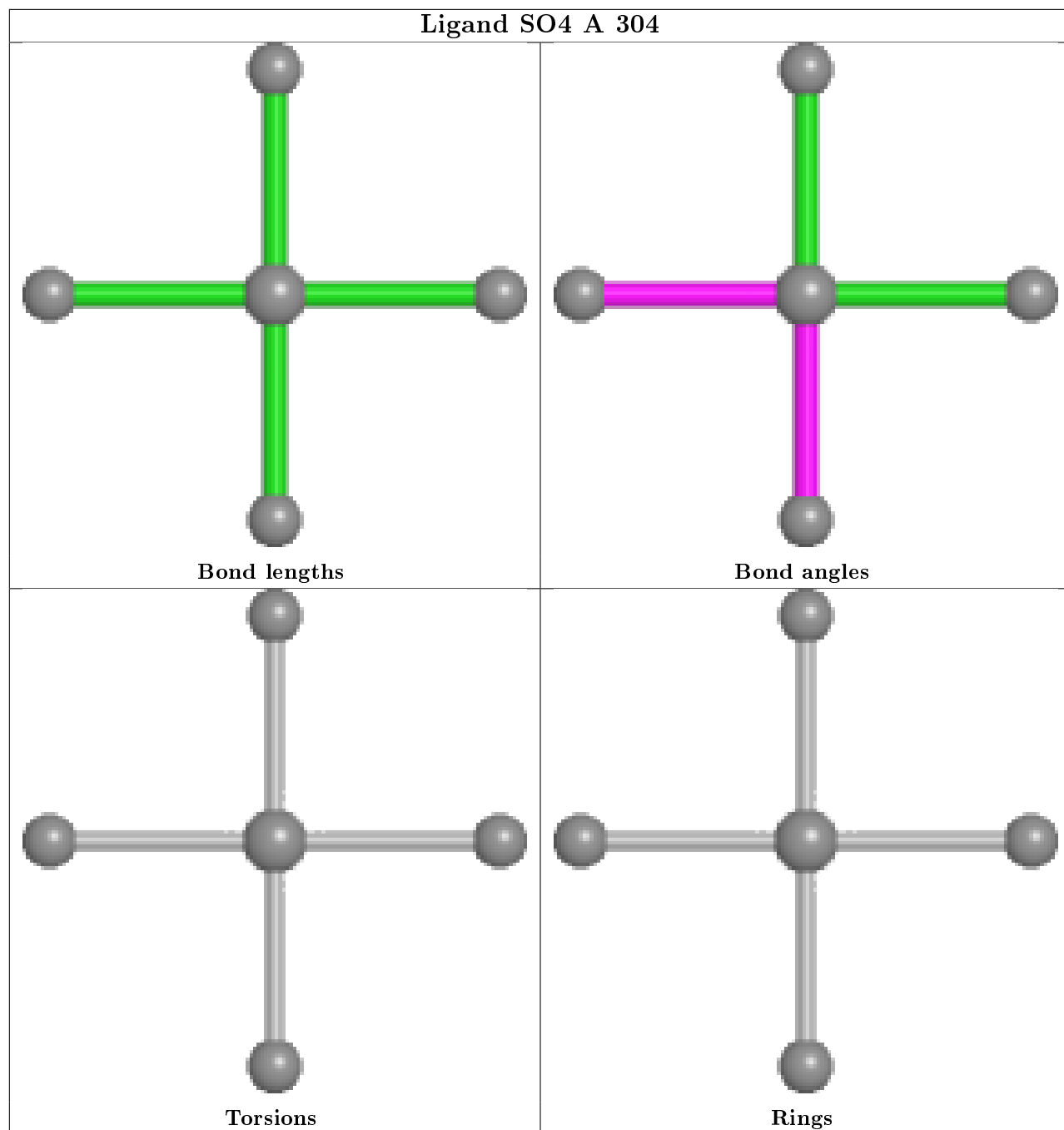


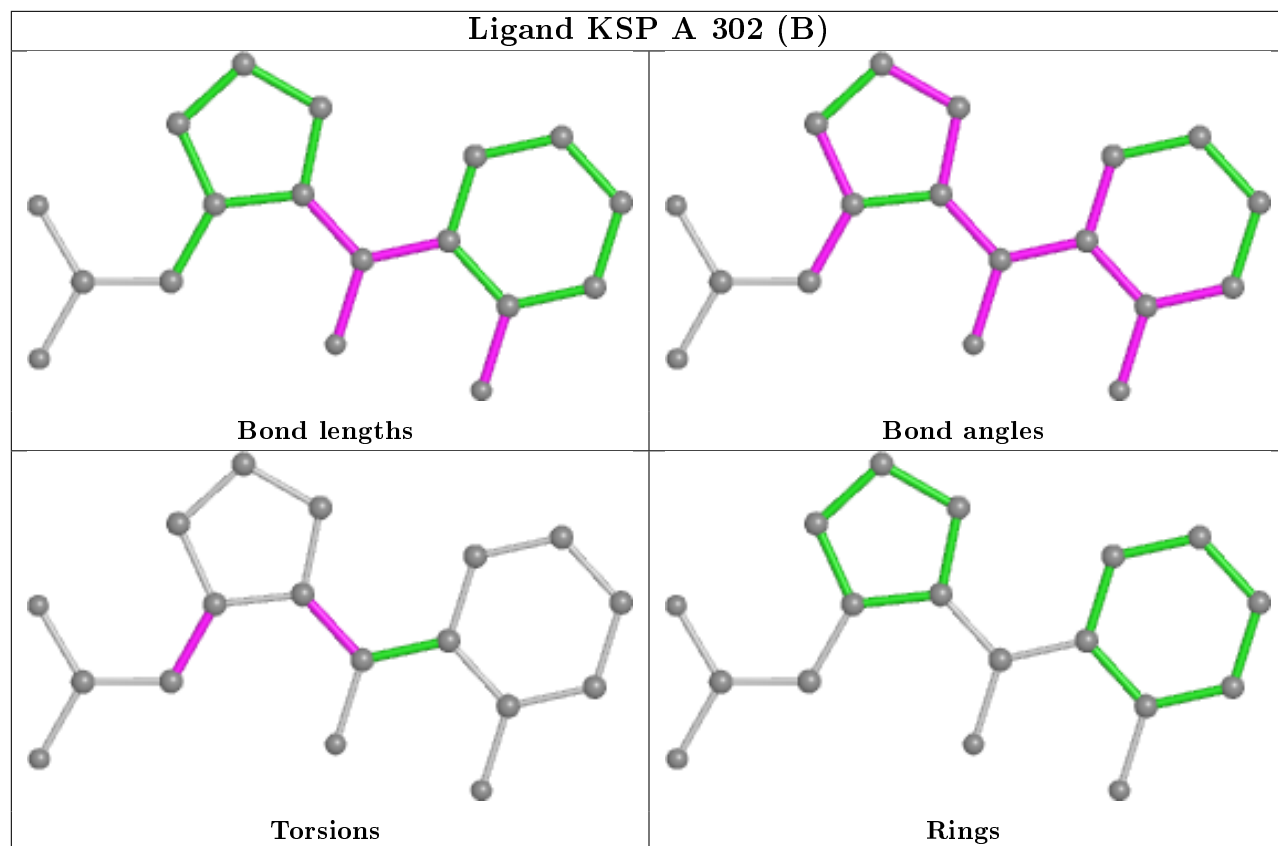


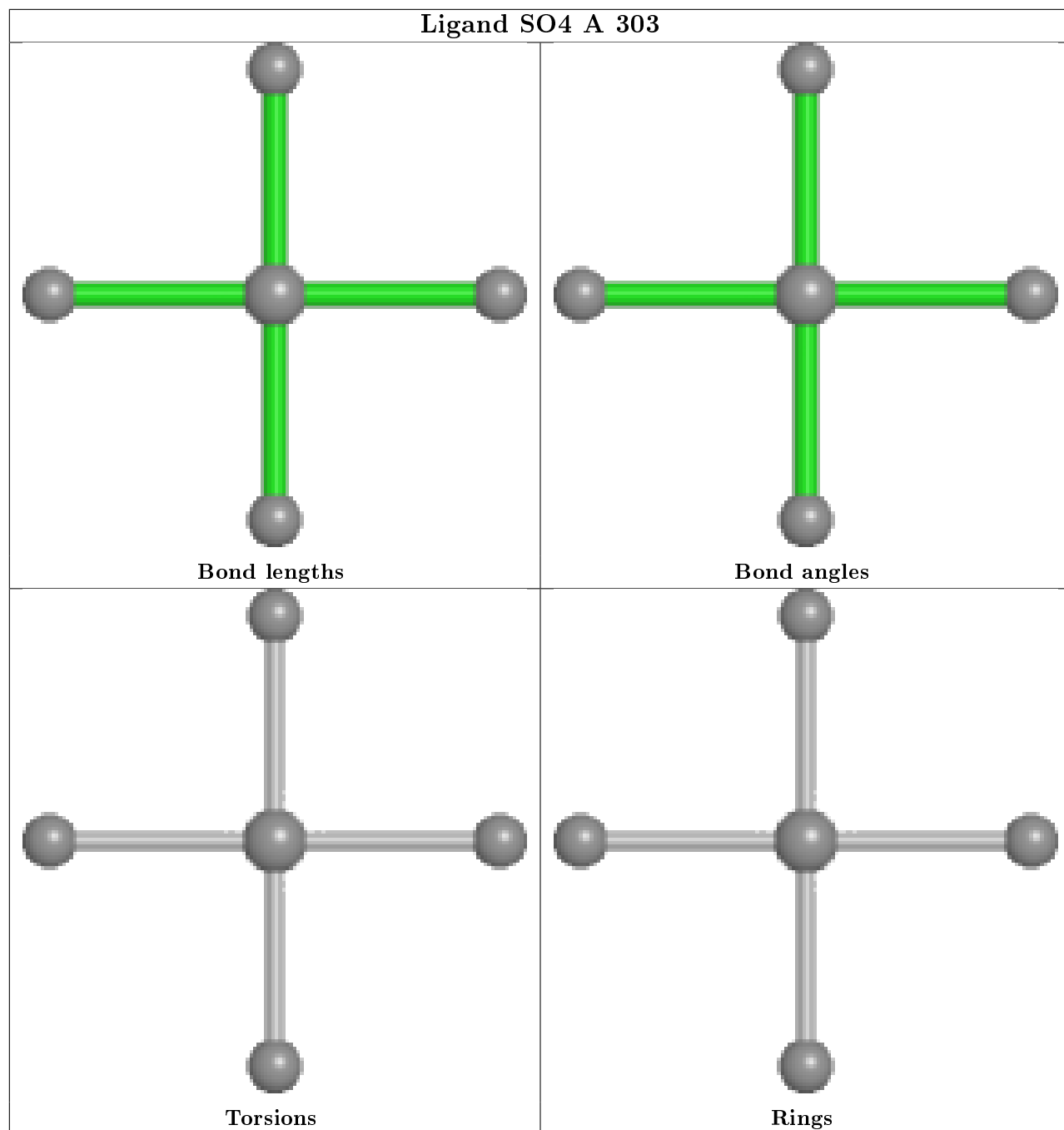


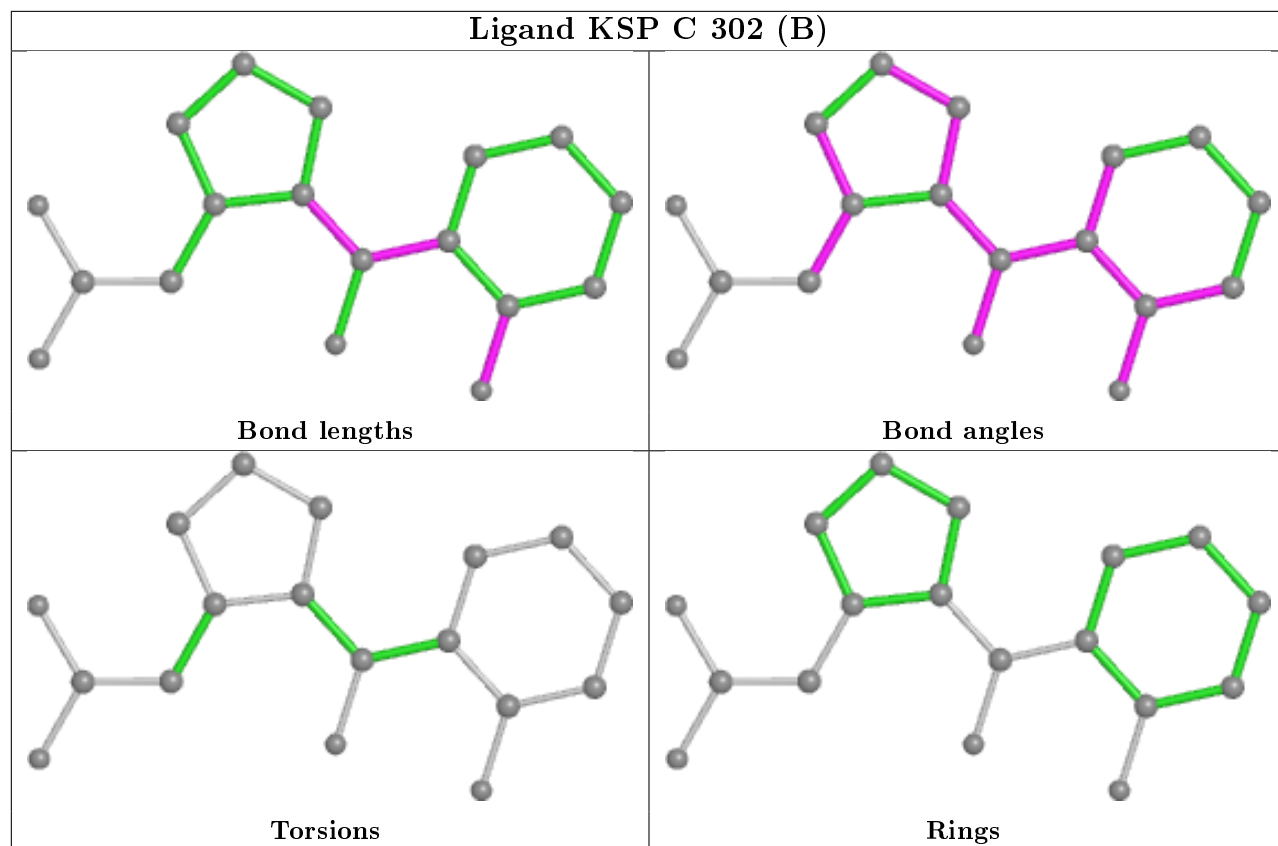


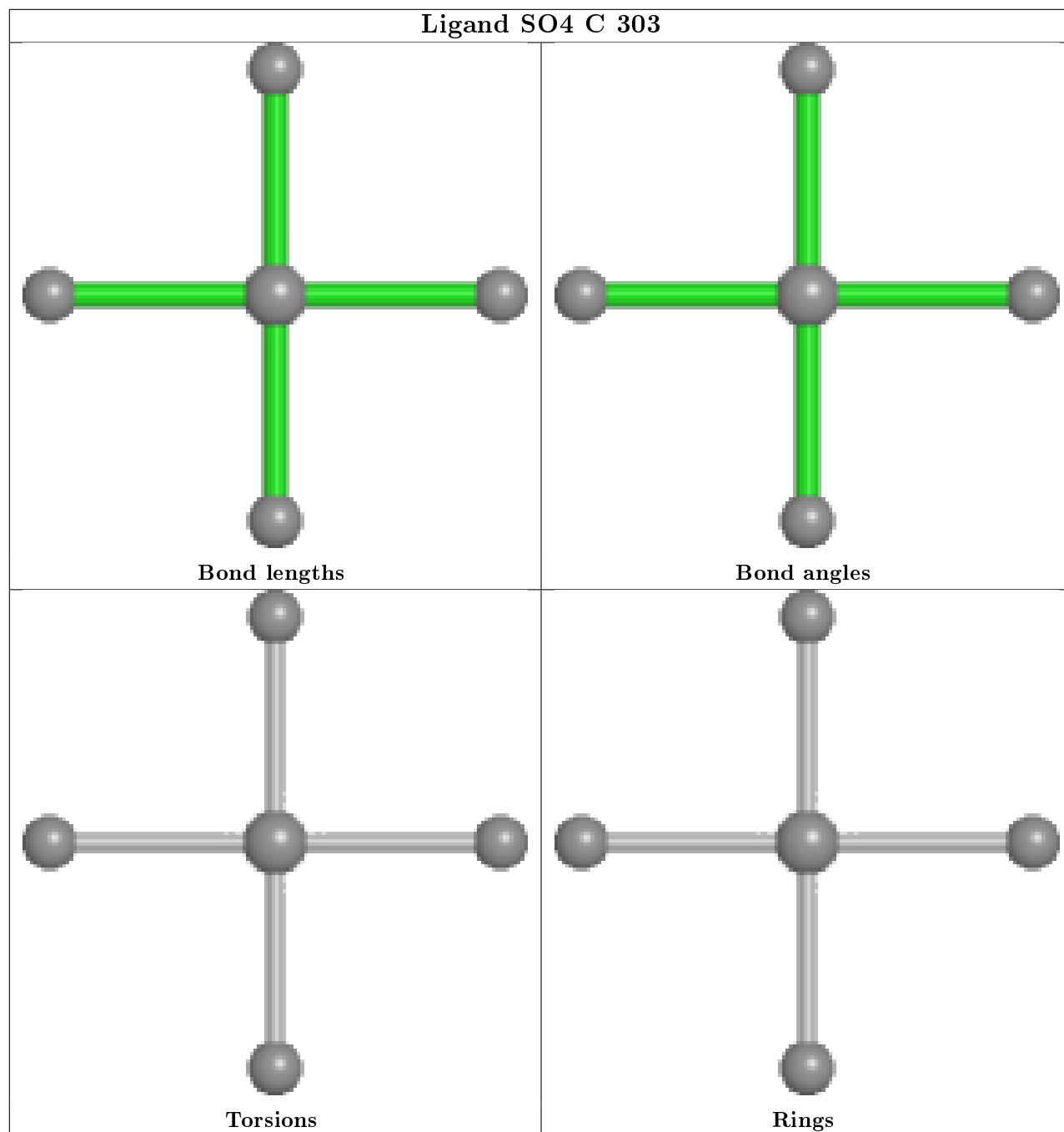


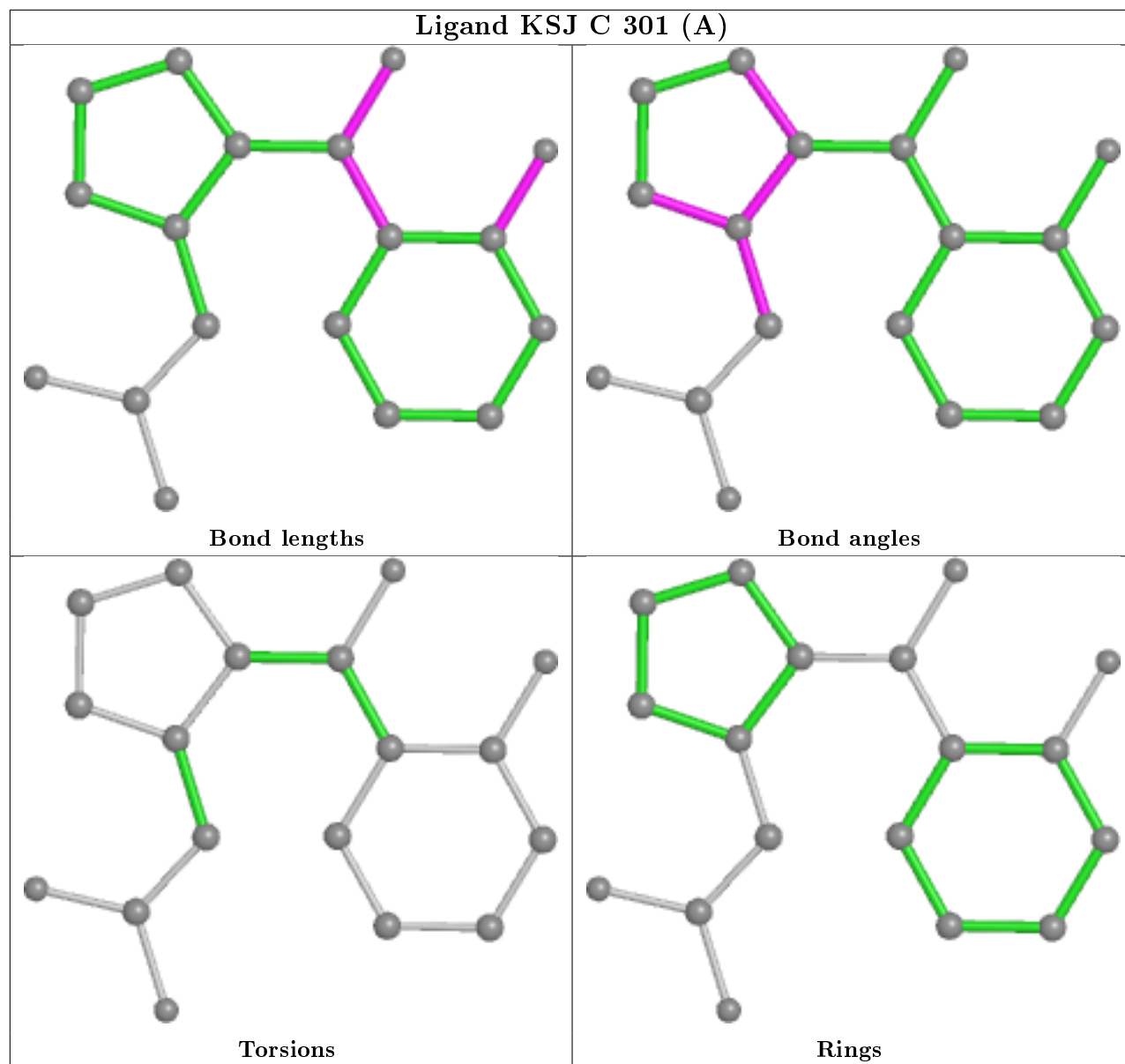


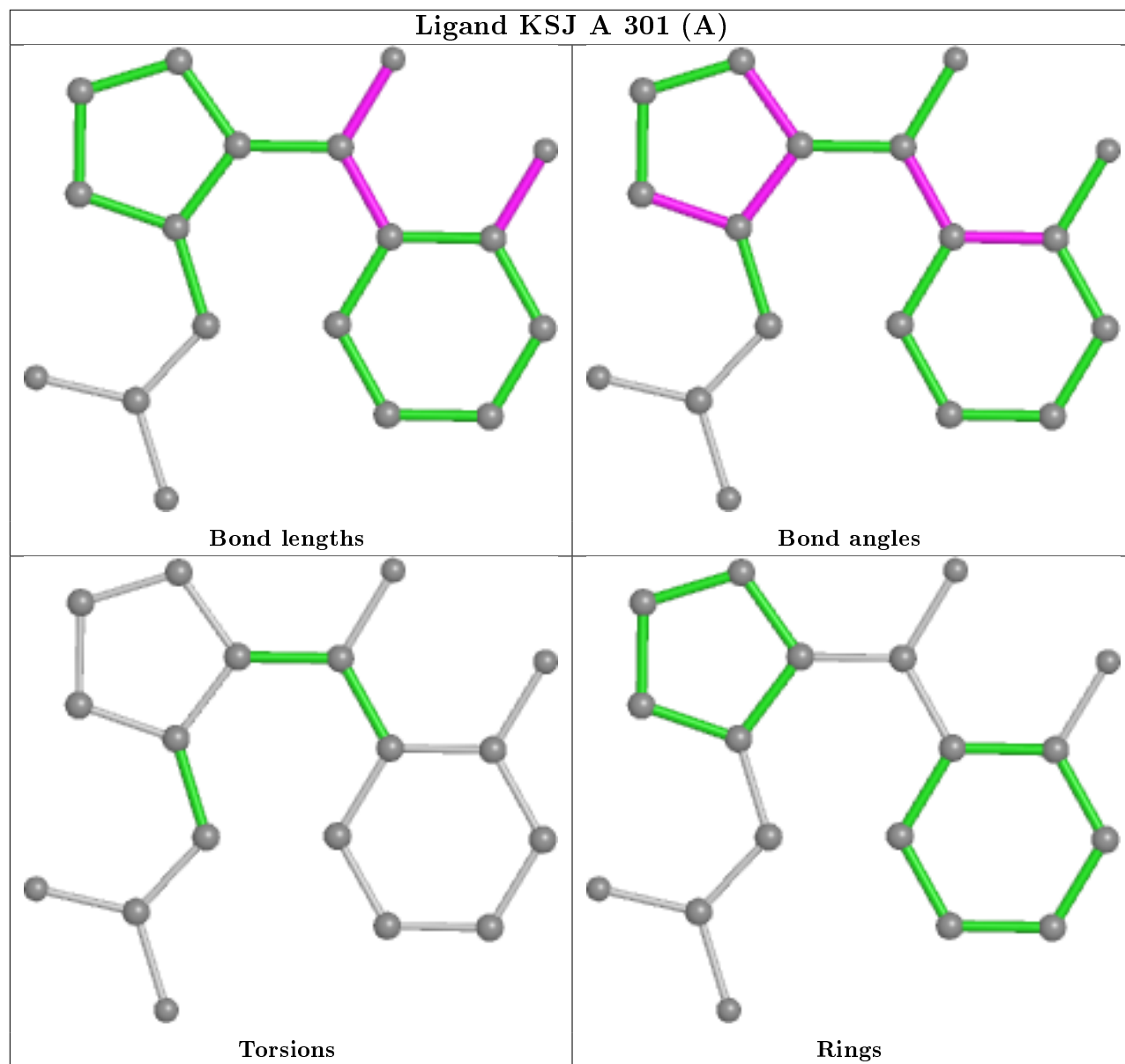


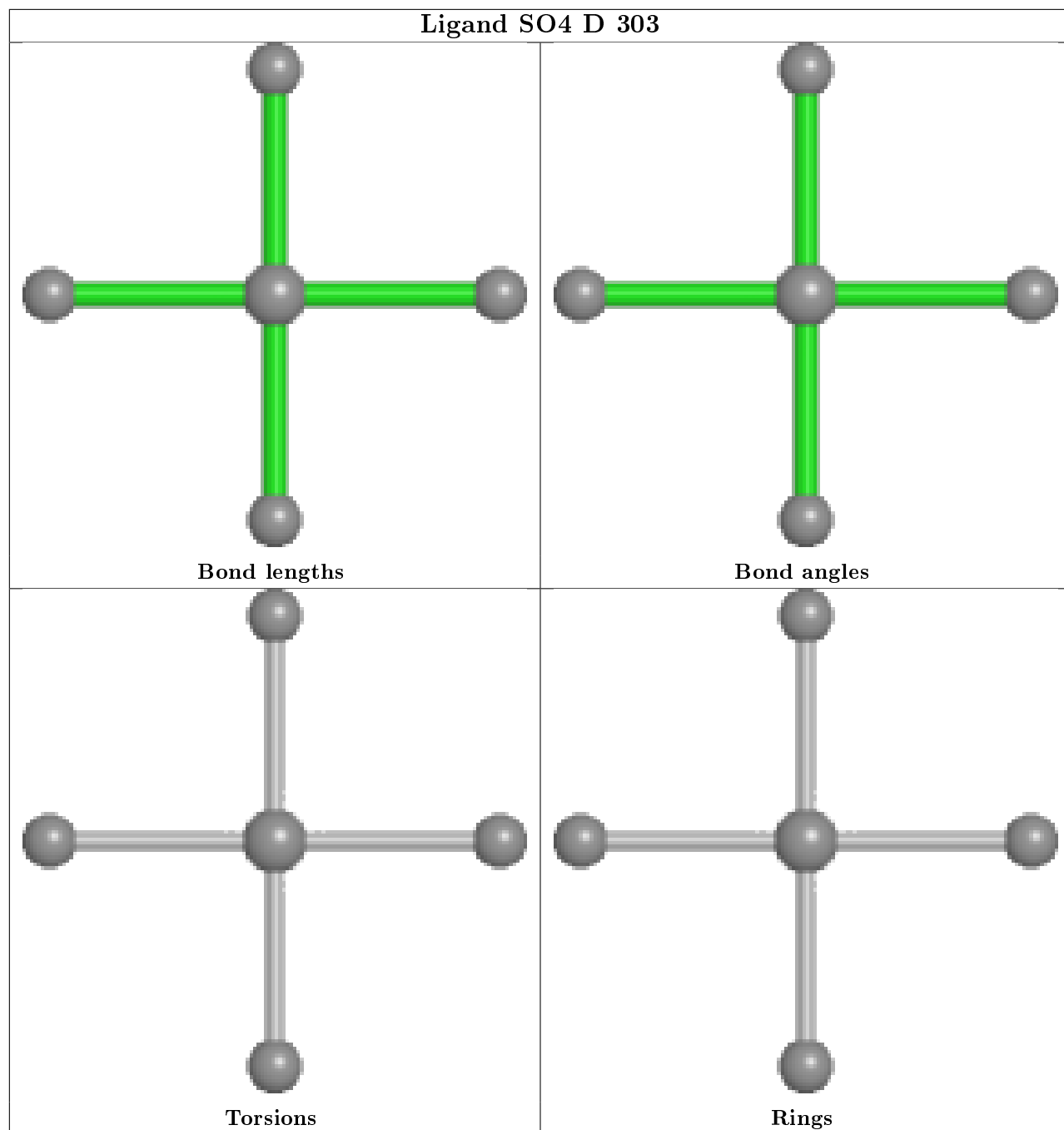




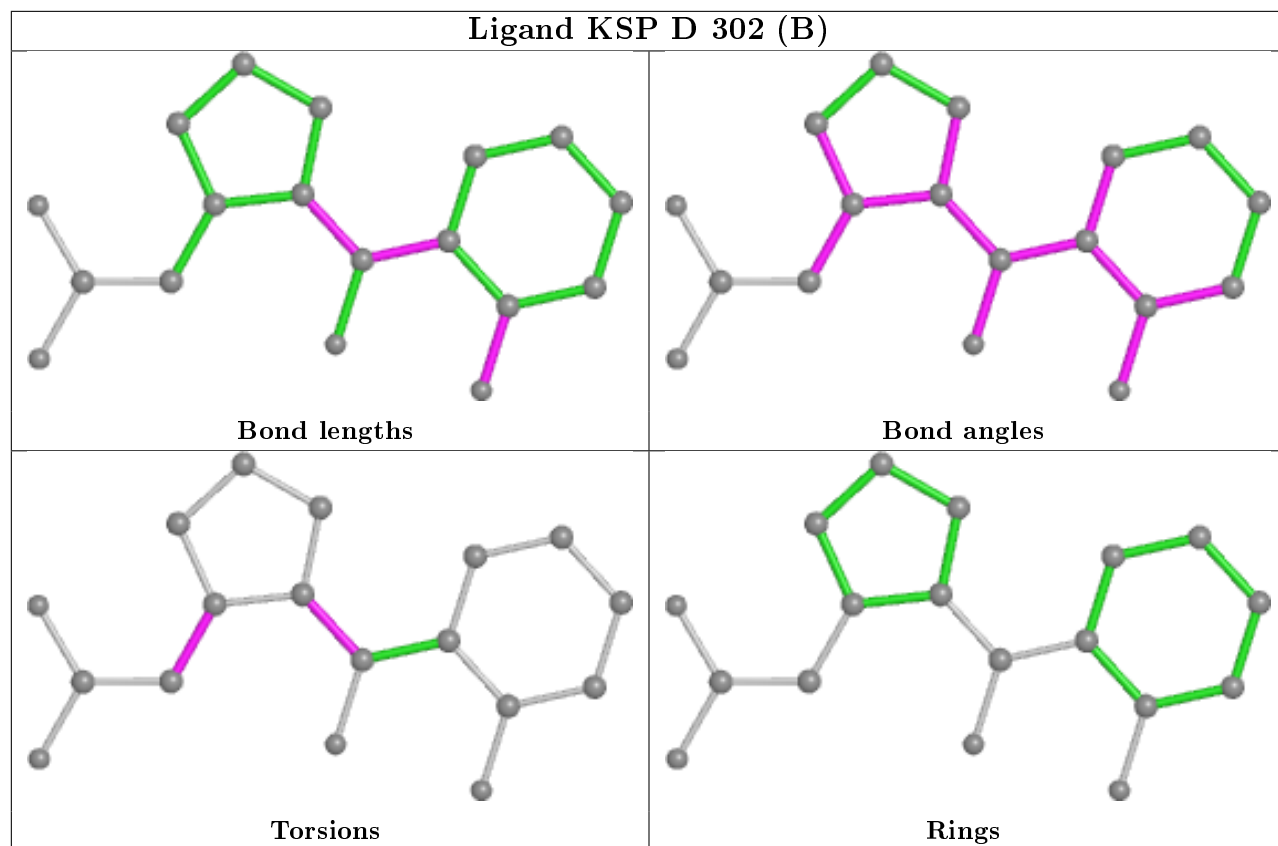


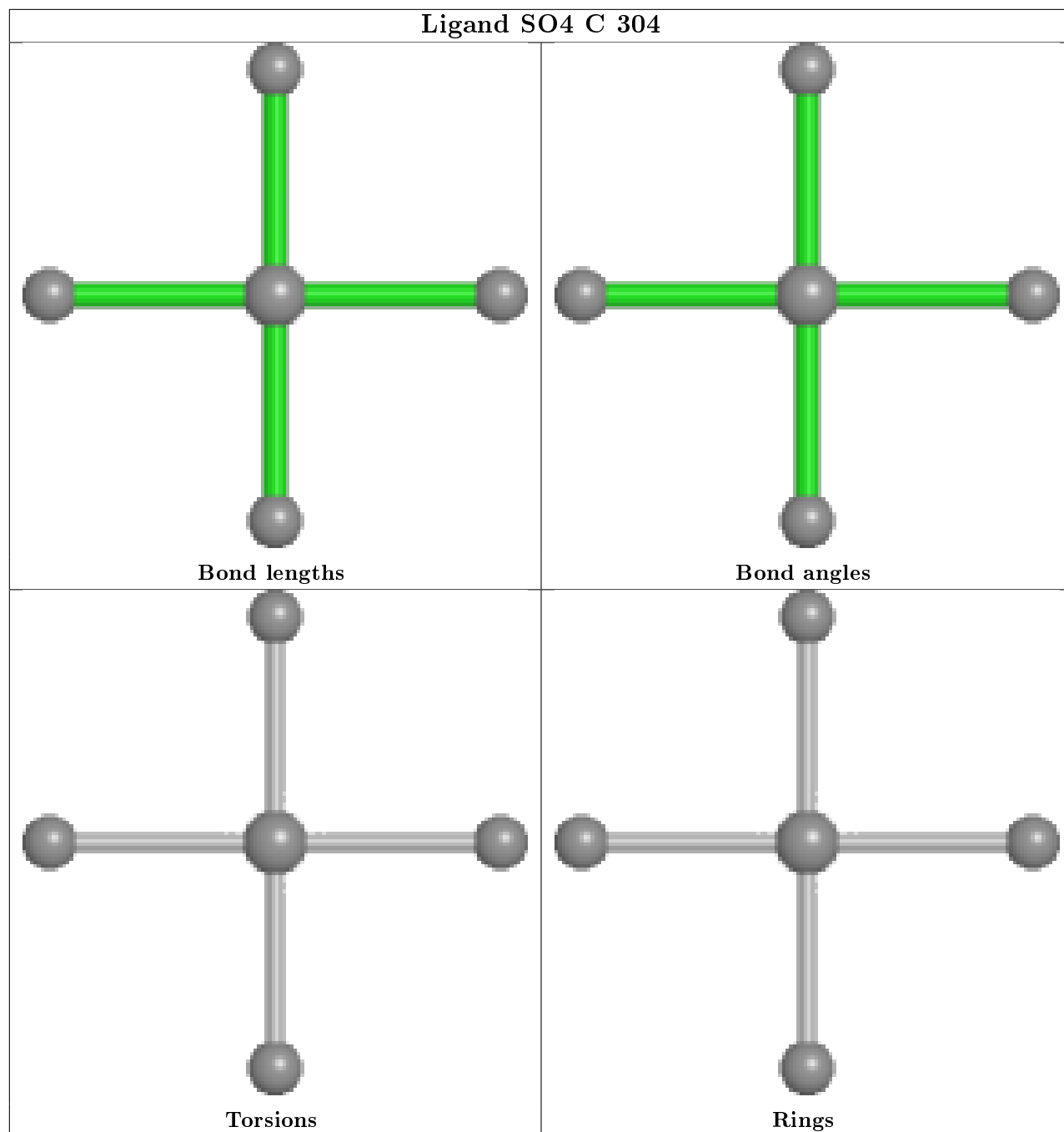












