



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2022 – 01:14 am BST

PDB ID : 7Q2W
Title : Mutant T91S of uridine phosphorylase from Shewanella oneidensis
Authors : Polyakov, K.; Safonova, T.
Deposited on : 2021-10-26
Resolution : 1.65 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, 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

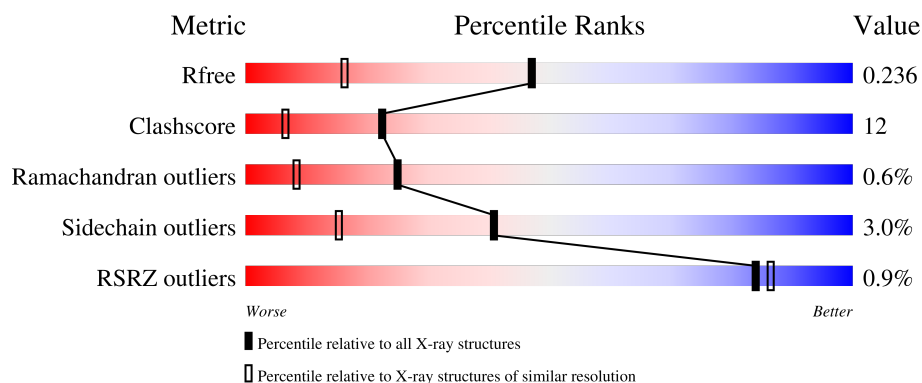
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 ≥ 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	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
1	BBB	251	<div> <div></div> <div> <div>71%</div> <div>21%</div> <div>.</div> <div>.</div> </div> </div>
1	CCC	251	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	DDD	251	<div> <div></div> <div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
1	EEE	251	<div> <div></div> <div> <div>76%</div> <div>18%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	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	SO4	BBB	301[A]	-	-	X	-
2	SO4	EEE	301	-	-	X	-
2	SO4	FFF	303	-	-	X	-
3	GOL	DDD	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22765 atoms, of which 10920 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	H	N	O	S	87	2	0
			3718	1169	1851	322	362	14			
1	FFF	244	Total	C	H	N	O	S	86	3	0
			3649	1146	1824	315	351	13			
1	AAA	245	Total	C	H	N	O	S	85	2	0
			3643	1145	1818	316	350	14			
1	CCC	250	Total	C	H	N	O	S	86	2	0
			3711	1166	1851	321	358	15			
1	EEE	242	Total	C	H	N	O	S	83	1	0
			3583	1126	1789	311	344	13			
1	BBB	240	Total	C	H	N	O	S	83	0	0
			3542	1114	1767	307	341	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	91	SER	THR	engineered mutation	UNP Q8E9X9
FFF	91	SER	THR	engineered mutation	UNP Q8E9X9
AAA	91	SER	THR	engineered mutation	UNP Q8E9X9
CCC	91	SER	THR	engineered mutation	UNP Q8E9X9
EEE	91	SER	THR	engineered mutation	UNP Q8E9X9
BBB	91	SER	THR	engineered mutation	UNP Q8E9X9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



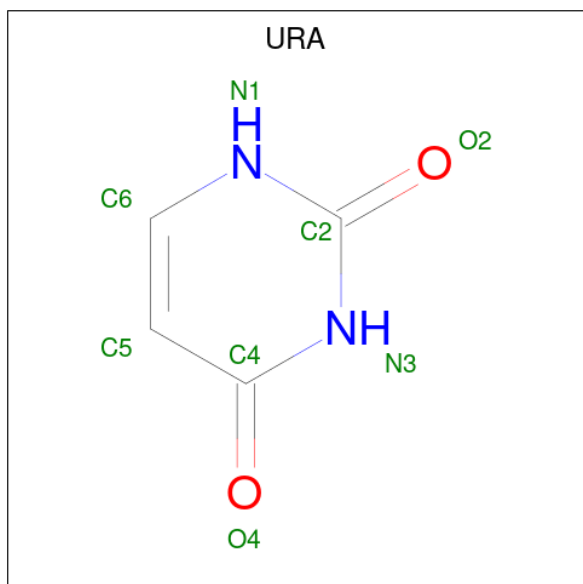
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	O	S	0	0
			5	4	1		
2	FFF	1	Total	O	S	0	1
			5	4	1		
2	FFF	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	EEE	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	1
			10	8	2		
2	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
3	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	FFF	1	Total	C	H	N	O	0
			12	4	4	2	2	

