



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2022 – 01:05 am BST

PDB ID : 7Q30  
Title : Mutant T91A of uridine phosphorylase from *Shewanella oneidensis*  
Authors : Polyakov, K.; Safonova, T.  
Deposited on : 2021-10-26  
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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

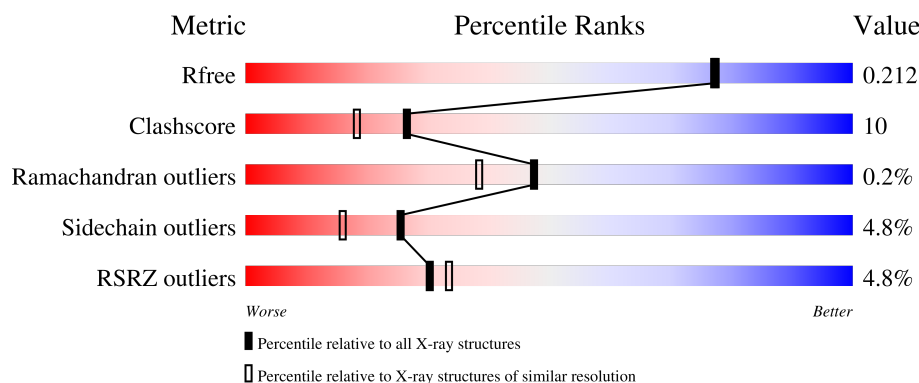
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

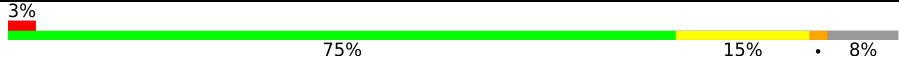

The reported resolution of this entry is 1.90 Å.

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 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	AAA	251	
1	DDD	251	

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	GOL	DDD	302	-	-	X	-
3	SO4	AAA	303	-	-	X	-
3	SO4	DDD	303	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3940 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.

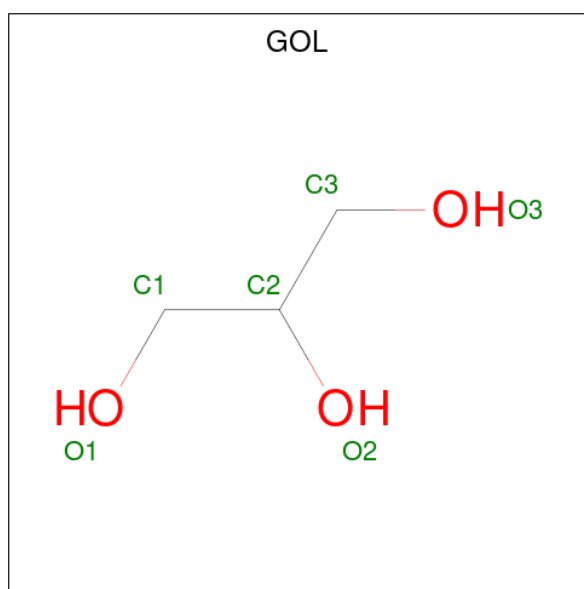
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DDD	251	Total	C	N	O	S	0	2	0
			1876	1176	324	362	14			
1	AAA	232	Total	C	N	O	S	0	2	0
			1714	1077	292	331	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	91	ALA	THR	engineered mutation	UNP Q8E9X9
AAA	91	ALA	THR	engineered mutation	UNP Q8E9X9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



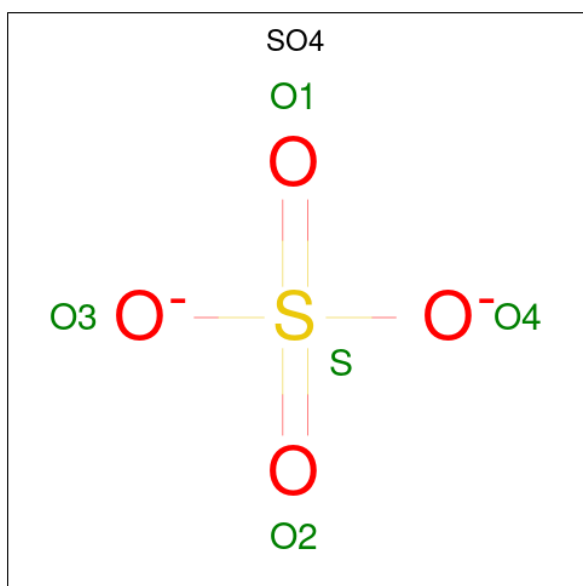
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	C	O	0	0
			6	3	3		
2	AAA	1	Total	C	O	0	0
			6	3	3		
2	AAA	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 4 is LITHIUM ION (three-letter code: LI) (formula: Li) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total 1	Li 1	0	0

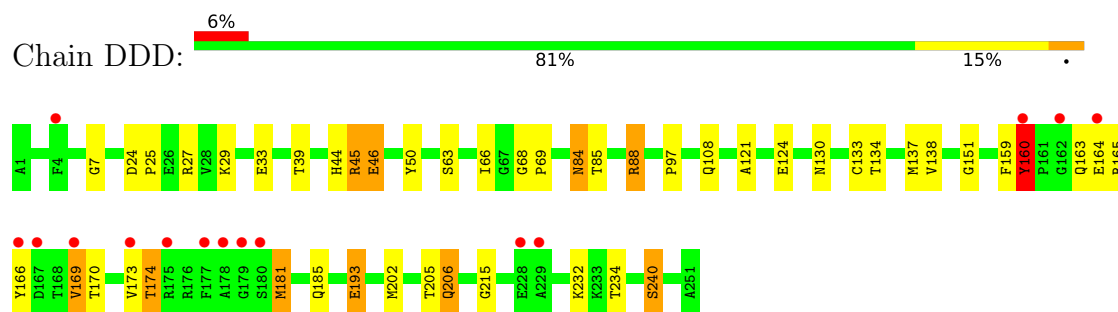
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	DDD	158	Total 158	O 158	0	0
5	AAA	137	Total 137	O 137	0	0