### 5.7 Other polymers [i](#)

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	227/233 (97%)	0.21	7 (3%) 49 51	16, 28, 62, 85	1 (0%)
1	B	226/233 (96%)	0.09	2 (0%) 84 85	18, 32, 52, 71	0
1	C	229/233 (98%)	0.62	21 (9%) 9 10	25, 48, 75, 88	0
1	D	227/233 (97%)	0.22	5 (2%) 62 64	25, 40, 69, 83	1 (0%)
All	All	909/932 (97%)	0.28	35 (3%) 39 42	16, 37, 70, 88	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	ARG	3.7
1	D	177	LEU	3.5
1	A	177	LEU	3.1
1	D	171	TRP	3.1
1	D	-1	HIS	2.9
1	C	222	ALA	2.8
1	C	22	LEU	2.8
1	B	218	ARG	2.8
1	C	25	ALA	2.8
1	C	224	LEU	2.6
1	A	171	TRP	2.6
1	A	218	ARG	2.5
1	C	101	PRO	2.5
1	A	178	VAL	2.5
1	C	-1	HIS	2.4
1	C	226	GLY	2.4
1	C	29	ALA	2.4
1	C	27	ARG	2.4
1	C	91	ILE	2.4
1	C	57	ALA	2.3
1	C	94	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASP	2.3
1	C	26	ALA	2.3
1	C	61	GLN	2.2
1	C	3	ILE	2.2
1	A	174	PRO	2.2
1	C	98	LEU	2.1
1	D	120	PRO	2.1
1	C	31	ILE	2.1
1	D	224	LEU	2.1
1	C	216	PHE	2.1
1	C	225	VAL	2.1
1	C	210	ALA	2.0
1	B	173	ASP	2.0
1	A	219	ASN	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 carbohydrates 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.