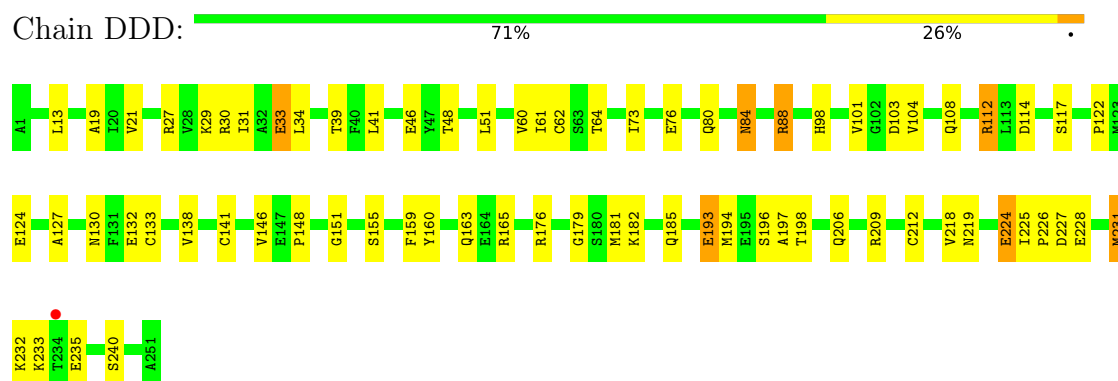
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	DDD	150	Total 150	O 150	0	0
5	FFF	123	Total 123	O 123	0	0
5	AAA	156	Total 156	O 156	0	0
5	CCC	152	Total 152	O 152	0	0
5	EEE	126	Total 126	O 126	0	0
5	BBB	132	Total 132	O 132	0	0

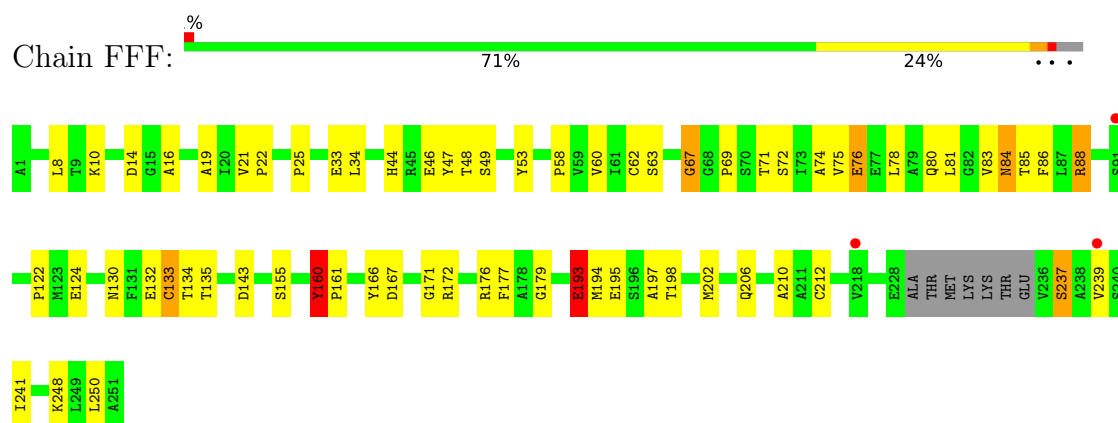
3 Residue-property plots [i](#)