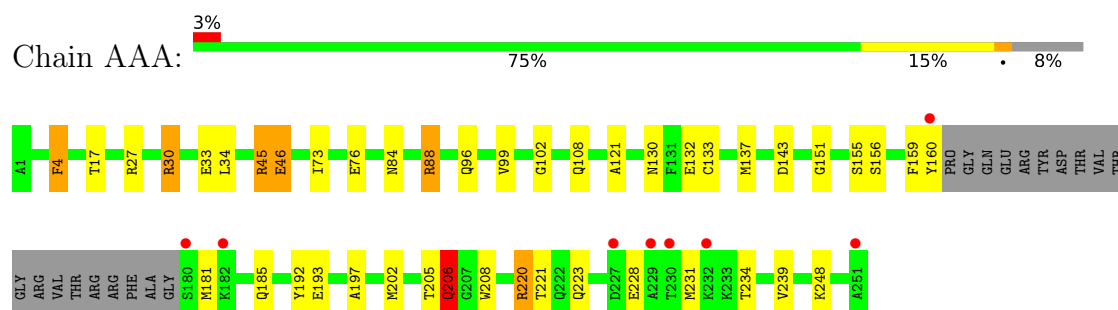
### 3 Residue-property plots

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

- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.66Å 91.66Å 47.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.47 – 1.90 26.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.47-1.90) 99.9 (26.46-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.157 , 0.211 0.159 , 0.212	Depositor DCC
$R_{free}$ test set	1696 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.908	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l 0.036 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LI, GOL, 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	AAA	0.85	5/1751 (0.3%)	1.25	12/2380 (0.5%)
1	DDD	0.79	3/1919 (0.2%)	1.19	8/2608 (0.3%)
All	All	0.82	8/3670 (0.2%)	1.22	20/4988 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	46	GLU	CD-OE2	8.91	1.35	1.25
1	AAA	76	GLU	CD-OE2	8.76	1.35	1.25
1	DDD	46	GLU	CD-OE2	8.07	1.34	1.25
1	AAA	76	GLU	CD-OE1	6.44	1.32	1.25
1	AAA	46	GLU	CD-OE1	6.19	1.32	1.25
1	DDD	124	GLU	CD-OE1	-5.54	1.19	1.25
1	AAA	33	GLU	CD-OE1	5.36	1.31	1.25
1	DDD	33	GLU	CD-OE2	-5.31	1.19	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	88[A]	ARG	CG-CD-NE	-9.71	91.41	111.80
1	AAA	88[B]	ARG	CG-CD-NE	-9.71	91.41	111.80
1	AAA	45	ARG	NE-CZ-NH2	-8.71	115.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	88[A]	ARG	CB-CG-CD	7.43	130.91	111.60
1	DDD	88[B]	ARG	CB-CG-CD	7.43	130.91	111.60
1	AAA	27	ARG	CG-CD-NE	6.68	125.82	111.80
1	AAA	45	ARG	CB-CG-CD	-6.67	94.26	111.60
1	DDD	45	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	AAA	45	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	AAA	192	TYR	CB-CA-C	-5.51	99.38	110.40
1	AAA	88[A]	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	AAA	88[B]	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	AAA	206	GLN	CB-CA-C	-5.50	99.41	110.40
1	AAA	137	MET	CG-SD-CE	-5.34	91.66	100.20
1	DDD	39	THR	CA-CB-OG1	-5.28	97.91	109.00
1	DDD	45	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	DDD	137	MET	CG-SD-CE	-5.09	92.05	100.20
1	DDD	160	TYR	CB-CA-C	5.04	120.49	110.40
1	AAA	17	THR	CA-CB-OG1	-5.04	98.42	109.00
1	DDD	240	SER	N-CA-CB	5.02	118.03	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	159	PHE	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1714	0	1710	33	0
1	DDD	1876	0	1866	40	0
2	AAA	12	0	16	2	0
2	DDD	12	0	16	4	0
3	AAA	15	0	0	2	0
3	DDD	15	0	0	2	0
4	AAA	1	0	0	0	0
5	AAA	137	0	0	9	2
5	DDD	158	0	0	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3940	0	3608	75	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (75) 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:DDD:88[A]:ARG:NH1	5:DDD:405:HOH:O	1.65	1.30
2:DDD:302:GOL:O1	5:DDD:404:HOH:O	1.61	1.15
2:DDD:302:GOL:H11	5:DDD:503:HOH:O	1.61	1.00
3:AAA:303:SO4:O2	5:AAA:406:HOH:O	1.85	0.92
1:AAA:160:TYR:CB	5:AAA:524:HOH:O	2.17	0.91
1:DDD:169:VAL:HG12	1:DDD:170:THR:N	1.88	0.88
1:DDD:130:ASN:OD1	2:DDD:302:GOL:H12	1.75	0.86
3:DDD:303:SO4:O1	5:DDD:405:HOH:O	1.96	0.84
1:DDD:130:ASN:HD22	1:DDD:133:CYS:H	1.25	0.81
1:AAA:202:MET:O	1:AAA:206:GLN:HG2	1.79	0.80
3:AAA:303:SO4:O2	5:AAA:407:HOH:O	2.00	0.80
1:DDD:169:VAL:HG11	1:AAA:208:TRP:CZ2	2.16	0.80
1:DDD:169:VAL:HG12	1:DDD:170:THR:HG23	1.65	0.79
1:DDD:169:VAL:HG11	1:AAA:208:TRP:HZ2	1.48	0.77
1:DDD:88[A]:ARG:HD2	5:DDD:401:HOH:O	1.85	0.75
3:DDD:303:SO4:O4	5:DDD:407:HOH:O	2.05	0.75
1:DDD:169:VAL:CG1	1:DDD:170:THR:N	2.52	0.73
1:AAA:88[A]:ARG:NE	5:AAA:401:HOH:O	2.13	0.72
1:AAA:88[A]:ARG:NH1	5:AAA:401:HOH:O	2.16	0.71
1:AAA:130:ASN:HD22	1:AAA:133:CYS:H	1.39	0.70
1:AAA:132:GLU:HG3	5:AAA:528:HOH:O	1.92	0.68
1:AAA:130:ASN:OD1	2:AAA:302:GOL:H12	1.94	0.67
1:AAA:220:ARG:HG3	1:AAA:220:ARG:HH11	1.60	0.67
1:DDD:169:VAL:HG12	1:DDD:170:THR:H	1.60	0.67
1:AAA:228:GLU:HA	1:AAA:231:MET:CE	2.25	0.67
1:AAA:202:MET:O	1:AAA:206:GLN:CG	2.43	0.67
1:AAA:34:LEU:CD1	1:AAA:239:VAL:HG12	2.26	0.66
1:AAA:30:ARG:HD2	5:AAA:516:HOH:O	1.95	0.66
1:AAA:228:GLU:HA	1:AAA:231:MET:HE2	1.80	0.63
1:DDD:46:GLU:HB3	1:AAA:46:GLU:HB3	1.79	0.63
1:DDD:169:VAL:CG1	1:DDD:170:THR:HG23	2.30	0.61
1:AAA:34:LEU:CD1	1:AAA:239:VAL:CG1	2.79	0.61
1:AAA:108:GLN:HE21	1:AAA:151:GLY:HA2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:174:THR:HG23	5:DDD:412:HOH:O	2.01	0.60
1:DDD:166:TYR:CE1	1:DDD:173:VAL:HG23	2.36	0.59
1:AAA:155:SER:HB3	1:AAA:197:ALA:HB2	1.84	0.59
1:DDD:202:MET:O	1:DDD:206:GLN:HG2	2.04	0.56
1:DDD:181:MET:O	1:DDD:185:GLN:HG3	2.05	0.56
1:DDD:159:PHE:O	1:DDD:163:GLN:HB2	2.06	0.56
1:DDD:130:ASN:ND2	1:DDD:133:CYS:H	2.00	0.56
1:AAA:130:ASN:ND2	1:AAA:133:CYS:H	2.03	0.56
1:DDD:170:THR:HG21	1:AAA:206:GLN:HB3	1.87	0.54
1:DDD:84:ASN:HD22	1:DDD:84:ASN:C	2.13	0.52
1:DDD:88[B]:ARG:NH1	5:DDD:401:HOH:O	0.67	0.52
1:DDD:170:THR:CG2	1:AAA:206:GLN:HB3	2.40	0.52
1:DDD:108:GLN:NE2	5:DDD:414:HOH:O	2.42	0.51
1:AAA:34:LEU:HD13	1:AAA:239:VAL:HG12	1.93	0.51
2:AAA:302:GOL:H2	5:AAA:503:HOH:O	2.10	0.51
1:AAA:181:MET:O	1:AAA:185:GLN:HG3	2.11	0.51
1:DDD:202:MET:O	1:DDD:206:GLN:CG	2.59	0.50
1:AAA:121:ALA:HB2	1:AAA:205:THR:HG21	1.94	0.49
1:DDD:24:ASP:HB3	1:DDD:27:ARG:HG2	1.94	0.49
1:AAA:45:ARG:HD3	5:AAA:431:HOH:O	2.12	0.49
1:DDD:121:ALA:HB2	1:DDD:205:THR:HG21	1.97	0.47
1:DDD:174:THR:CG2	5:DDD:412:HOH:O	2.59	0.47
1:DDD:25:PRO:HA	1:DDD:63:SER:HB3	1.97	0.46
1:DDD:215:GLY:HA3	1:DDD:234:THR:HG22	1.98	0.46
1:AAA:102:GLY:HA2	1:AAA:234:THR:OG1	2.15	0.46
1:DDD:108:GLN:HE21	1:DDD:151:GLY:HA2	1.80	0.45
1:AAA:228:GLU:HA	1:AAA:231:MET:HE3	1.98	0.45
1:DDD:160:TYR:HA	1:DDD:165:ARG:HB2	1.98	0.45
1:DDD:88[A]:ARG:NH2	1:DDD:193:GLU:OE2	2.49	0.45
1:AAA:96:GLN:HB2	1:AAA:99:VAL:HG23	2.00	0.44
1:DDD:66:ILE:HG21	1:AAA:73:ILE:HD12	1.99	0.44
1:DDD:29:LYS:HD2	1:DDD:50:TYR:OH	2.17	0.44
1:DDD:84:ASN:HD22	1:DDD:85:THR:N	2.17	0.43
1:DDD:7:GLY:HA3	1:DDD:44:HIS:CD2	2.53	0.43
1:DDD:164:GLU:HG3	1:DDD:166:TYR:CE2	2.53	0.43
1:DDD:68:GLY:N	1:DDD:69:PRO:CD	2.81	0.43
1:AAA:34:LEU:HD11	1:AAA:239:VAL:CG1	2.49	0.43
2:DDD:302:GOL:C1	5:DDD:503:HOH:O	2.39	0.41
1:DDD:45:ARG:HD3	5:DDD:453:HOH:O	2.21	0.41
5:DDD:539:HOH:O	1:AAA:4:PHE:HD1	2.03	0.41
1:AAA:143:ASP:OD2	1:AAA:248:LYS:NZ	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:134:THR:O	1:DDD:138:VAL:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:537:HOH:O	5:AAA:537:HOH:O[2_545]	1.92	0.28
5:DDD:510:HOH:O	5:AAA:526:HOH:O[2_444]	2.12	0.08

## 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	AAA	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
1	DDD	251/251 (100%)	241 (96%)	9 (4%)	1 (0%)	34	24
All	All	481/502 (96%)	467 (97%)	13 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	160	TYR

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	181/196 (92%)	172 (95%)	9 (5%)	24	15
1	DDD	198/196 (101%)	189 (96%)	9 (4%)	27	18
All	All	379/392 (97%)	361 (95%)	18 (5%)	25	16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	84	ASN
1	DDD	97	PRO
1	DDD	169	VAL
1	DDD	174	THR
1	DDD	181	MET
1	DDD	193	GLU
1	DDD	206	GLN
1	DDD	232	LYS
1	DDD	240	SER
1	AAA	4	PHE
1	AAA	30	ARG
1	AAA	84	ASN
1	AAA	156	SER
1	AAA	193	GLU
1	AAA	206	GLN
1	AAA	220	ARG
1	AAA	221	THR
1	AAA	223	GLN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	$\# Z  > 2$
2	GOL	AAA	302	-	5,5,5	0.26	0	5,5,5	0.76	0
2	GOL	AAA	301	-	5,5,5	0.32	0	5,5,5	0.35	0
3	SO4	DDD	305	-	4,4,4	0.42	0	6,6,6	0.26	0
2	GOL	DDD	301	-	5,5,5	0.34	0	5,5,5	0.38	0
3	SO4	DDD	303	-	4,4,4	0.33	0	6,6,6	0.36	0
3	SO4	DDD	304	-	4,4,4	0.69	0	6,6,6	0.50	0
3	SO4	AAA	303	-	4,4,4	0.38	0	6,6,6	0.24	0
2	GOL	DDD	302	-	5,5,5	0.37	0	5,5,5	1.18	1 (20%)
3	SO4	AAA	304	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	AAA	305	-	4,4,4	0.63	0	6,6,6	0.22	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	GOL	AAA	302	-	-	2/4/4/4	-
2	GOL	AAA	301	-	-	0/4/4/4	-
2	GOL	DDD	302	-	-	0/4/4/4	-
2	GOL	DDD	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	302	GOL	O2-C2-C3	-2.02	100.23	109.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