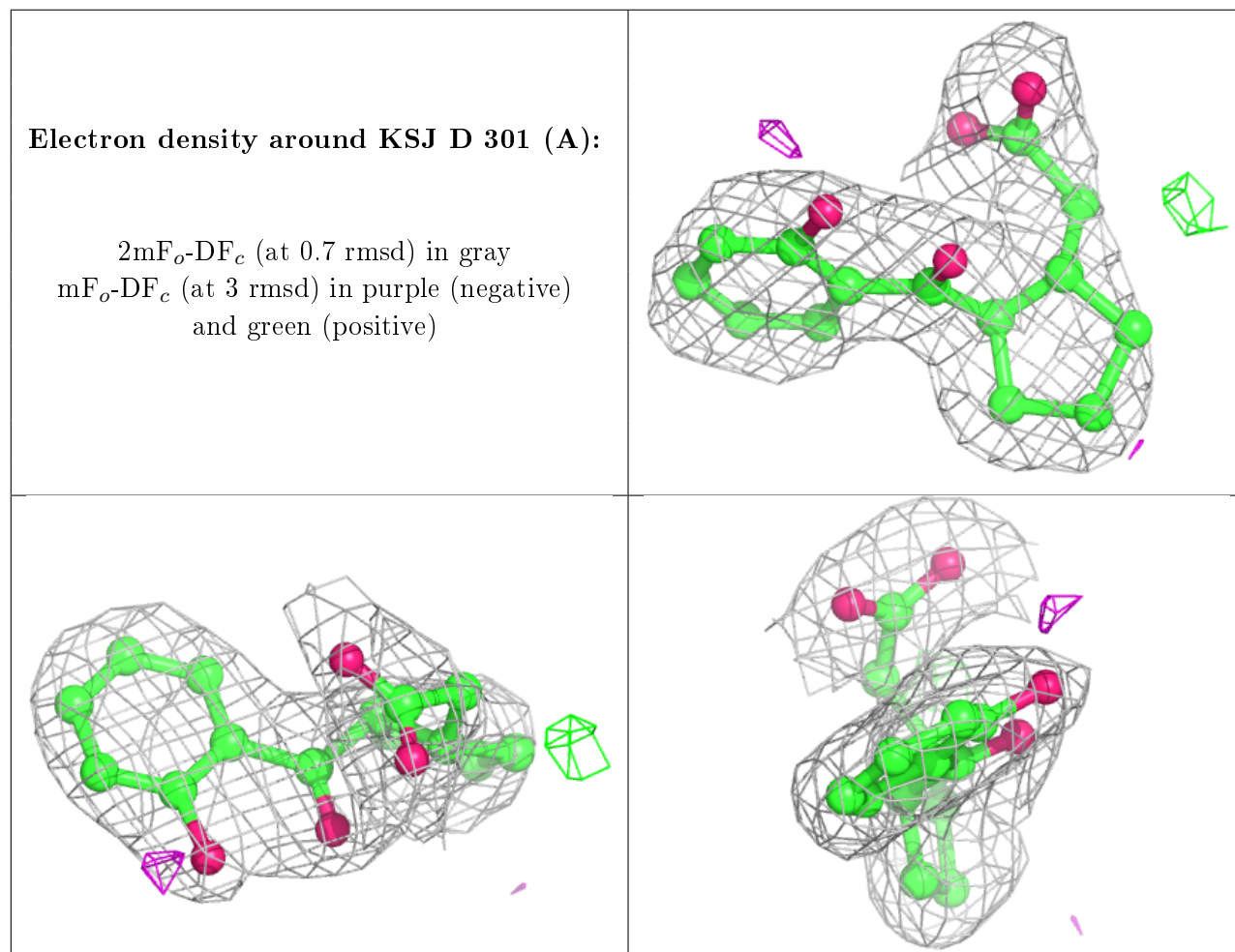
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	KSJ	D	301[A]	18/18	0.90	0.14	30,35,41,41	18
3	KSP	D	302[B]	18/18	0.90	0.16	31,37,40,41	18
4	SO4	A	304	5/5	0.92	0.30	19,20,39,44	5
2	KSJ	C	301[A]	18/18	0.92	0.13	28,36,41,47	18
4	SO4	D	304	5/5	0.92	0.26	25,35,41,44	5
3	KSP	C	302[B]	18/18	0.93	0.16	32,36,41,47	18
3	KSP	B	302[B]	18/18	0.93	0.14	28,32,39,39	18
2	KSJ	B	301[A]	18/18	0.93	0.13	27,32,38,39	18
2	KSJ	A	301[A]	18/18	0.94	0.11	22,25,29,29	18