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

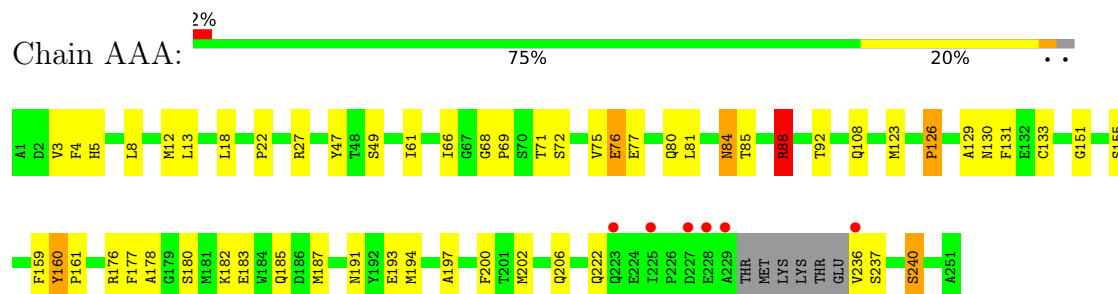
• Molecule 1: Uridine phosphorylase



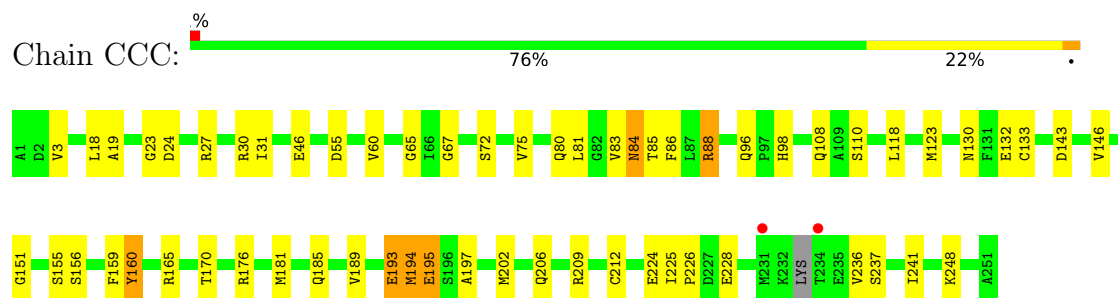
• Molecule 1: Uridine phosphorylase



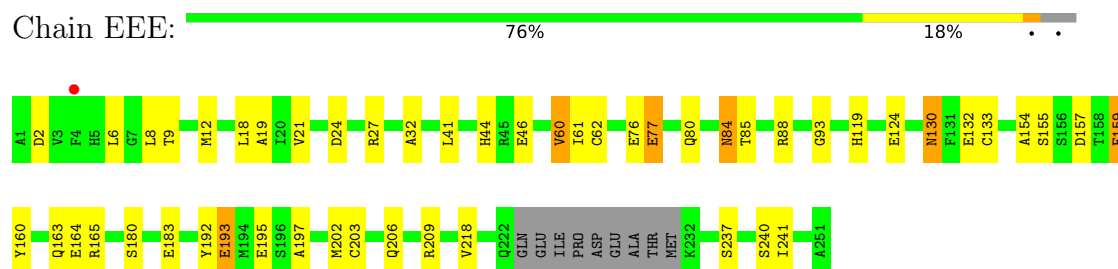
• Molecule 1: Uridine phosphorylase



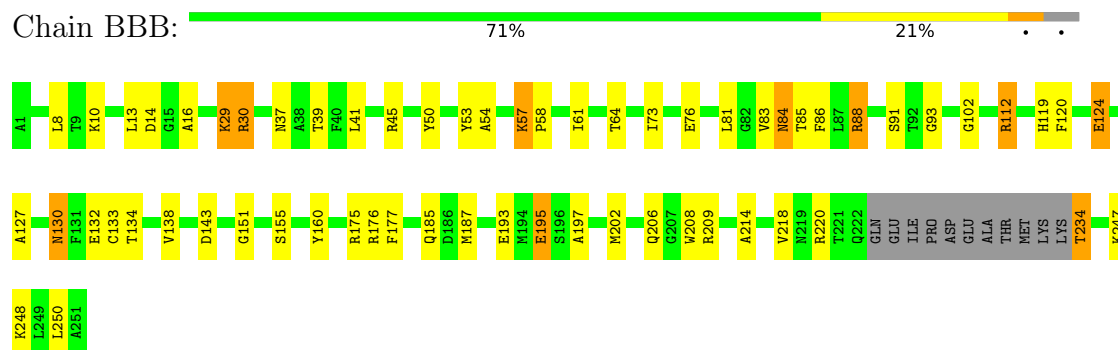
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.40Å 95.49Å 91.41Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	25.00 – 1.65 28.55 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.00-1.65) 98.4 (28.55-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.232 0.195 , 0.236	Depositor DCC
R_{free} test set	7780 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	1.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.338 for -h-l,k,h 0.338 for l,k,-h-l 0.310 for l,-k,h 0.370 for h,-k,-h-l 0.308 for -h-l,-k,l	Xtriage
Reported twinning fraction	0.082 for H, K, L 0.449 for -L, -K, -H 0.136 for -H-L, -K, L 0.040 for L, K, -H-L 0.208 for -H-L, K, H 0.084 for -H, -K, H+L	Depositor
Outliers	0 of 159146 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22765	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, URA, 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	1.06	1/1866 (0.1%)	1.22	3/2536 (0.1%)
1	BBB	1.13	8/1806 (0.4%)	1.22	2/2455 (0.1%)
1	CCC	1.13	4/1902 (0.2%)	1.23	1/2585 (0.0%)
1	DDD	1.13	5/1907 (0.3%)	1.23	5/2593 (0.2%)
1	EEE	1.09	6/1830 (0.3%)	1.22	0/2488
1	FFF	1.11	7/1869 (0.4%)	1.20	3/2542 (0.1%)
All	All	1.11	31/11180 (0.3%)	1.22	14/15199 (0.1%)

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	BBB	0	1
1	CCC	0	2
1	DDD	0	1
1	EEE	0	3
All	All	0	7

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	124	GLU	CD-OE2	9.05	1.35	1.25
1	AAA	76	GLU	CD-OE2	6.93	1.33	1.25
1	BBB	124	GLU	CD-OE2	-6.88	1.18	1.25
1	CCC	80	GLN	C-O	6.88	1.36	1.23
1	FFF	76	GLU	CD-OE2	6.73	1.33	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	209	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	DDD	165	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	FFF	172	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	CCC	195	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	DDD	227	ASP	CB-CA-C	6.10	122.60	110.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	194	MET	Mainchain
1	CCC	209	ARG	Mainchain
1	DDD	232	LYS	Peptide
1	EEE	44	HIS	Mainchain
1	EEE	60	VAL	Mainchain