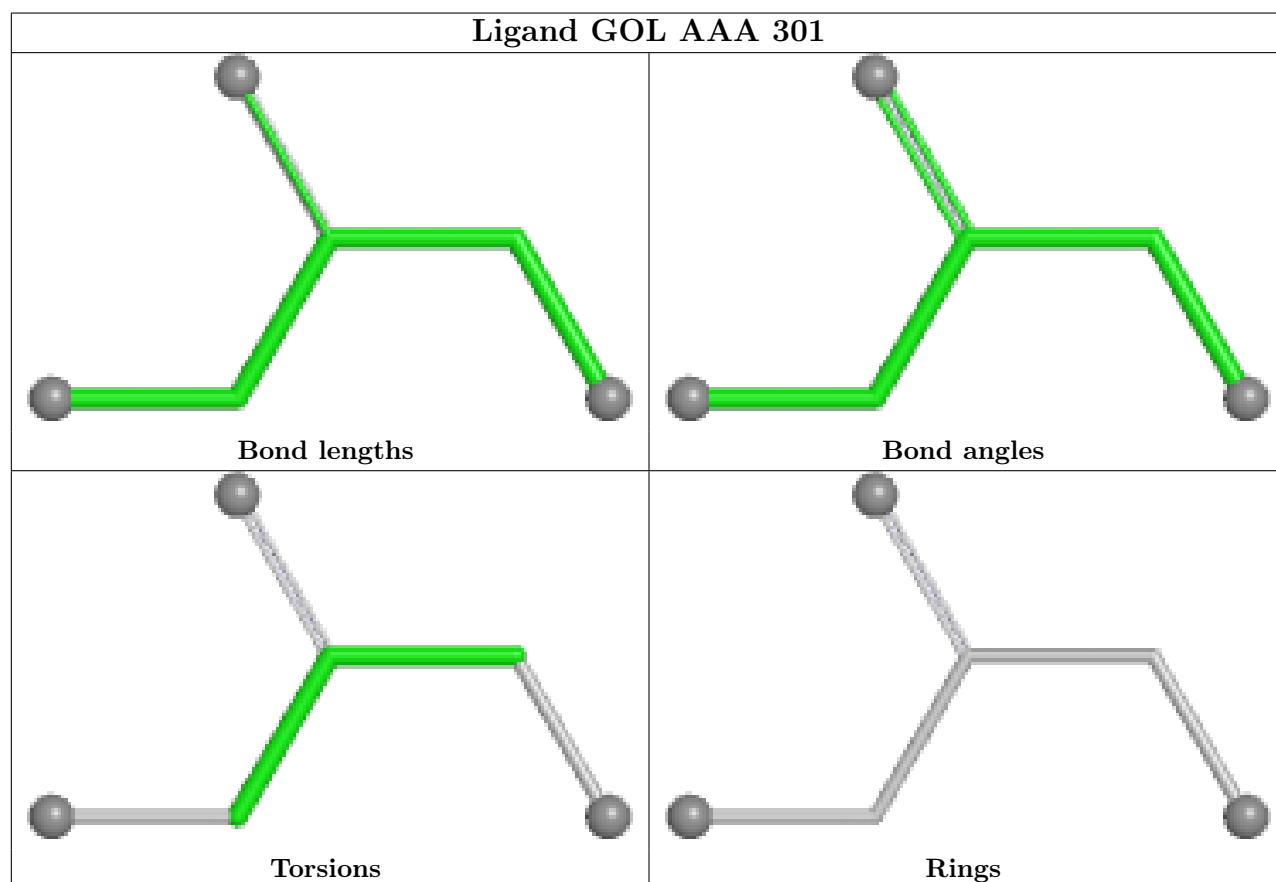
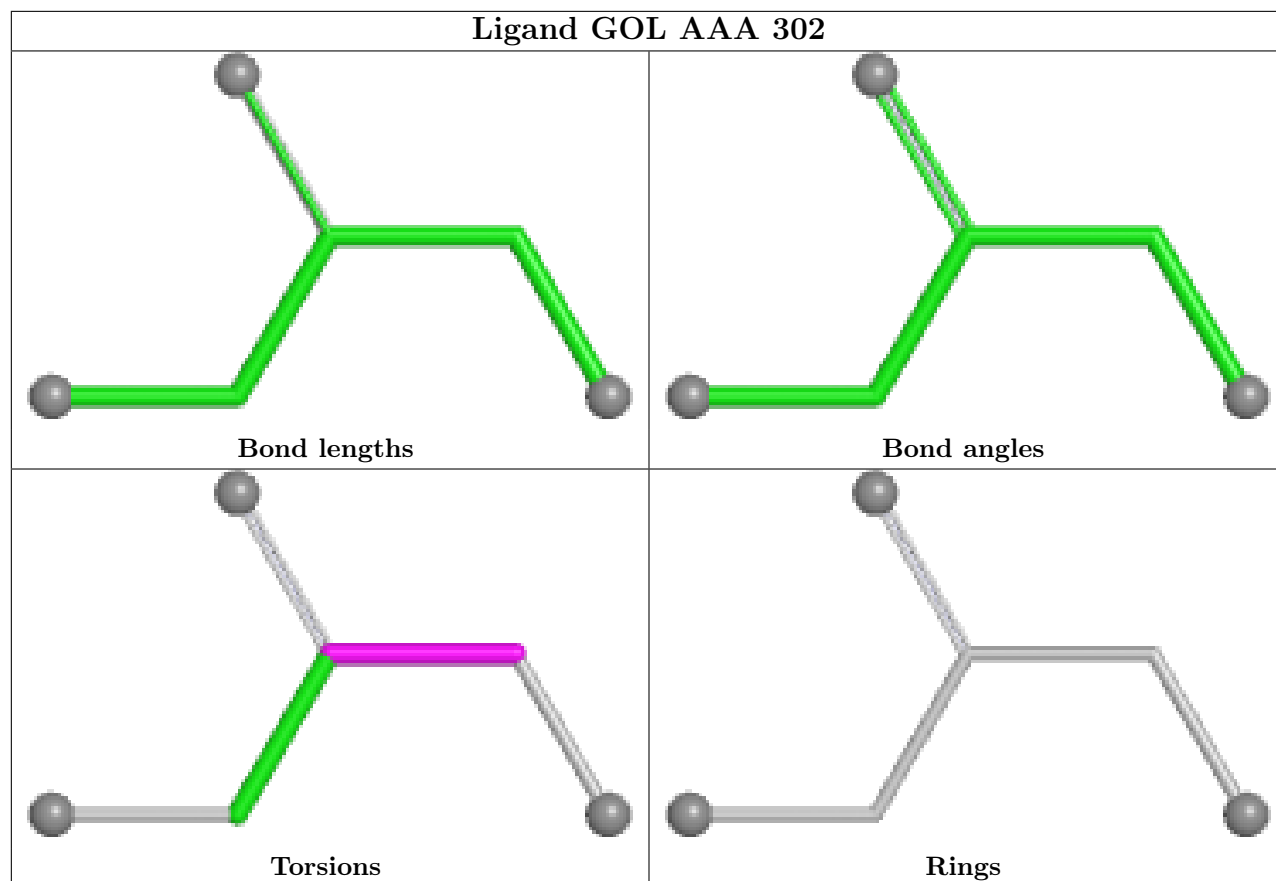
Mol	Chain	Res	Type	Atoms
2	AAA	302	GOL	O1-C1-C2-O2
2	AAA	302	GOL	O1-C1-C2-C3

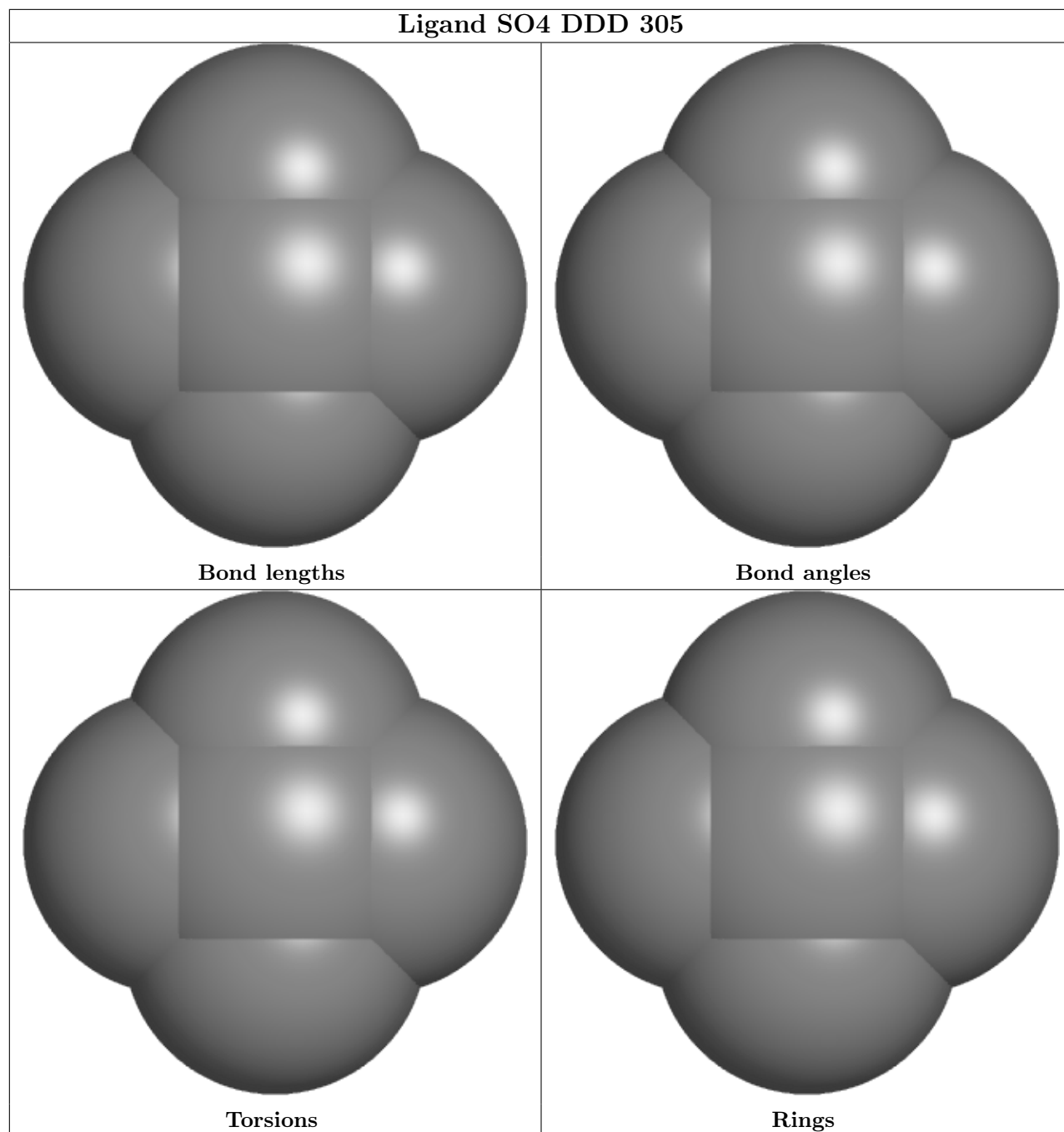
There are no ring outliers.

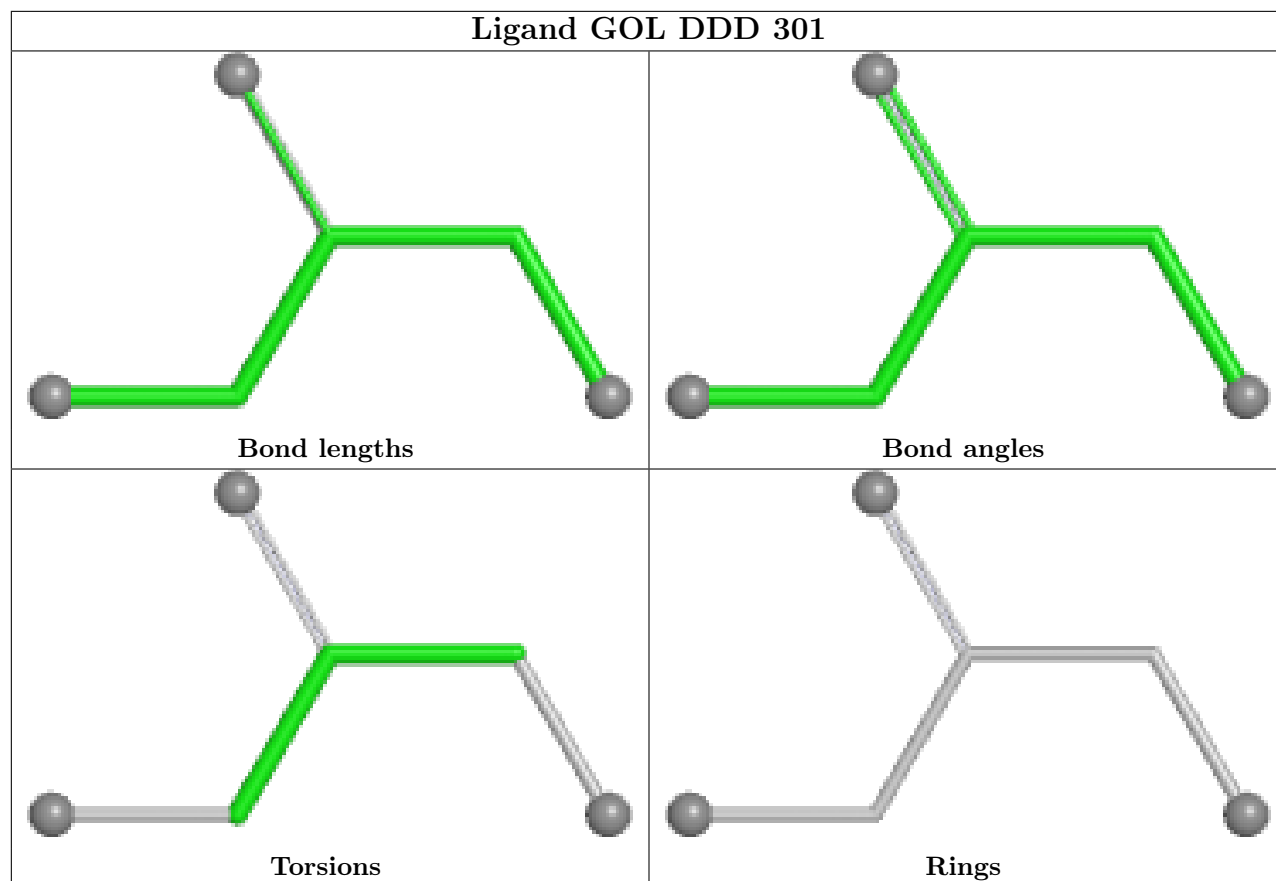
4 monomers are involved in 10 short contacts:

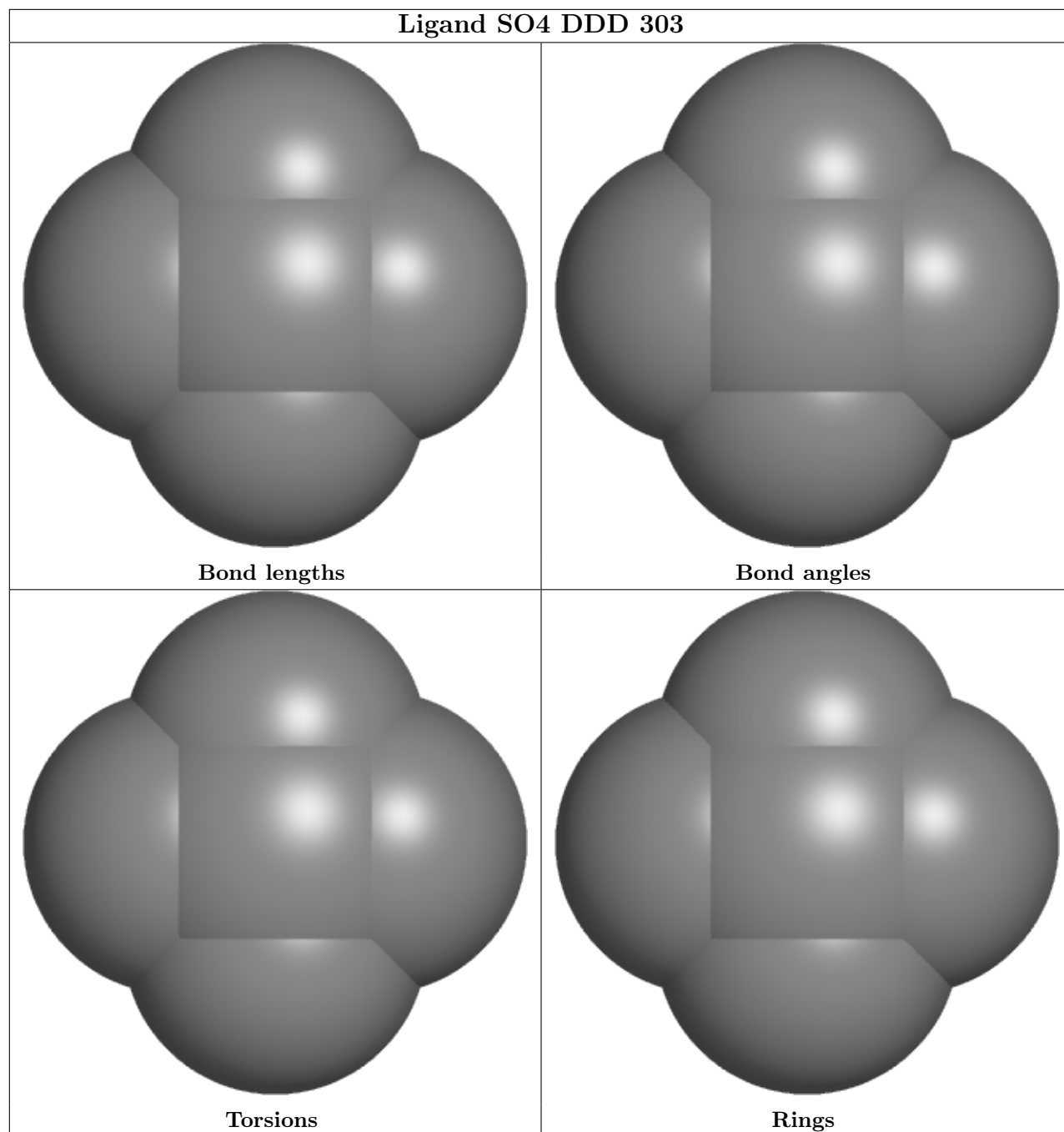
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	302	GOL	2	0
3	DDD	303	SO4	2	0
3	AAA	303	SO4	2	0
2	DDD	302	GOL	4	0

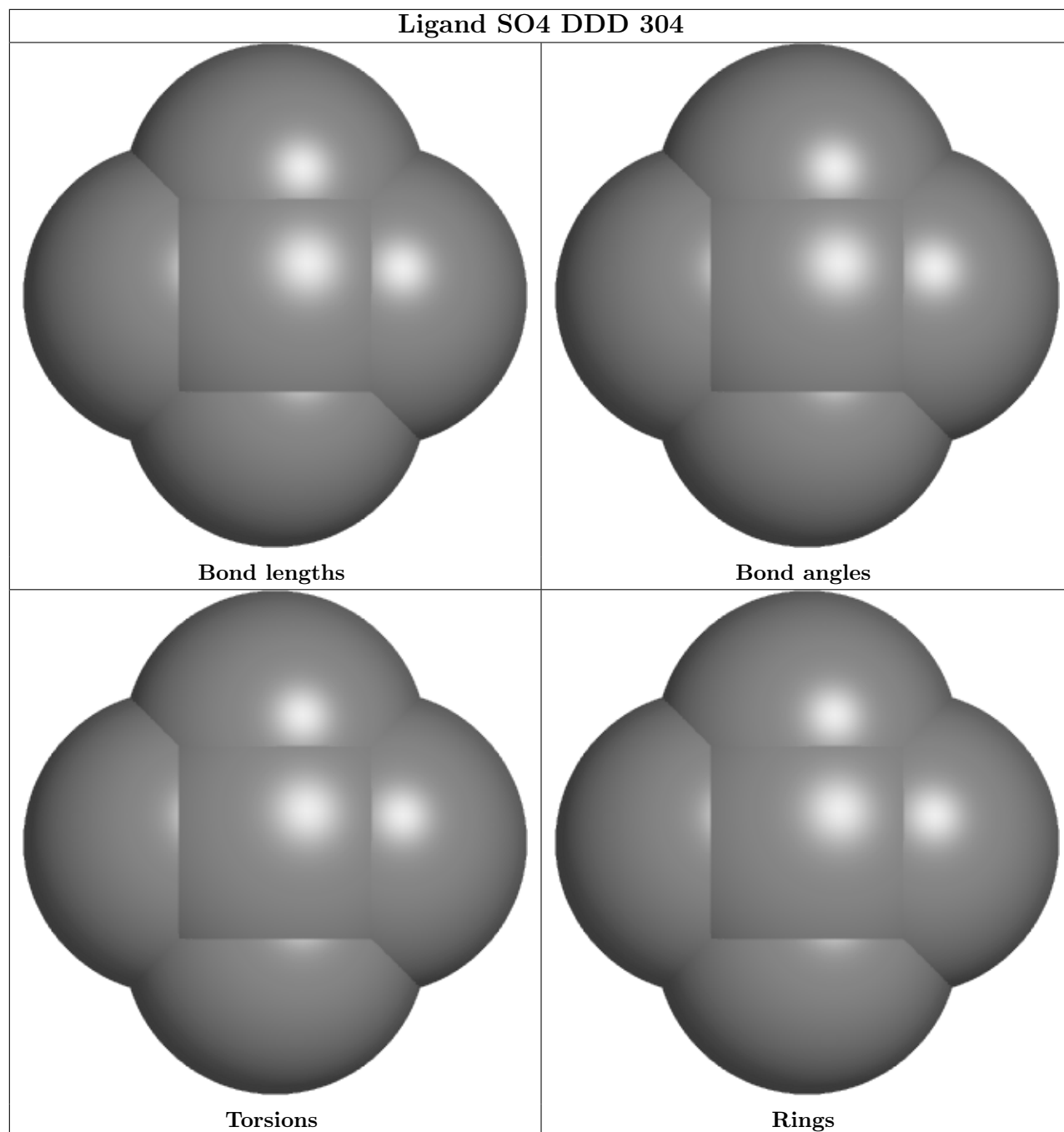
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