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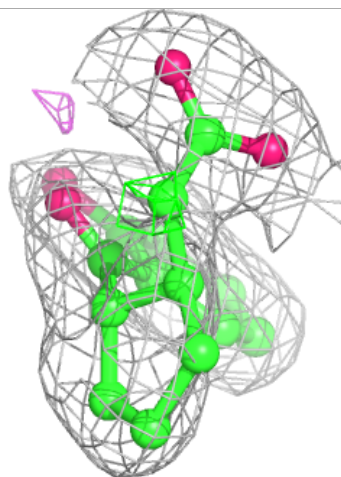
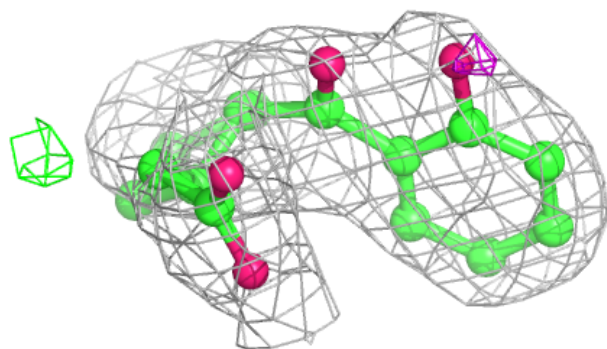
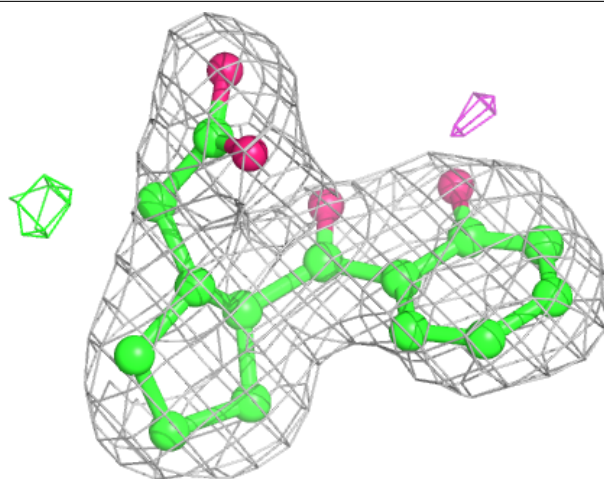
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	KSP	A	302[B]	18/18	0.95	0.12	22,27,30,31	18
4	SO4	B	304	5/5	0.96	0.24	10,22,31,37	5
4	SO4	C	304	5/5	0.98	0.23	15,27,36,38	5
4	SO4	B	303	5/5	0.99	0.11	21,21,27,28	0
4	SO4	D	303	5/5	0.99	0.08	27,32,35,36	0
4	SO4	C	303	5/5	0.99	0.11	27,29,34,41	0
4	SO4	A	303	5/5	0.99	0.10	12,17,21,22	5

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.



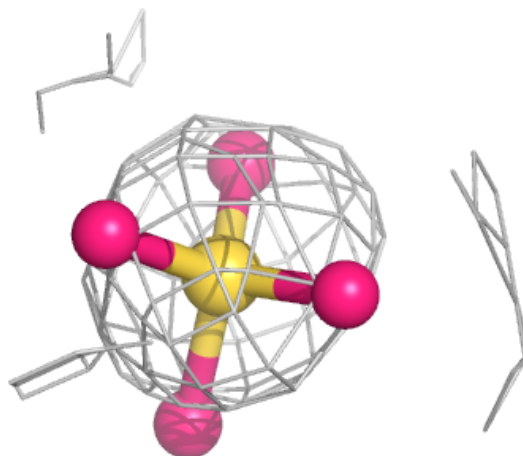
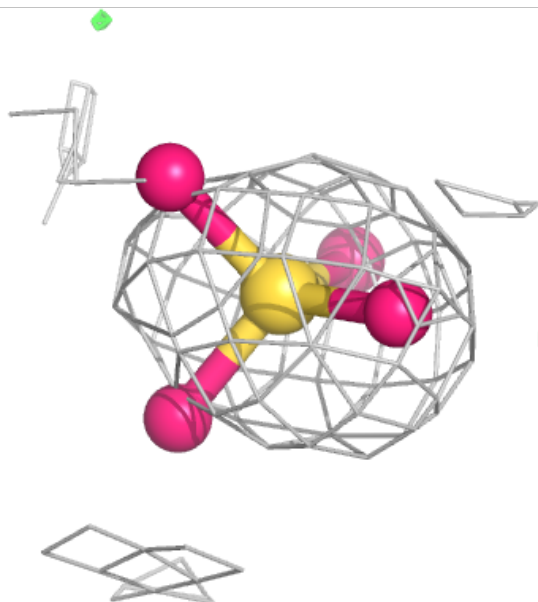
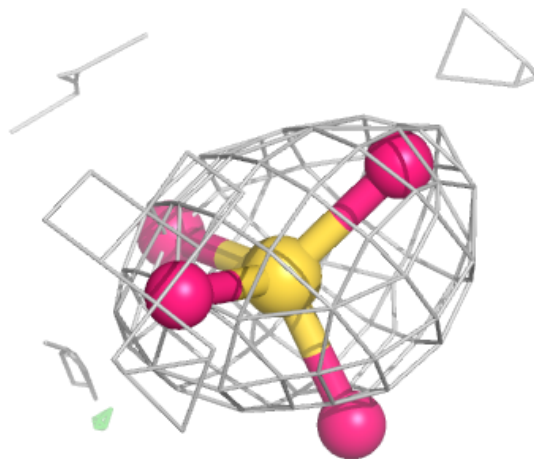
**Electron density around KSP D 302 (B):**

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



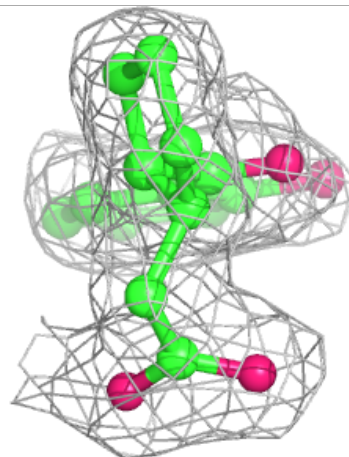
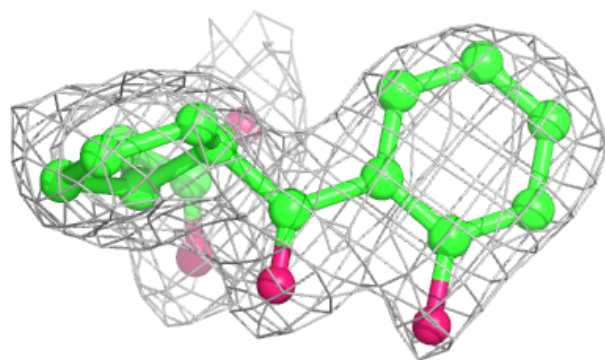
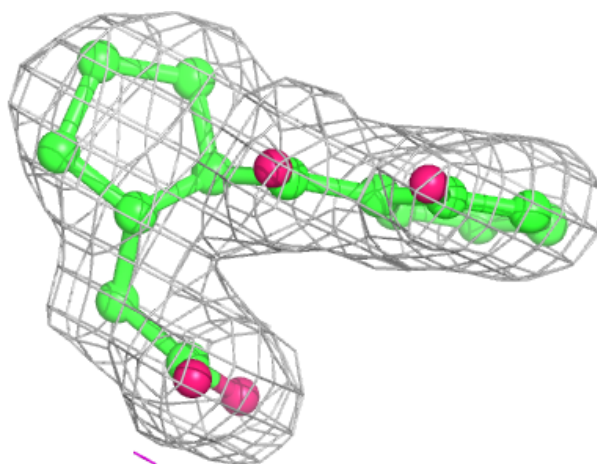
**Electron density around SO4 A 304:**

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



**Electron density around KSJ C 301 (A):**

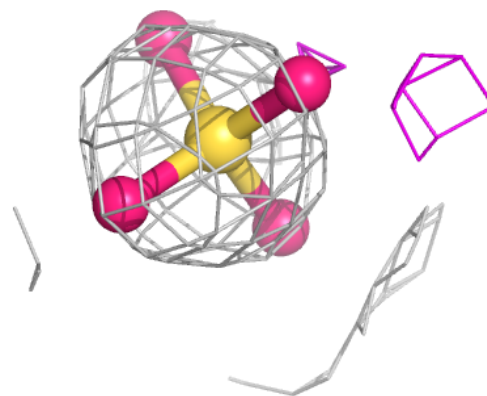
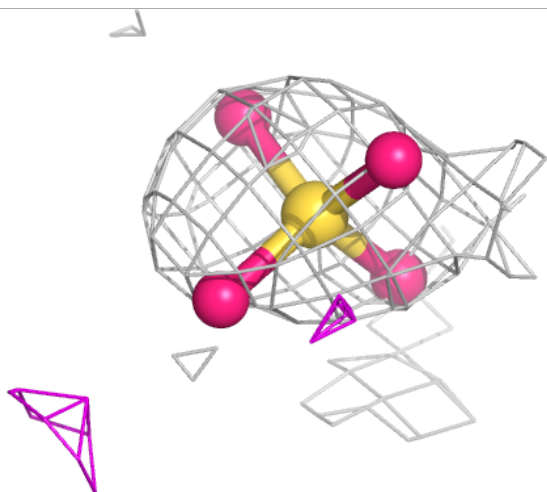
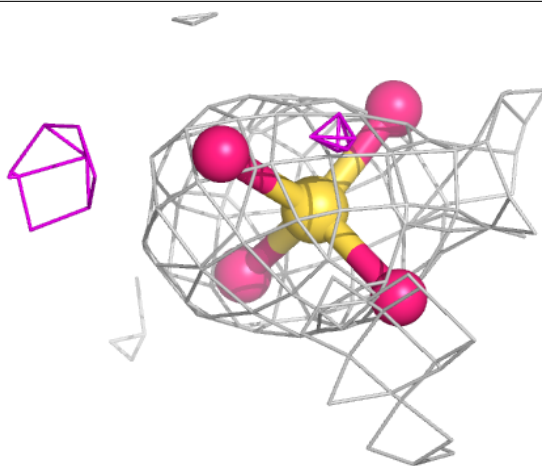
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