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	1825	1818	1807	44	0
1	BBB	1775	1767	1758	38	1
1	CCC	1860	1851	1836	44	1
1	DDD	1867	1851	1839	54	0
1	EEE	1794	1789	1777	29	0
1	FFF	1825	1824	1810	48	0
2	AAA	5	0	0	0	0
2	BBB	15	0	0	2	0
2	DDD	5	0	0	0	0
2	EEE	5	0	0	2	0
2	FFF	10	0	0	7	0
3	AAA	6	8	8	1	0
3	DDD	6	8	8	6	0
4	FFF	8	4	3	1	0
5	AAA	156	0	0	10	0
5	BBB	132	0	0	12	0
5	CCC	152	0	0	9	0
5	DDD	150	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	EEE	126	0	0	4	0
5	FFF	123	0	0	4	0
All	All	11845	10920	10846	253	1

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 12.

The worst 5 of 253 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:EEE:165[A]:ARG:HD2	5:EEE:401:HOH:O	1.16	1.34
1:CCC:123:MET:HE3	5:CCC:370:HOH:O	1.58	1.02
2:EEE:301:SO4:S	5:EEE:402:HOH:O	2.17	0.99
1:FFF:130:ASN:O	1:FFF:134[B]:THR:HG23	1.63	0.98
2:BBB:301[A]:SO4:O2	5:BBB:402:HOH:O	1.85	0.92

All (1) 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)
1:CCC:228:GLU:OE1	1:BBB:185:GLN:HE21[2_646]	1.51	0.09

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	243/251 (97%)	235 (97%)	7 (3%)	1 (0%)	34	16
1	BBB	236/251 (94%)	226 (96%)	9 (4%)	1 (0%)	34	16
1	CCC	248/251 (99%)	236 (95%)	11 (4%)	1 (0%)	34	16
1	DDD	251/251 (100%)	242 (96%)	6 (2%)	3 (1%)	13	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EEE	239/251 (95%)	226 (95%)	12 (5%)	1 (0%)	34	16
1	FFF	243/251 (97%)	234 (96%)	8 (3%)	1 (0%)	34	16
All	All	1460/1506 (97%)	1399 (96%)	53 (4%)	8 (0%)	25	11

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	160	TYR
1	DDD	235	GLU
1	FFF	160	TYR
1	AAA	160	TYR
1	CCC	160	TYR

5.3.2 Protein sidechains ⓘ

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	191/197 (97%)	182 (95%)	9 (5%)	26	6
1	BBB	185/197 (94%)	176 (95%)	9 (5%)	25	5
1	CCC	195/197 (99%)	190 (97%)	5 (3%)	46	21
1	DDD	195/197 (99%)	188 (96%)	7 (4%)	35	11
1	EEE	187/197 (95%)	185 (99%)	2 (1%)	73	57
1	FFF	193/197 (98%)	187 (97%)	6 (3%)	40	14
All	All	1146/1182 (97%)	1108 (97%)	38 (3%)	41	12

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	193	GLU
1	BBB	91	SER
1	BBB	29	LYS
1	BBB	57	LYS
1	BBB	234	THR

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
2	SO4	EEE	301	-	4,4,4	1.65	1 (25%)	6,6,6	1.24	0
3	GOL	AAA	302	-	5,5,5	0.19	0	5,5,5	0.64	0
4	URA	FFF	301	-	6,8,8	1.45	1 (16%)	4,10,10	12.35	4 (100%)
2	SO4	FFF	303	-	4,4,4	0.67	0	6,6,6	0.34	0
2	SO4	BBB	302	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	BBB	301[A]	-	4,4,4	0.72	0	6,6,6	0.37	0
2	SO4	BBB	301[B]	-	4,4,4	0.57	0	6,6,6	0.47	0
2	SO4	DDD	301	-	4,4,4	0.18	0	6,6,6	0.51	0
3	GOL	DDD	302	-	5,5,5	0.50	0	5,5,5	0.38	0
2	SO4	AAA	301	-	4,4,4	0.24	0	6,6,6	0.23	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
4	URA	FFF	301	-	-	-	0/1/1/1
3	GOL	DDD	302	-	-	1/4/4/4	-
3	GOL	AAA	302	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	301	SO4	O1-S	-2.54	1.32	1.46
4	FFF	301	URA	C4-N3	2.20	1.36	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	FFF	301	URA	C6-N1-C2	17.49	123.05	114.42
4	FFF	301	URA	N3-C2-N1	-16.91	114.98	128.43
4	FFF	301	URA	C5-C4-N3	-3.18	116.31	123.31
4	FFF	301	URA	C5-C6-N1	-2.86	120.40	123.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