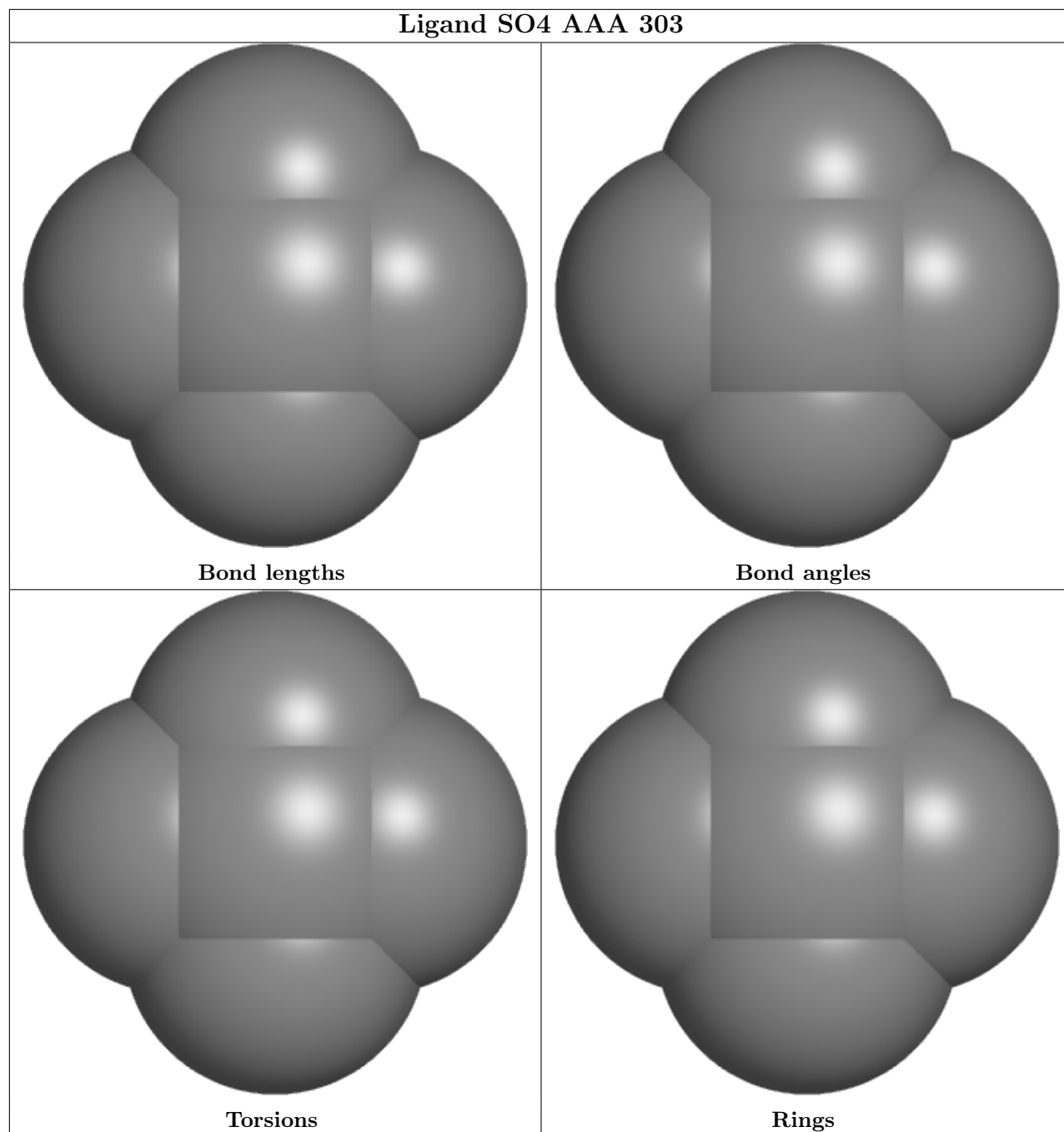


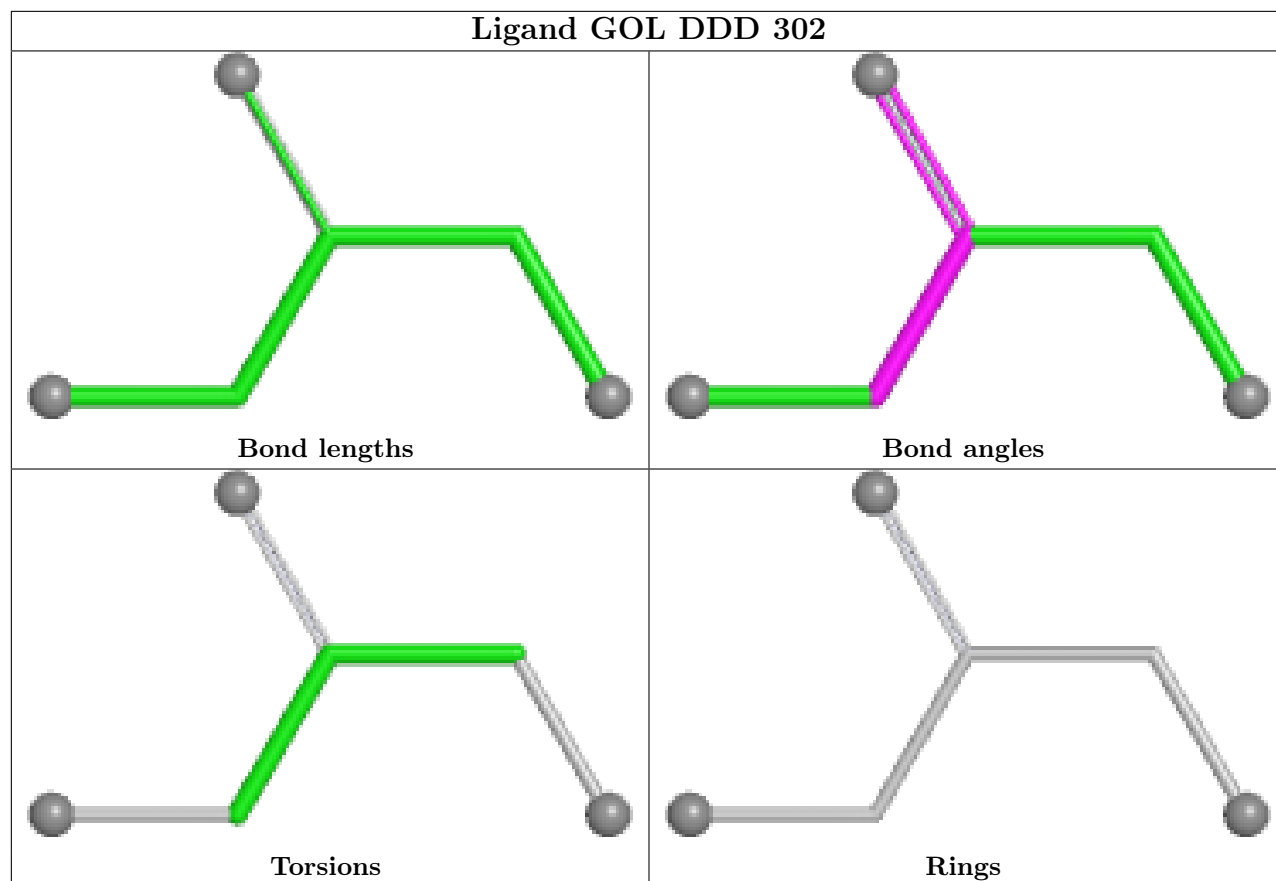


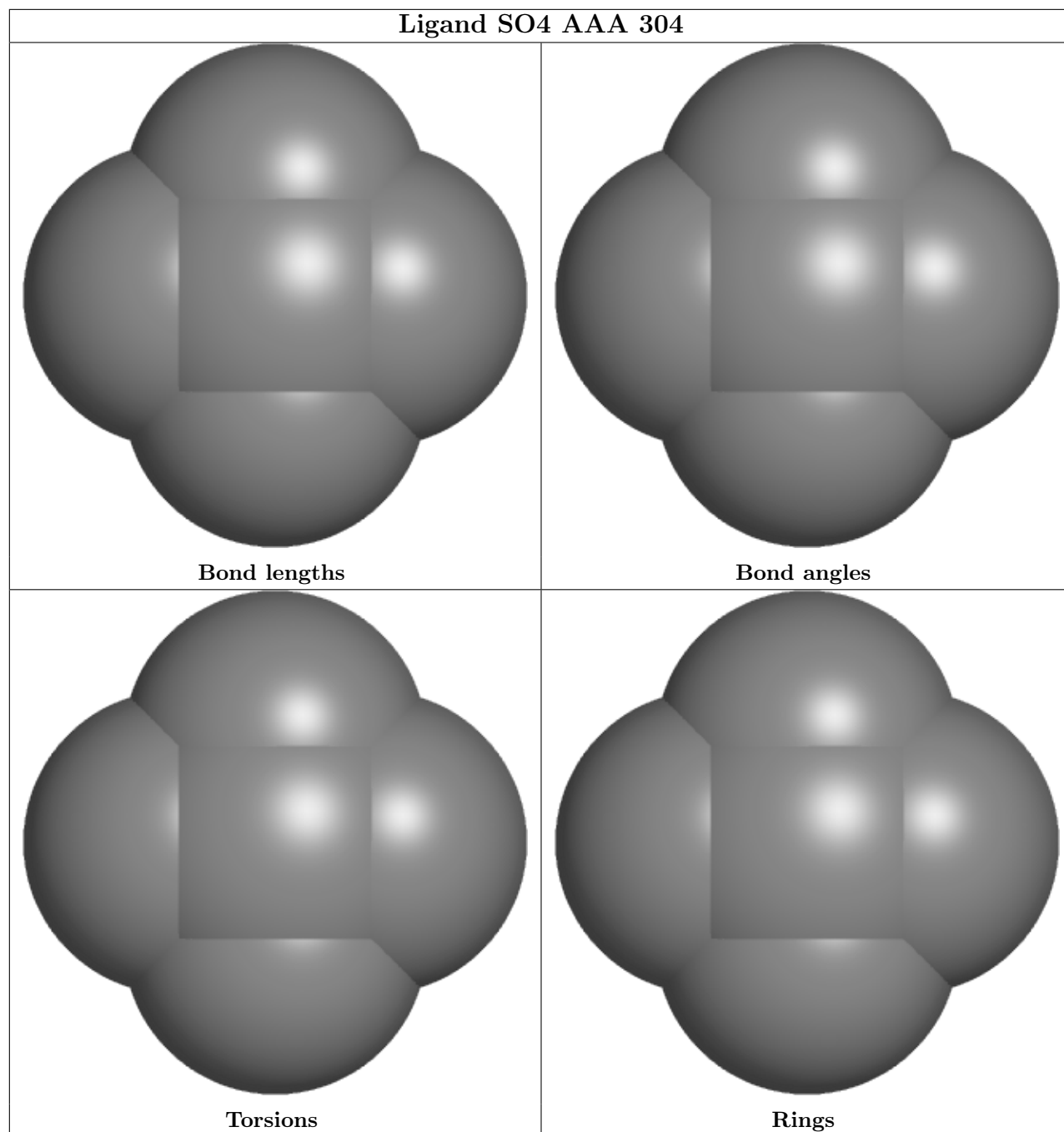


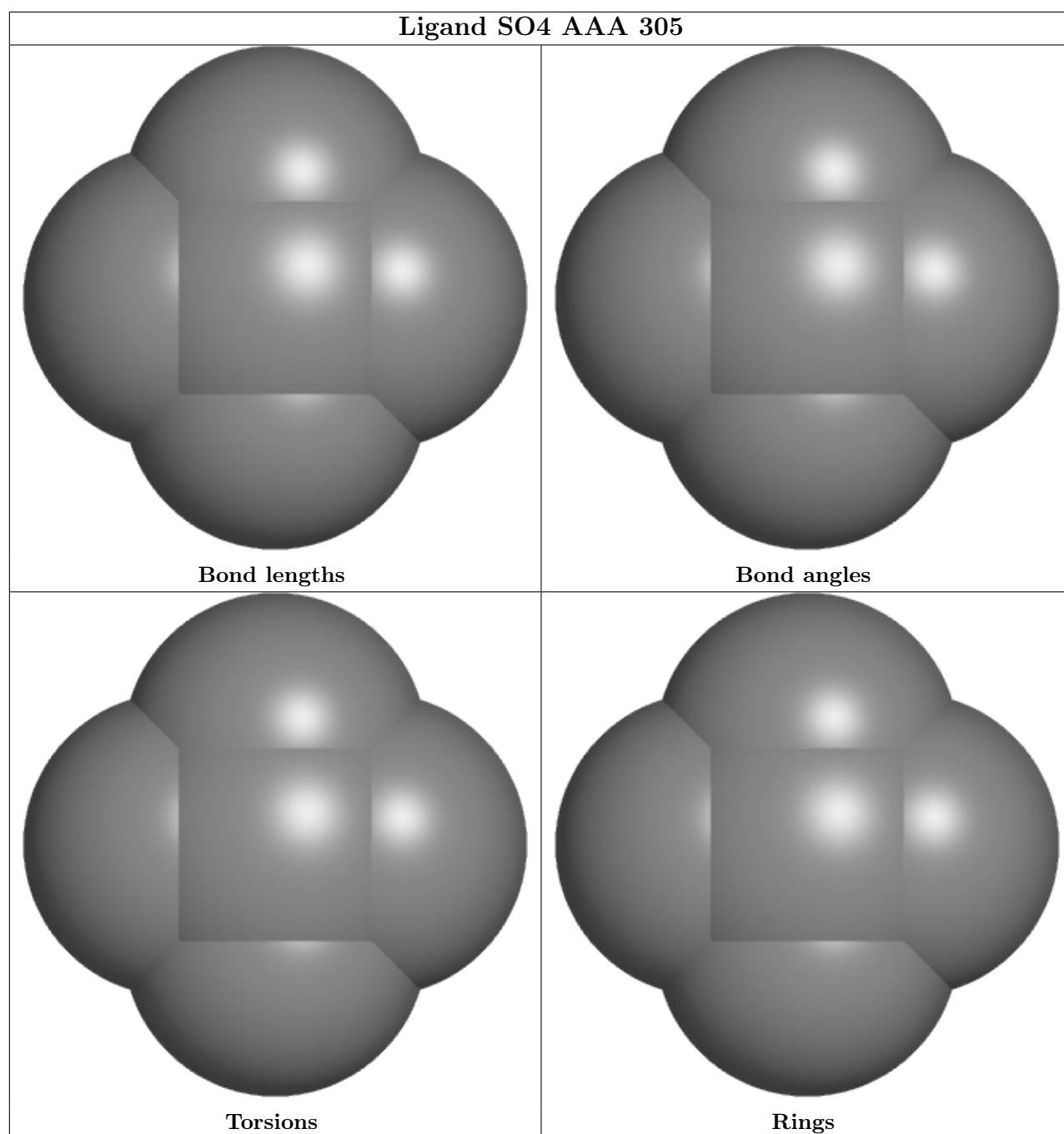












## 5.7 Other polymers [i](#)

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	AAA	232/251 (92%)	-0.20	8 (3%)	45	48	11, 19, 47, 62	0
1	DDD	251/251 (100%)	-0.06	15 (5%)	21	24	13, 21, 50, 71	8 (3%)
All	All	483/502 (96%)	-0.13	23 (4%)	30	33	11, 20, 50, 71	8 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	160	TYR	4.2
1	AAA	229	ALA	4.1
1	DDD	178	ALA	4.0
1	DDD	179	GLY	3.5
1	AAA	180	SER	3.5
1	DDD	160	TYR	3.4
1	DDD	169	VAL	3.4
1	DDD	175	ARG	3.0
1	DDD	167	ASP	2.8
1	DDD	173	VAL	2.6
1	DDD	228	GLU	2.6
1	AAA	227	ASP	2.5
1	DDD	166	TYR	2.5
1	DDD	164	GLU	2.5
1	AAA	182	LYS	2.3
1	DDD	177	PHE	2.3
1	DDD	4	PHE	2.2
1	DDD	162	GLY	2.2
1	AAA	232	LYS	2.2
1	DDD	180	SER	2.1
1	AAA	230	THR	2.1
1	DDD	229	ALA	2.1