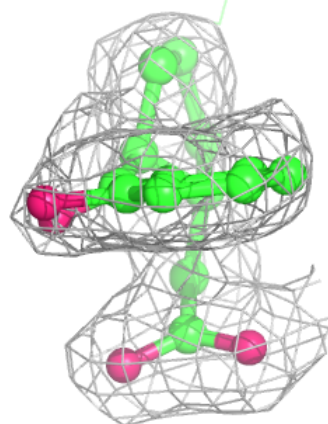
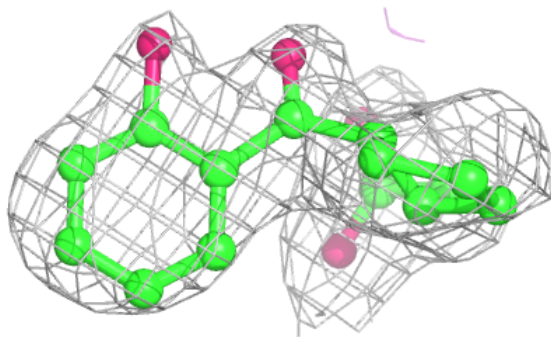
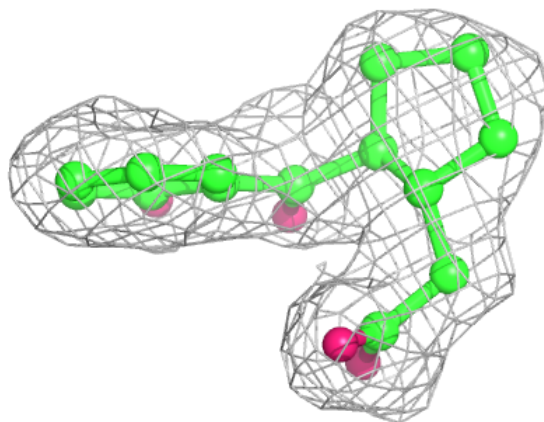
**Electron density around SO4 D 304:**

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



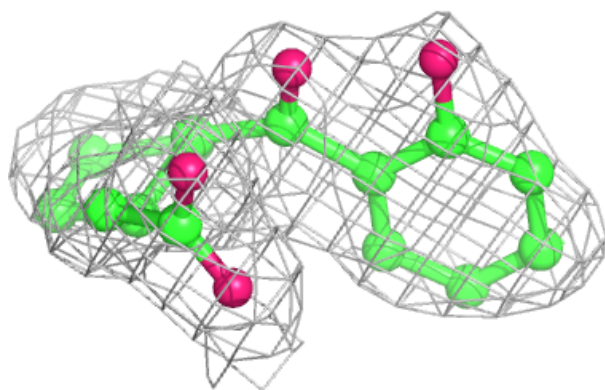
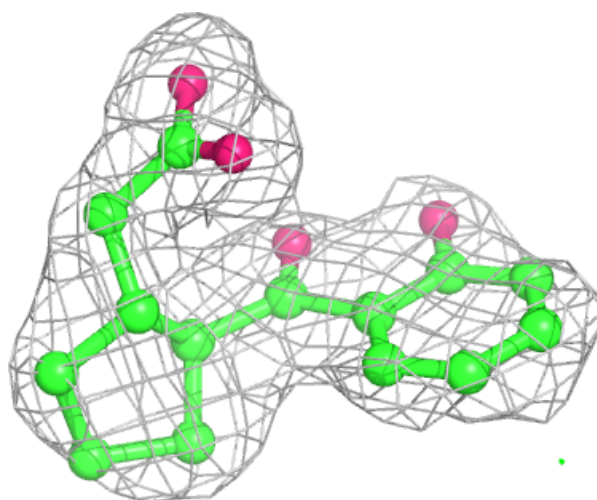
**Electron density around KSP C 302 (B):**

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



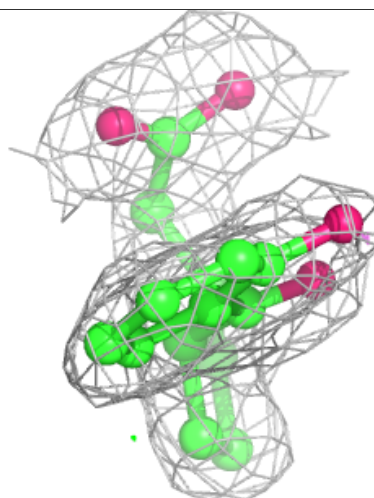
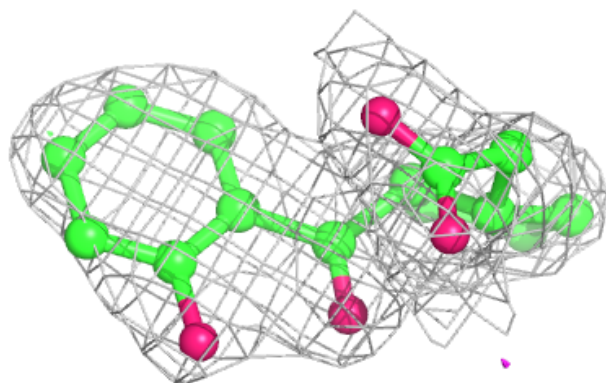
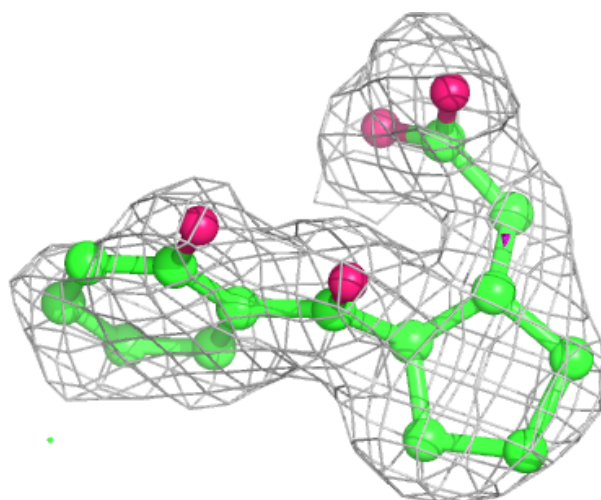
**Electron density around KSP B 302 (B):**

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



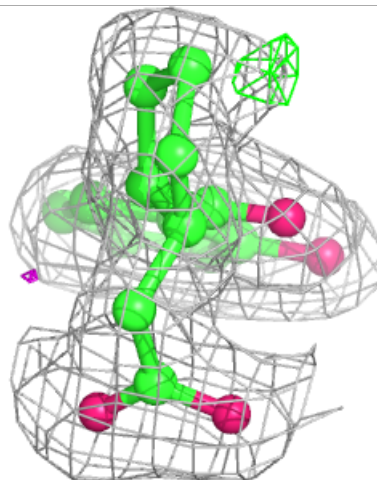
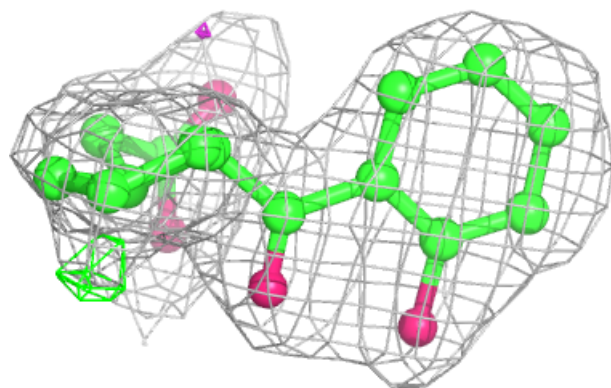
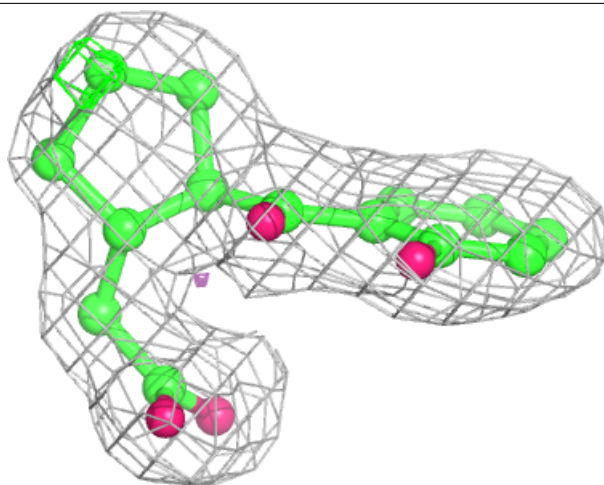
**Electron density around KSJ B 301 (A):**