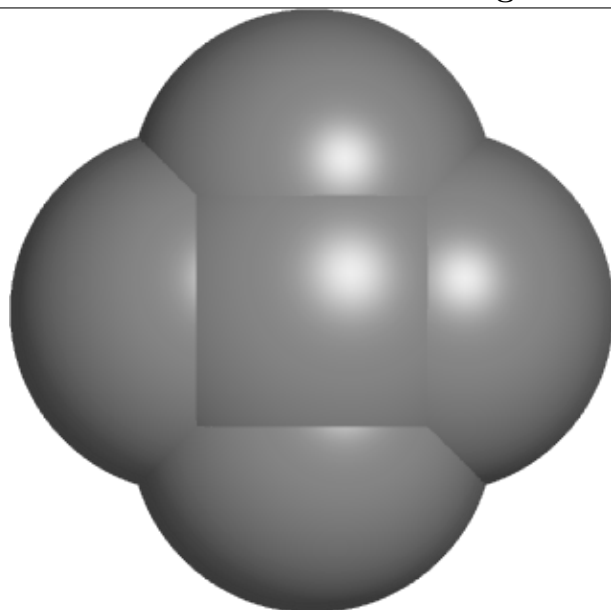
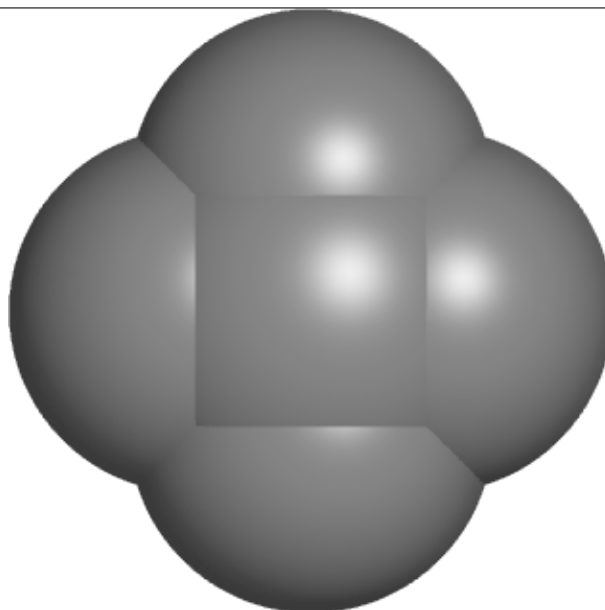
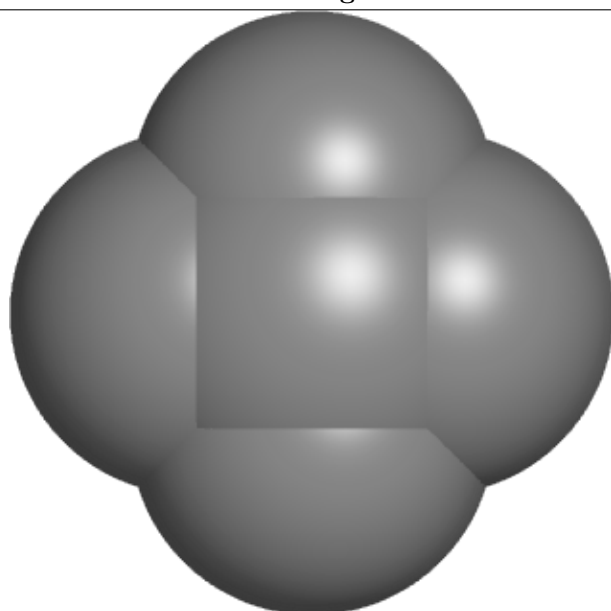
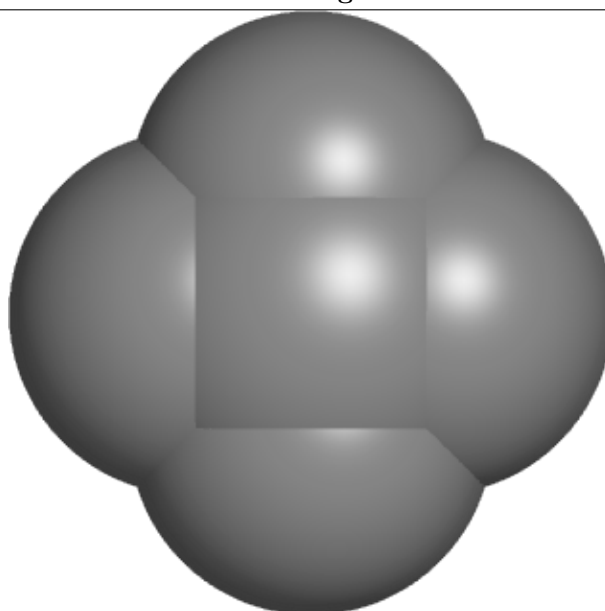
Mol	Chain	Res	Type	Atoms
3	AAA	302	GOL	O1-C1-C2-C3
3	AAA	302	GOL	C1-C2-C3-O3
3	AAA	302	GOL	O1-C1-C2-O2
3	AAA	302	GOL	O2-C2-C3-O3
3	DDD	302	GOL	O1-C1-C2-O2

There are no ring outliers.