1	AAA	251	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

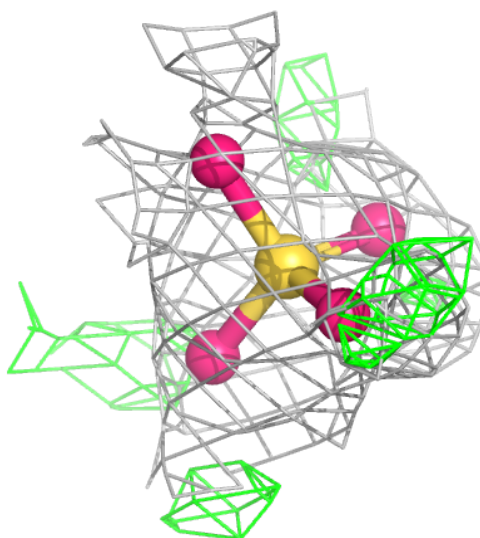
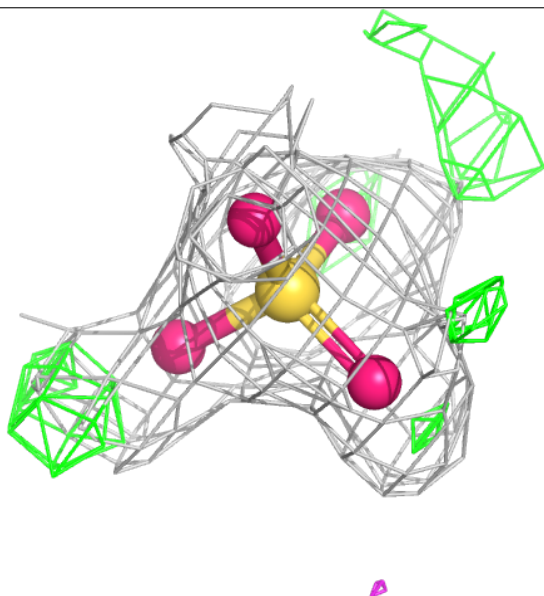
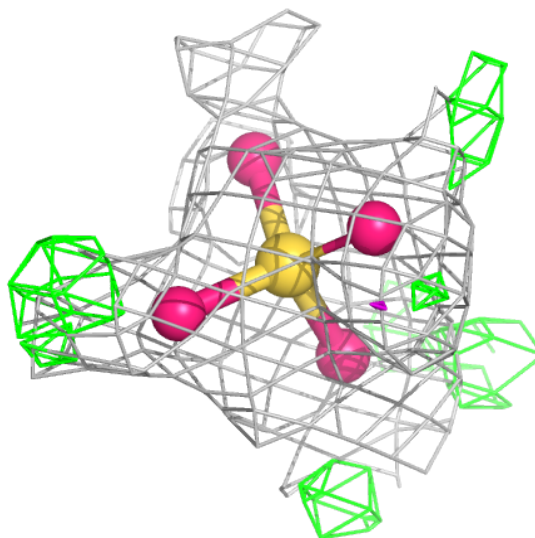
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	AAA	303	5/5	0.88	0.31	31,34,36,36	5
3	SO4	AAA	304	5/5	0.89	0.15	78,82,92,92	5
2	GOL	DDD	302	6/6	0.93	0.20	12,14,16,18	6
3	SO4	DDD	303	5/5	0.93	0.30	23,24,31,31	5
3	SO4	DDD	305	5/5	0.94	0.13	24,25,30,33	5
4	LI	AAA	306	1/1	0.94	0.48	8,8,8,8	0
2	GOL	AAA	302	6/6	0.95	0.13	8,12,12,14	6
2	GOL	DDD	301	6/6	0.96	0.10	20,28,33,36	0
3	SO4	DDD	304	5/5	0.96	0.11	26,26,27,30	5
2	GOL	AAA	301	6/6	0.97	0.07	20,23,28,29	0
3	SO4	AAA	305	5/5	0.98	0.07	26,26,31,33	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.

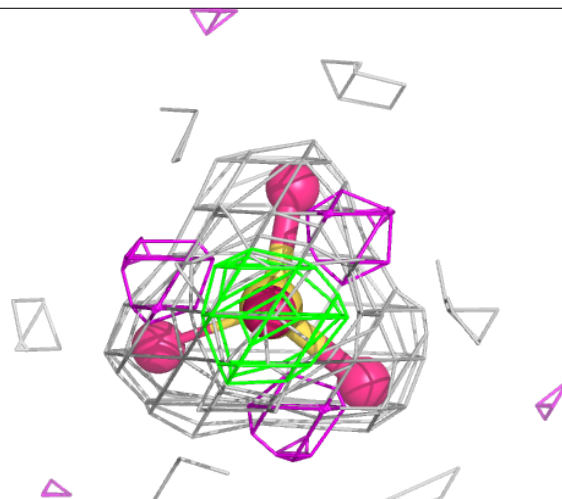
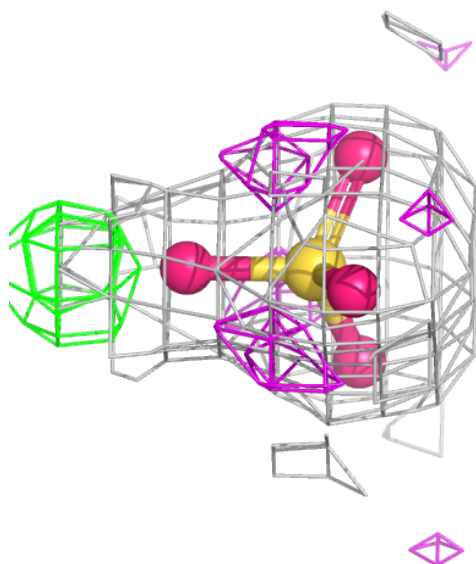
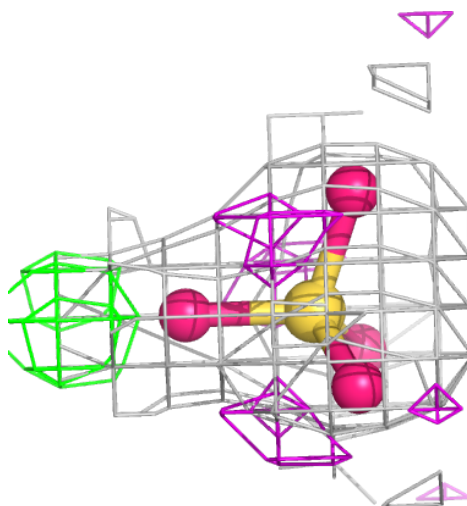
**Electron density around SO4 AAA 303:**