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



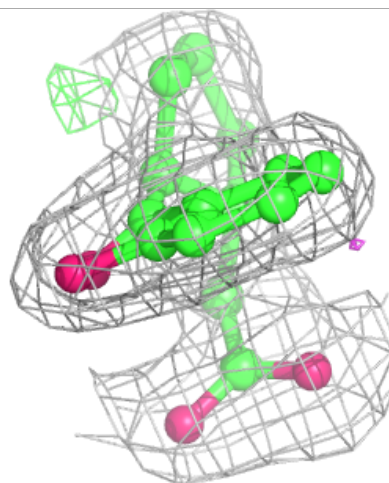
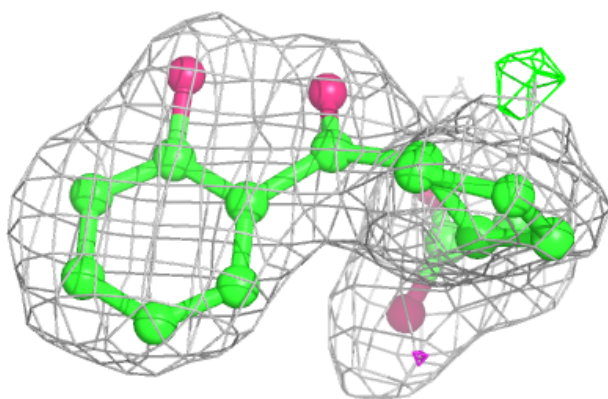
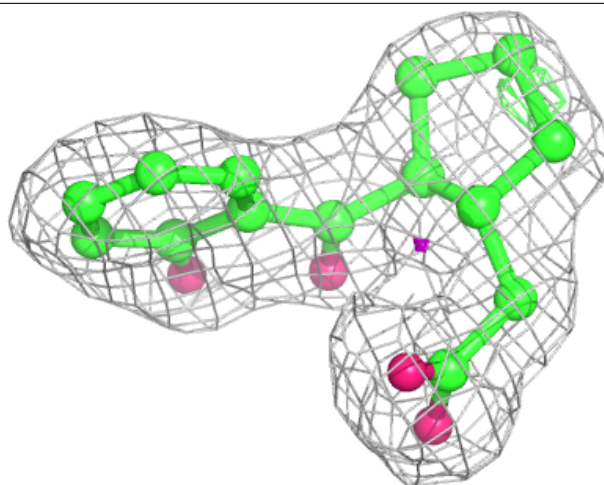
**Electron density around KSJ A 301 (A):**

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



**Electron density around KSP A 302 (B):**

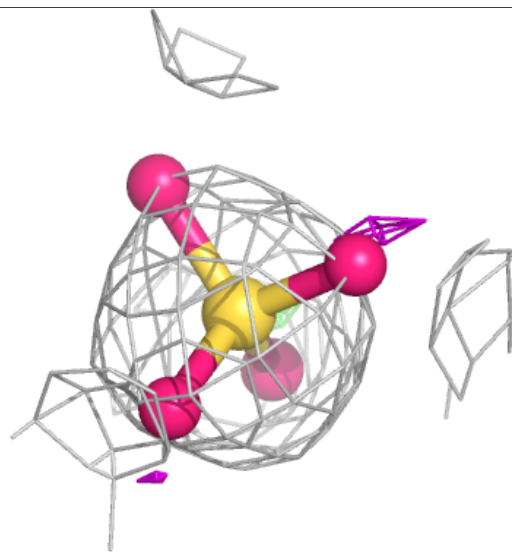
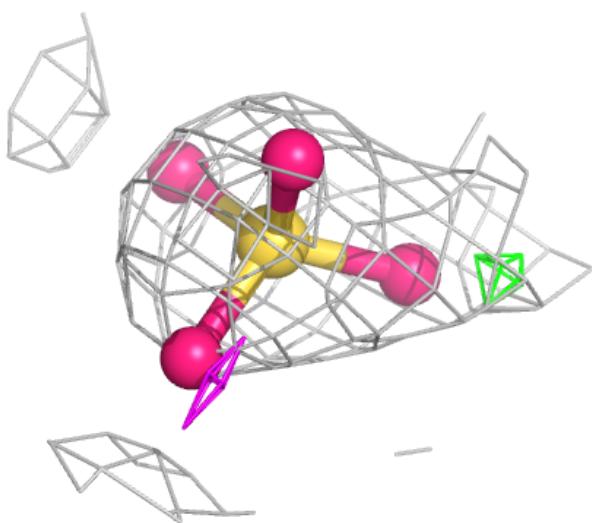
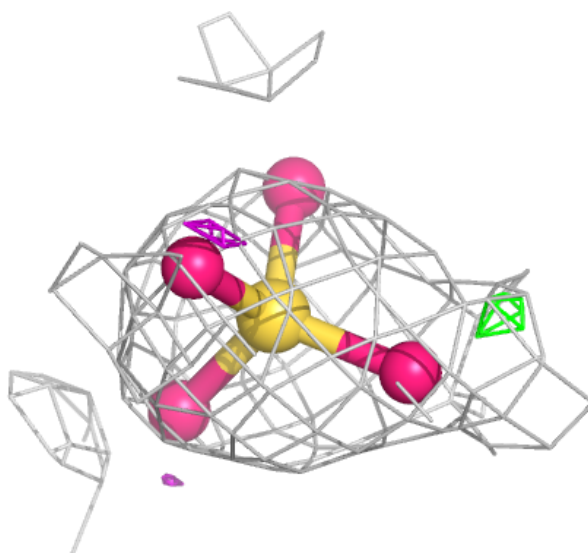
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





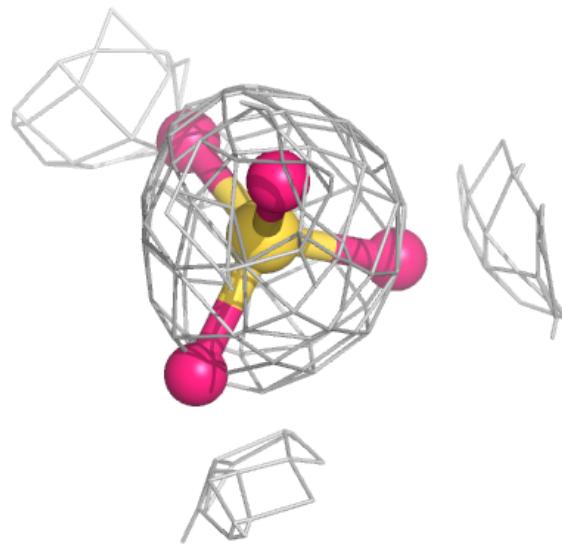
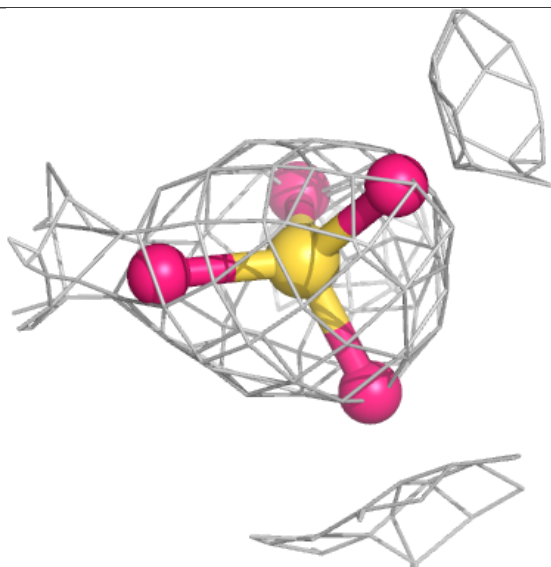
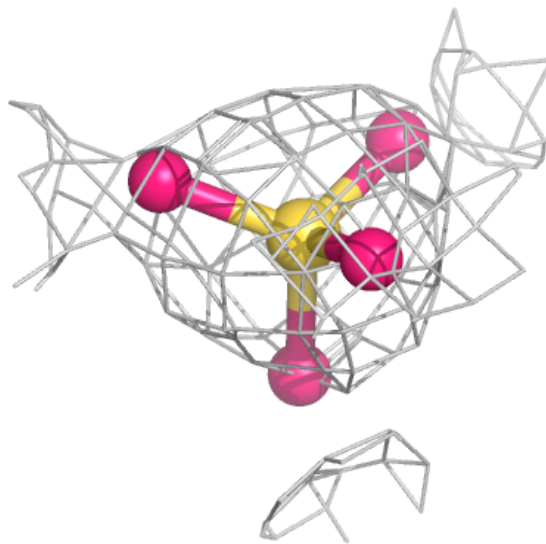
**Electron density around SO4 B 304:**

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



**Electron density around SO4 C 304:**

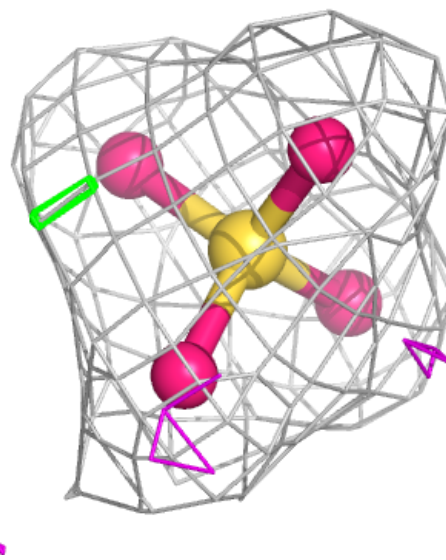
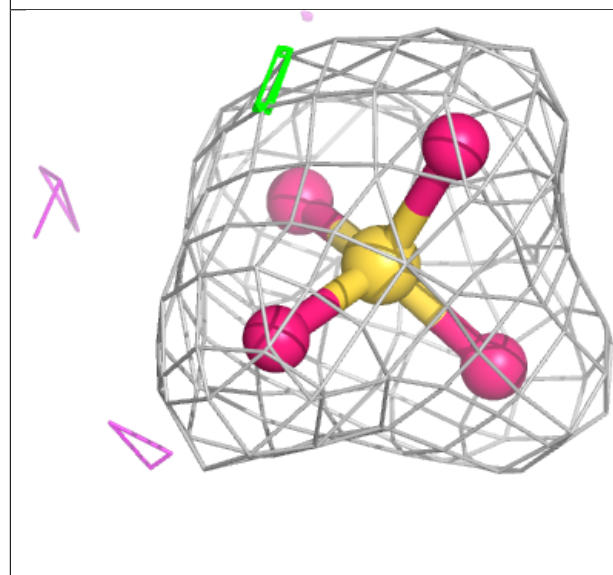
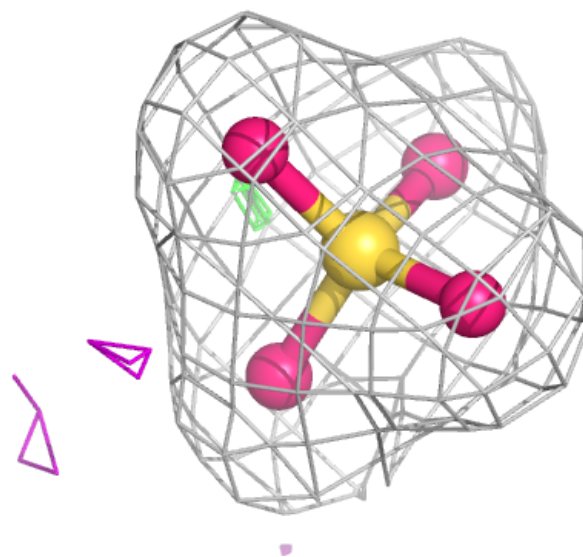
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