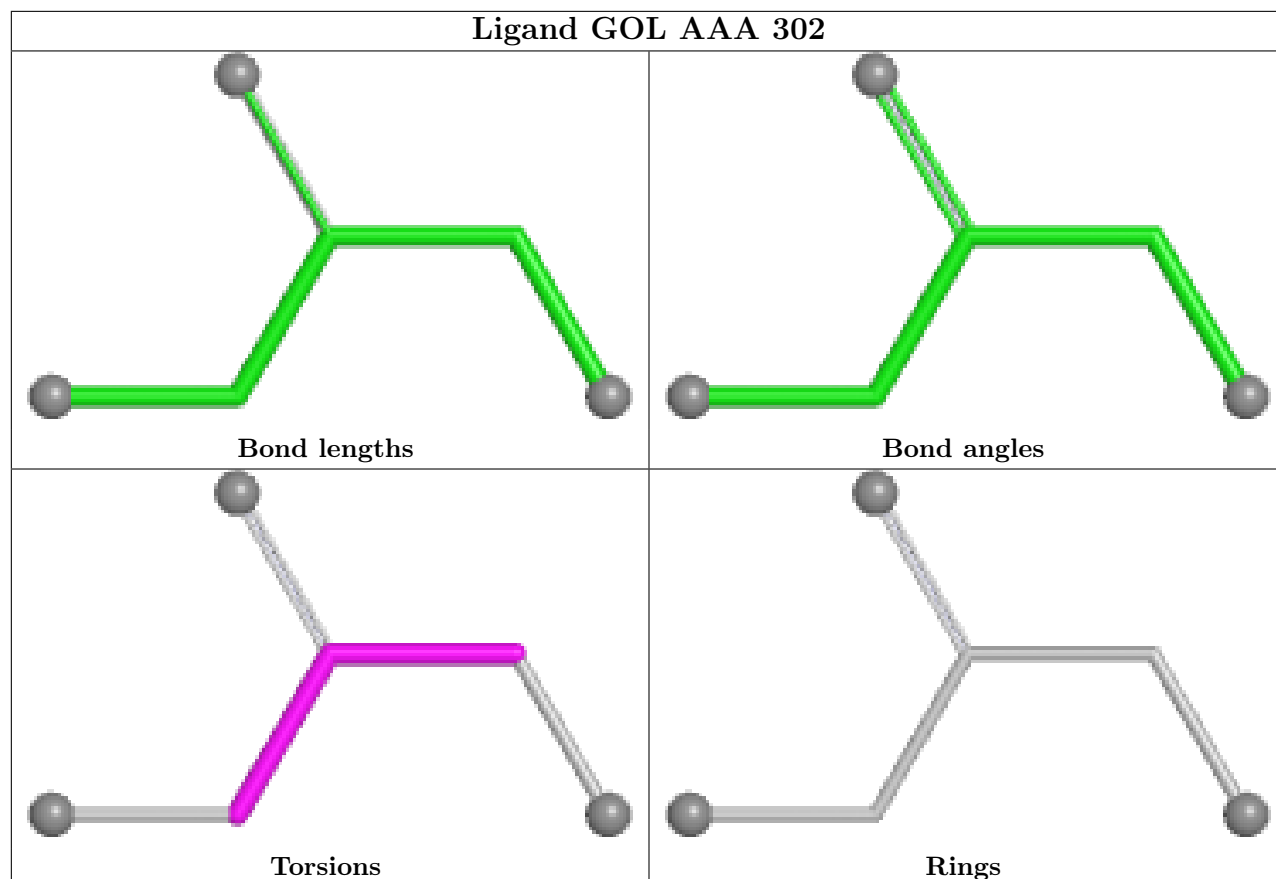
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EEE	301	SO4	2	0
3	AAA	302	GOL	1	0
4	FFF	301	URA	1	0
2	FFF	303	SO4	7	0
2	BBB	301[A]	SO4	2	0
3	DDD	302	GOL	6	0