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



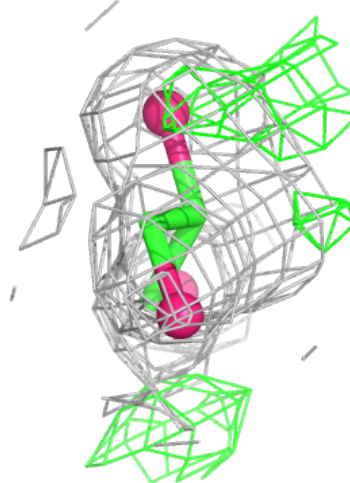
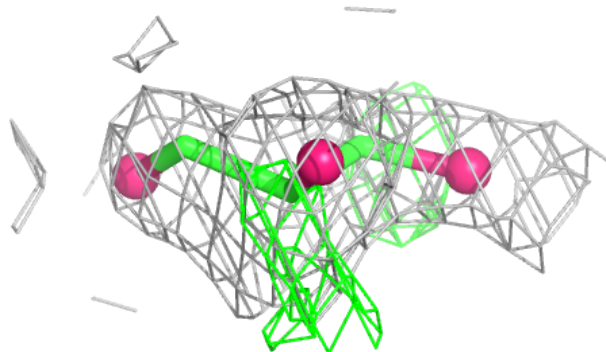
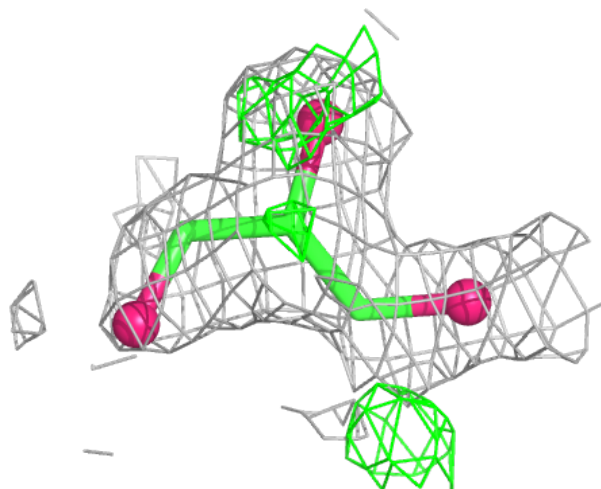
**Electron density around SO4 AAA 304:**

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



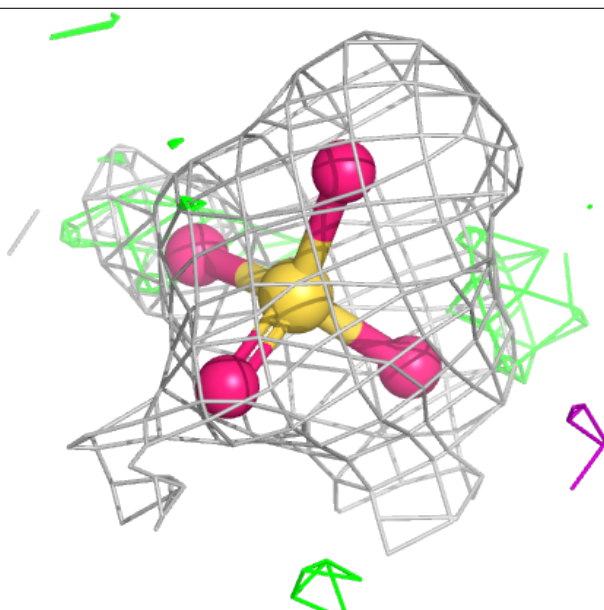
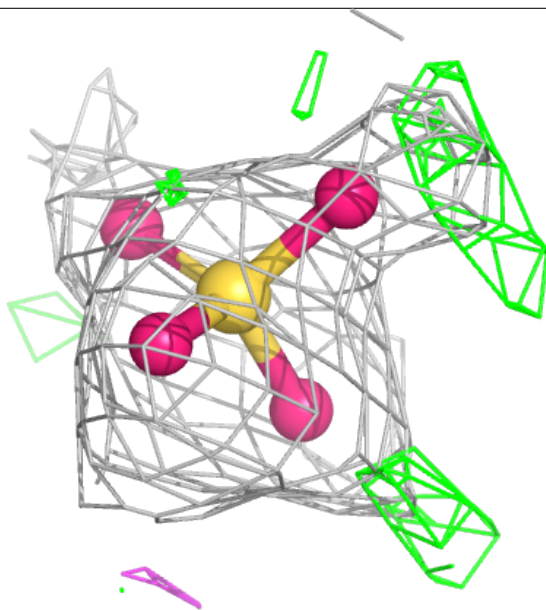
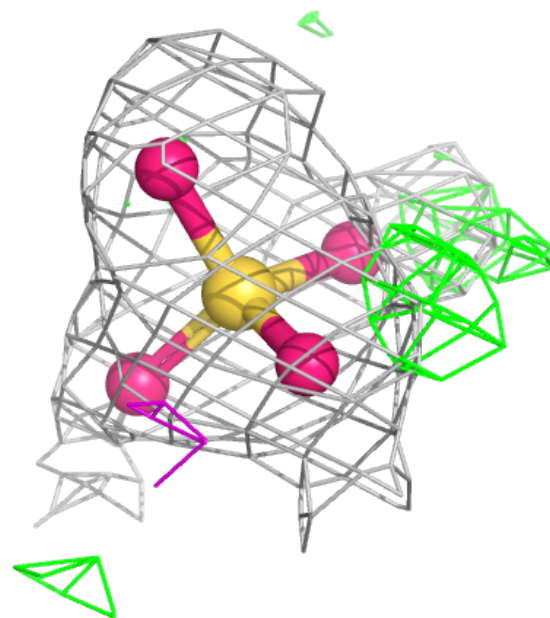
**Electron density around GOL DDD 302:**

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



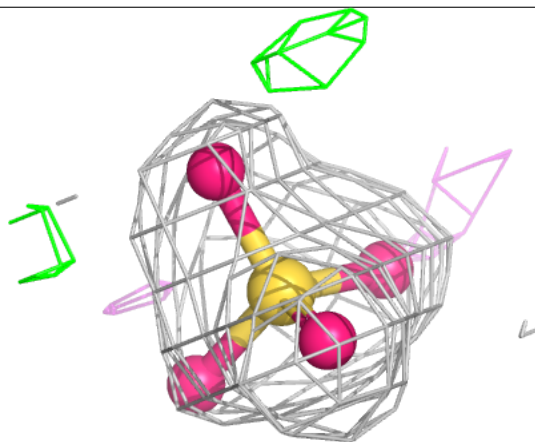
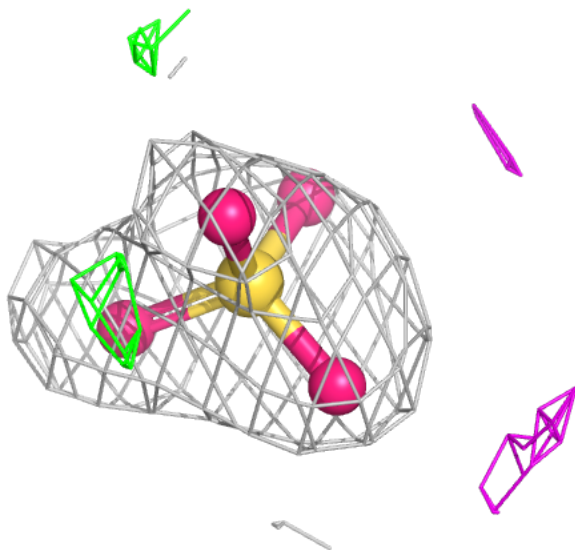
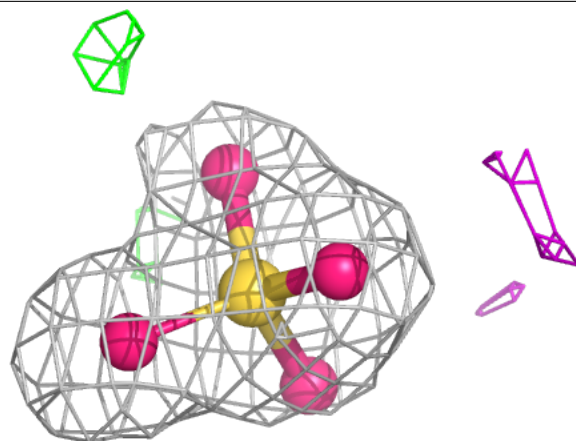
**Electron density around SO4 DDD 303:**

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



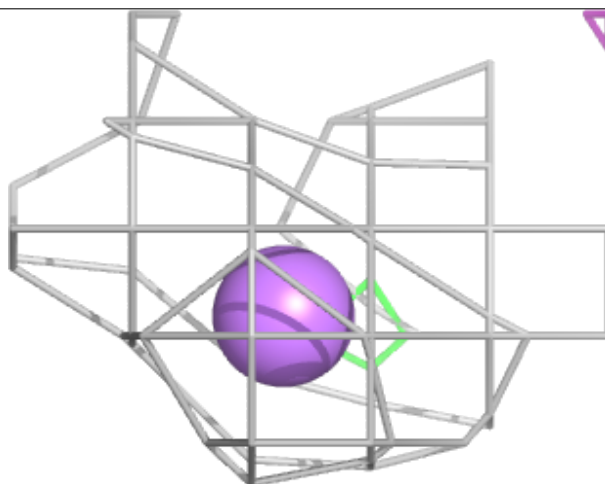
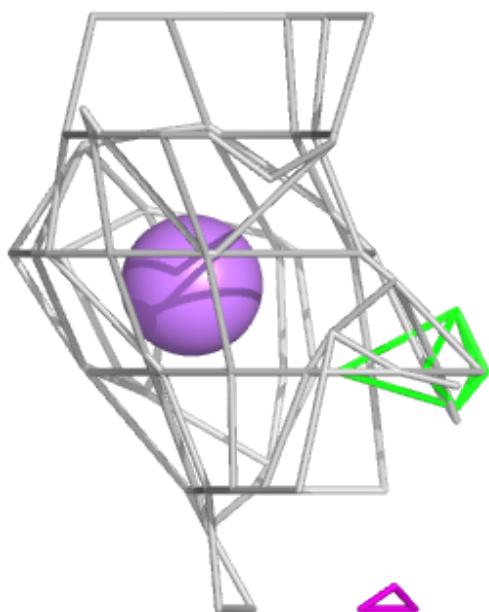
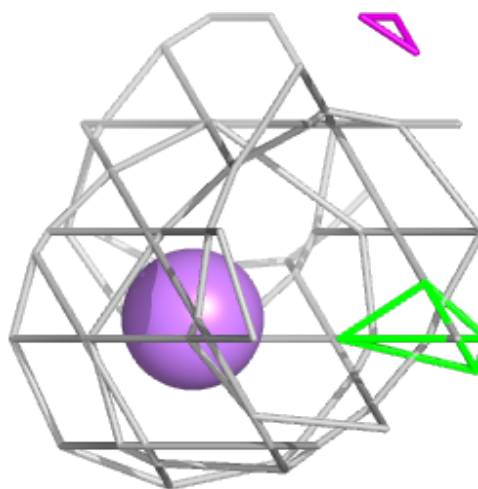
**Electron density around SO4 DDD 305:**