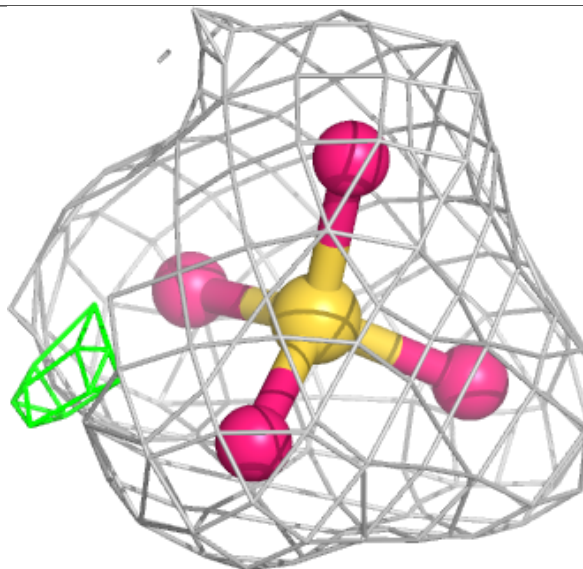
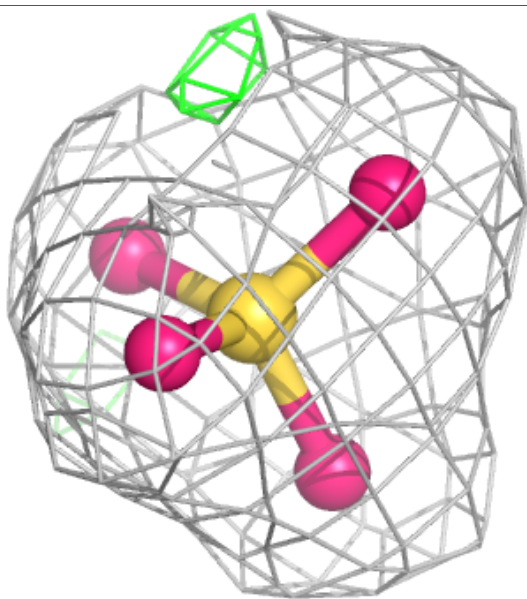
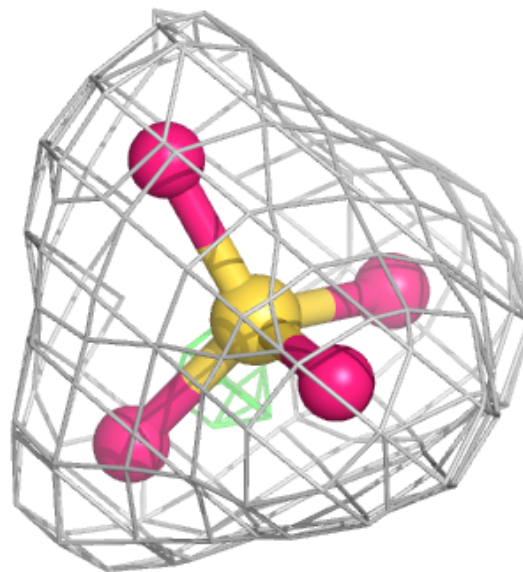
**Electron density around SO4 B 303:**

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



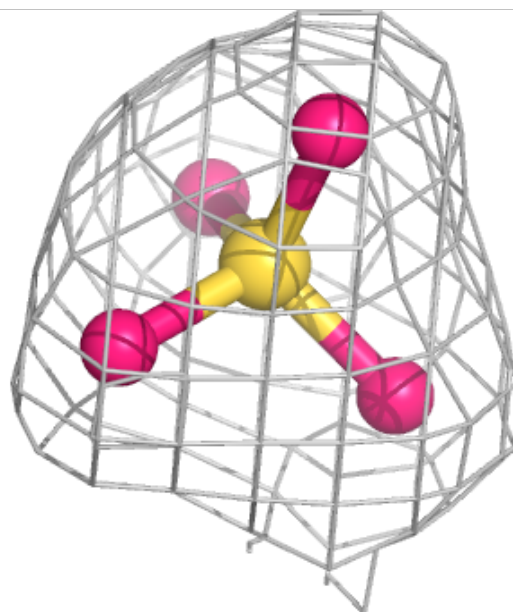
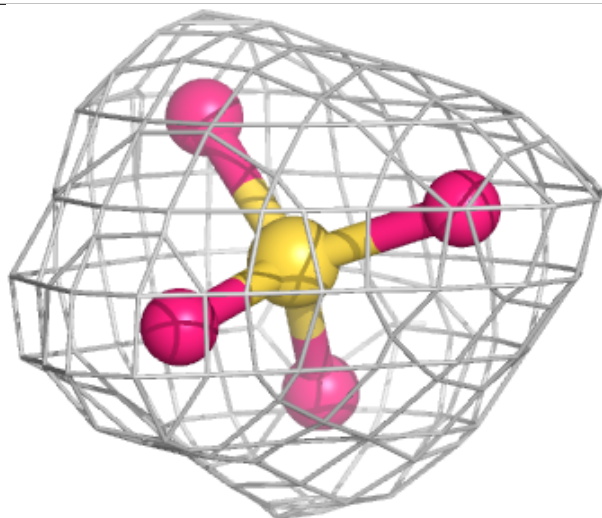
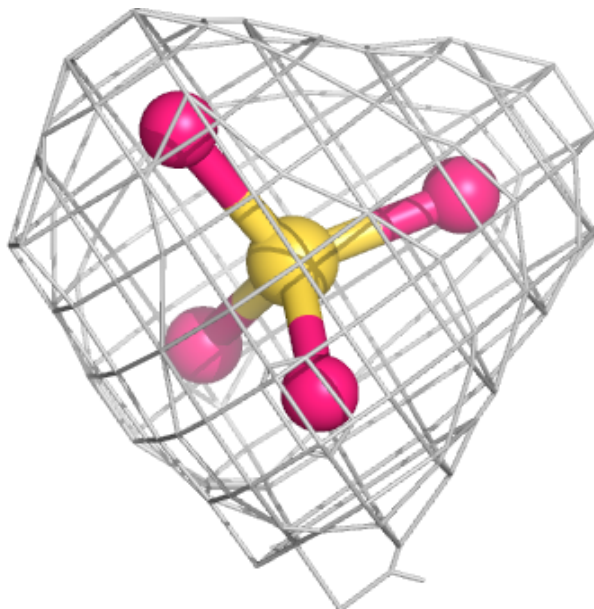
**Electron density around SO4 D 303:**

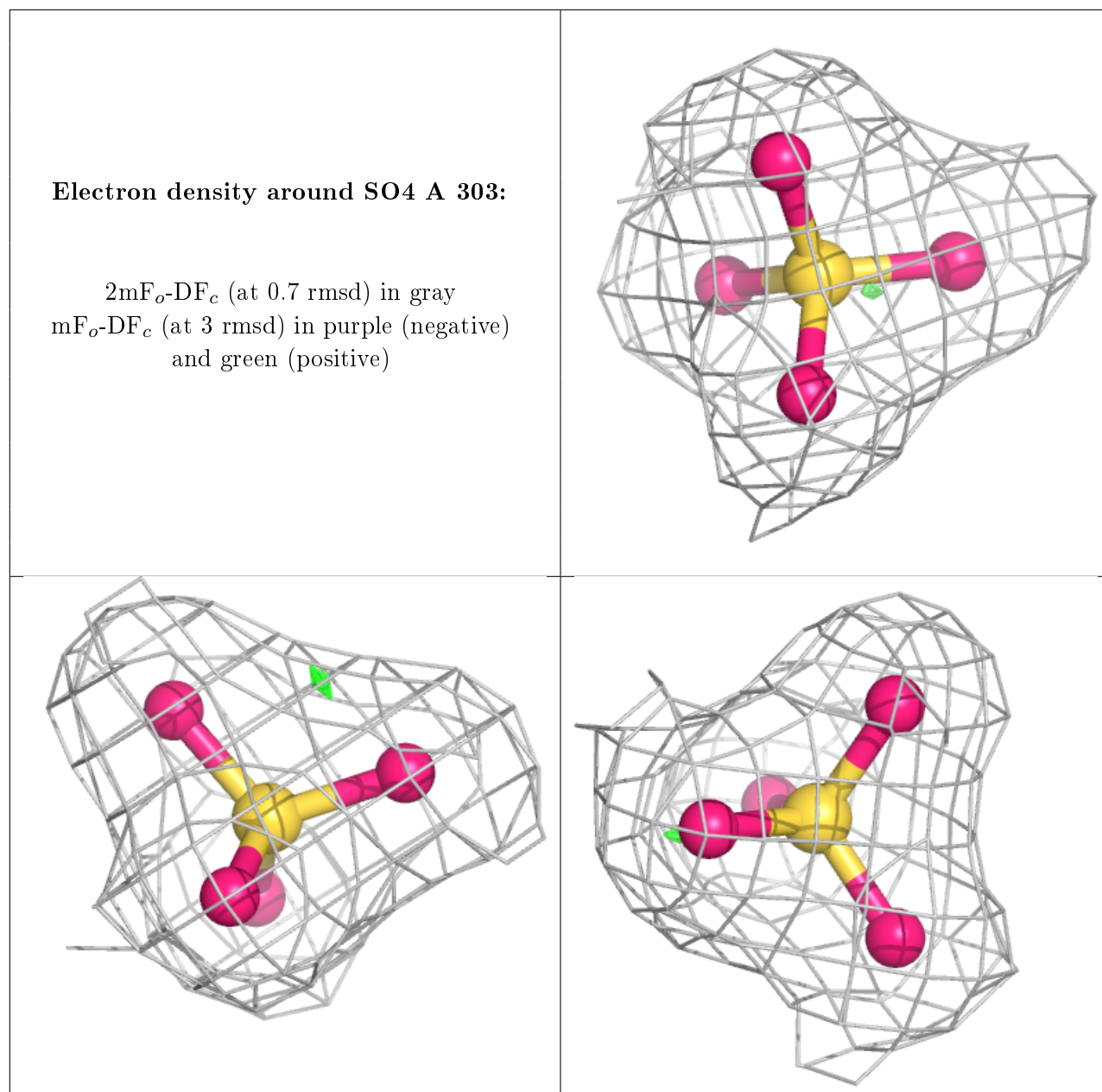
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SO4 C 303:**

$2mF_o-DF_c$  (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.