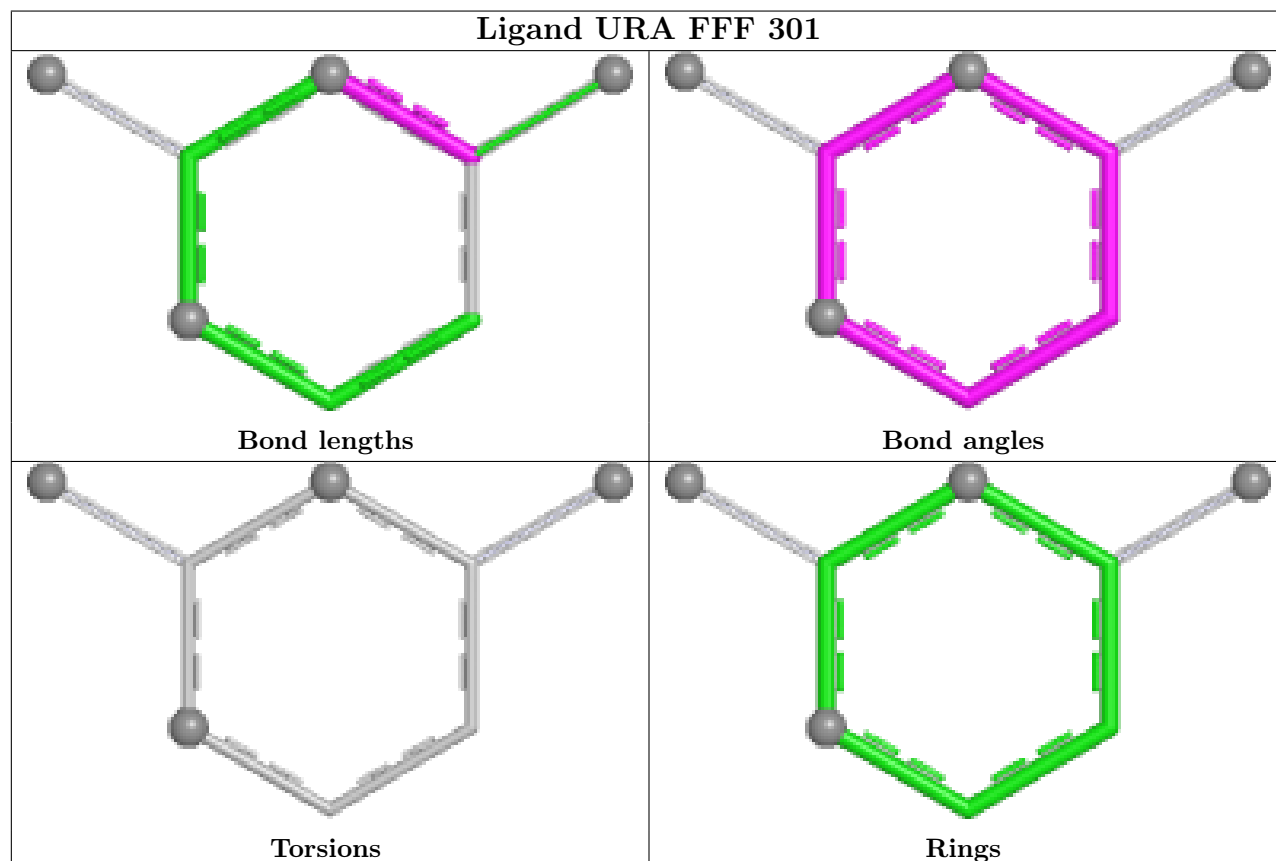
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