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



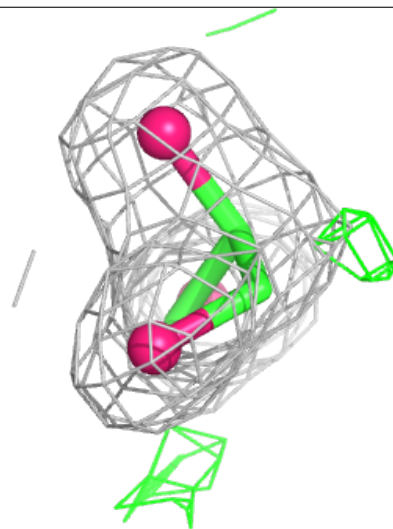
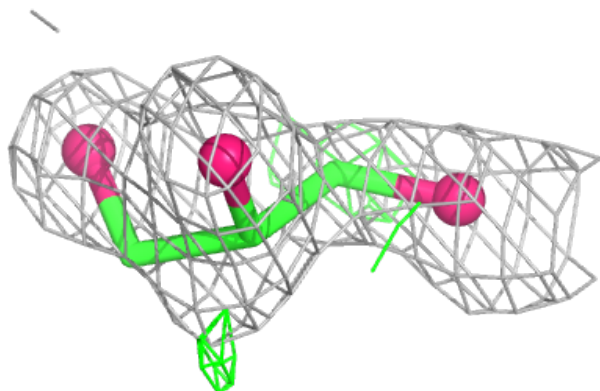
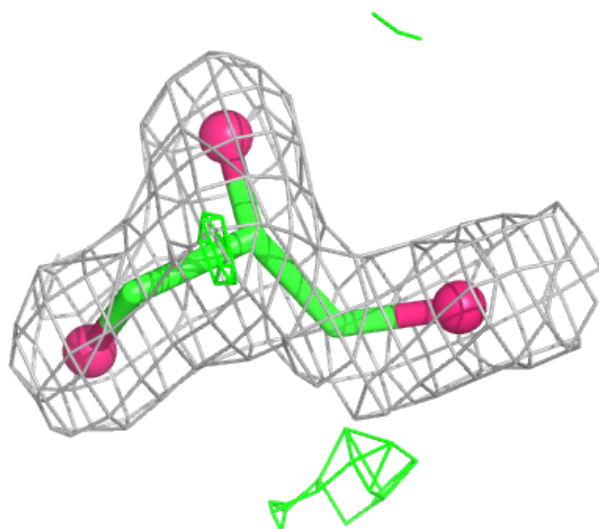
**Electron density around LI AAA 306:**

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



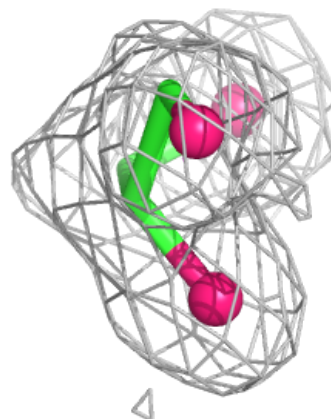
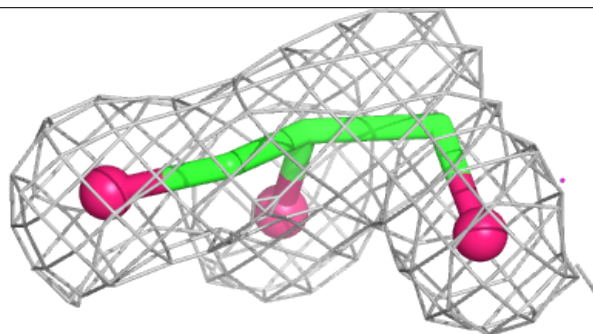
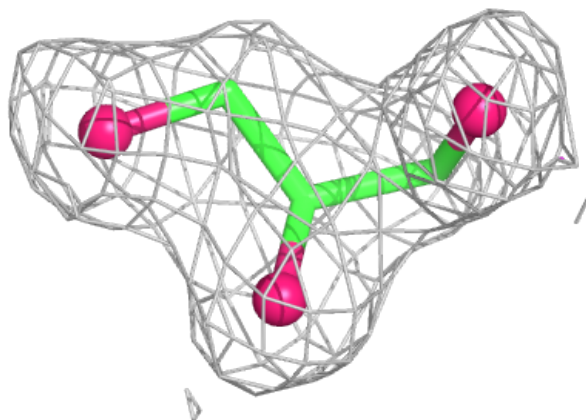
**Electron density around GOL AAA 302:**

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



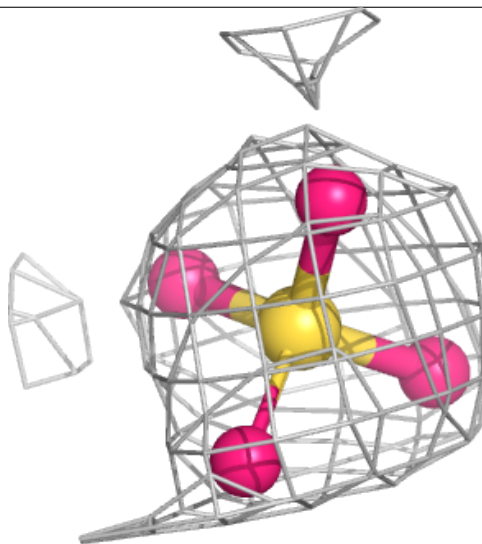
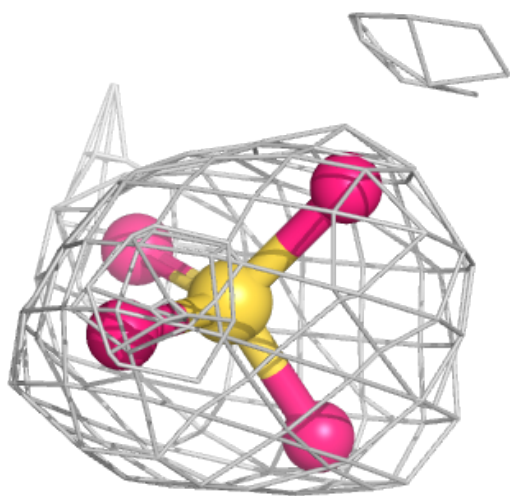
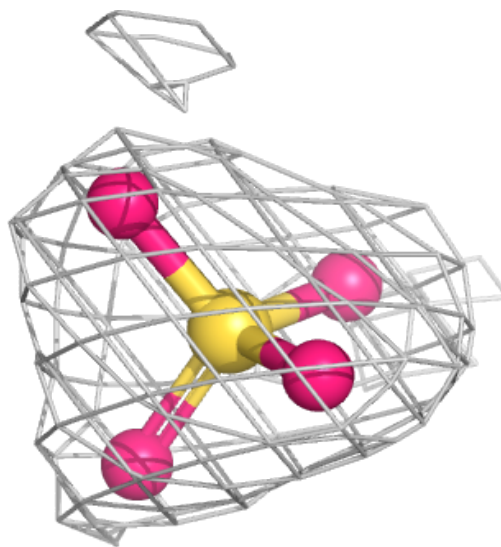
**Electron density around GOL DDD 301:**

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and green (positive)



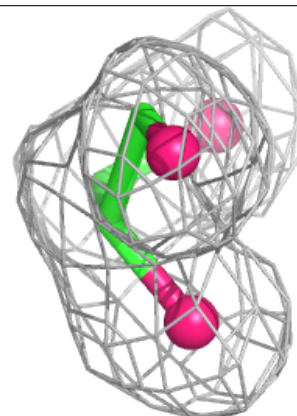
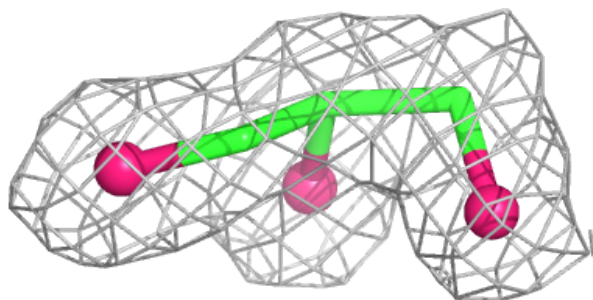
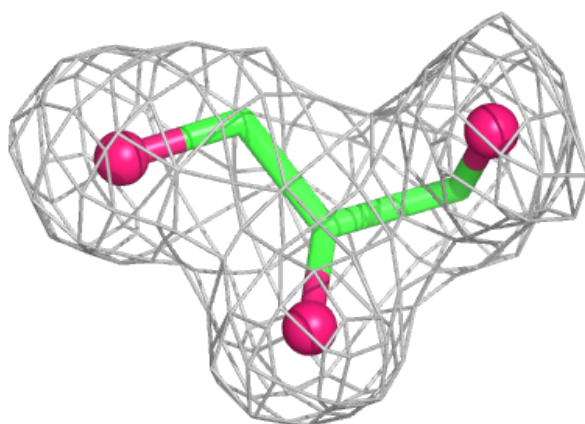
**Electron density around SO4 DDD 304:**

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



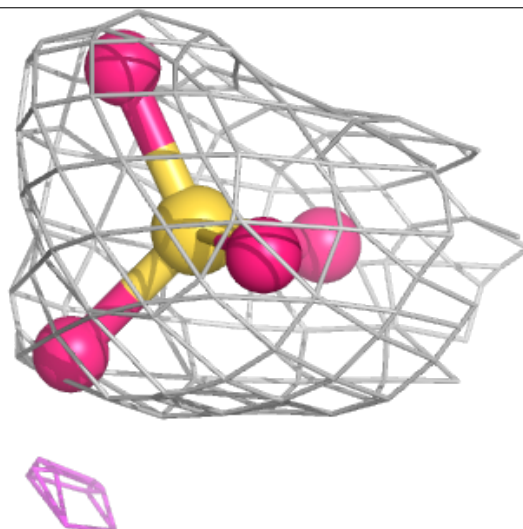
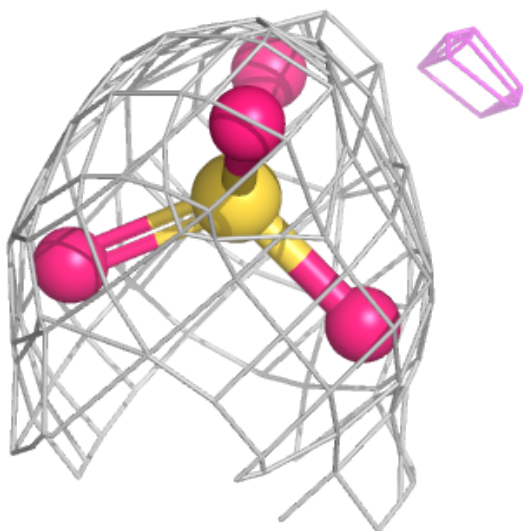
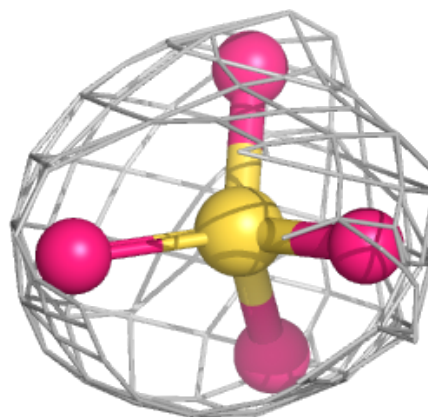
**Electron density around GOL AAA 301:**

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



**Electron density around SO4 AAA 305:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.