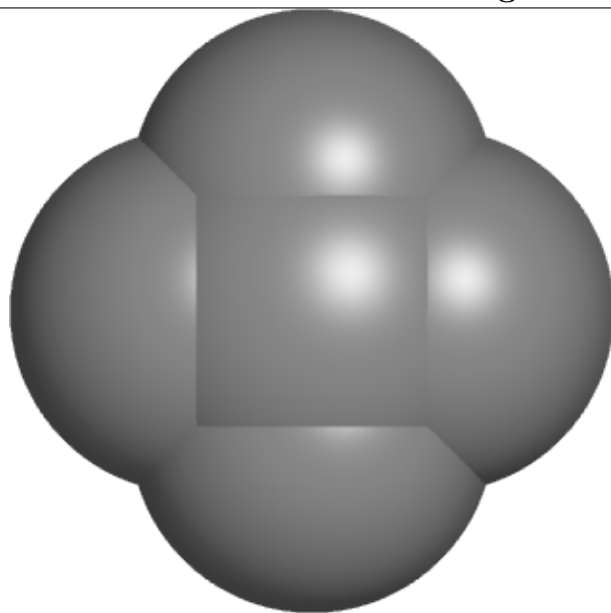
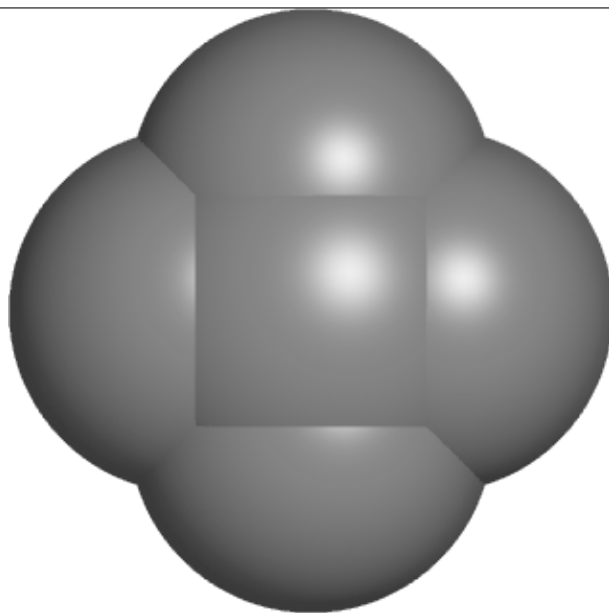
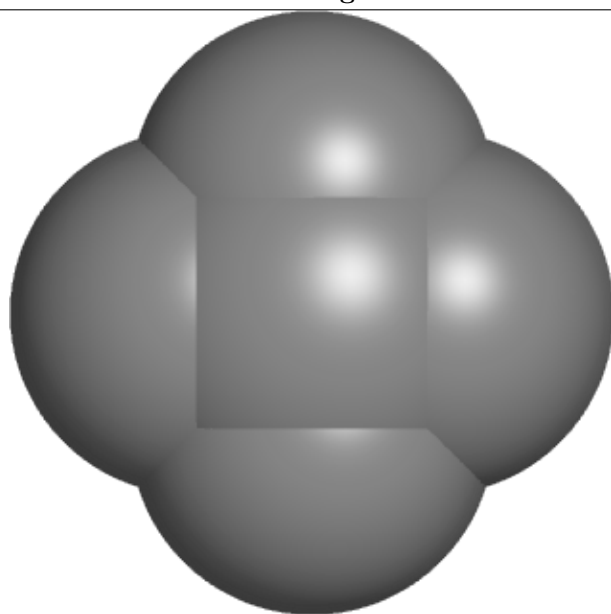
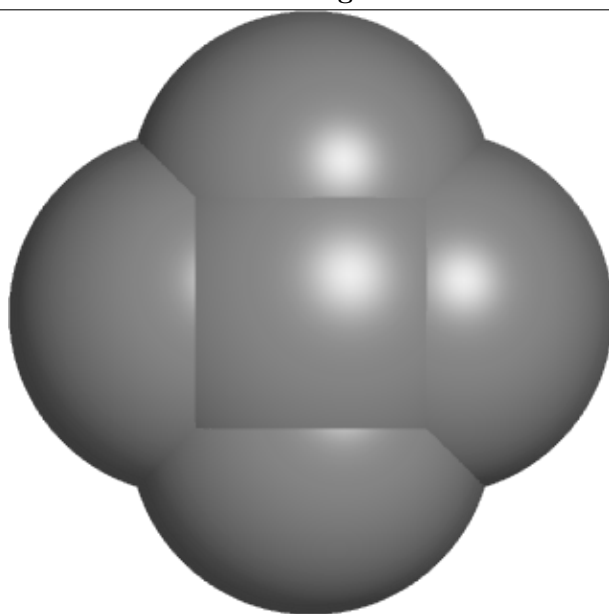
Ligand SO4 EEE 301**Bond lengths****Bond angles****Torsions****Rings**

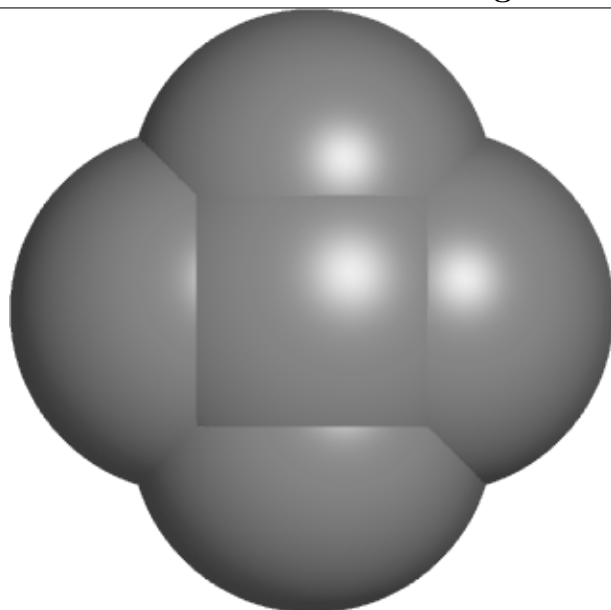
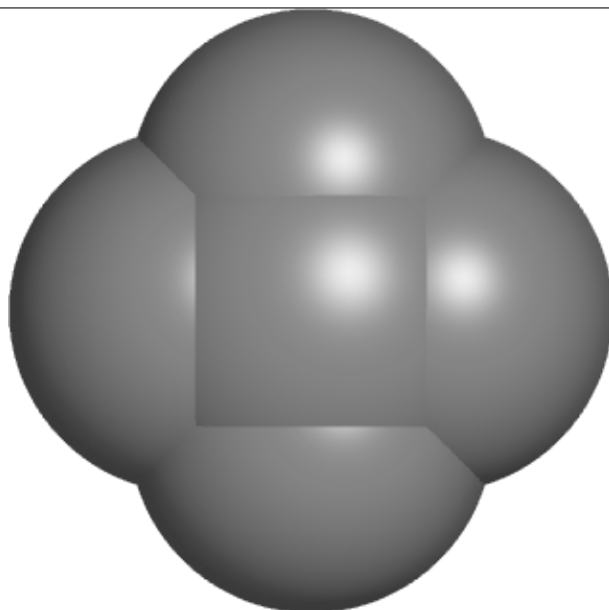
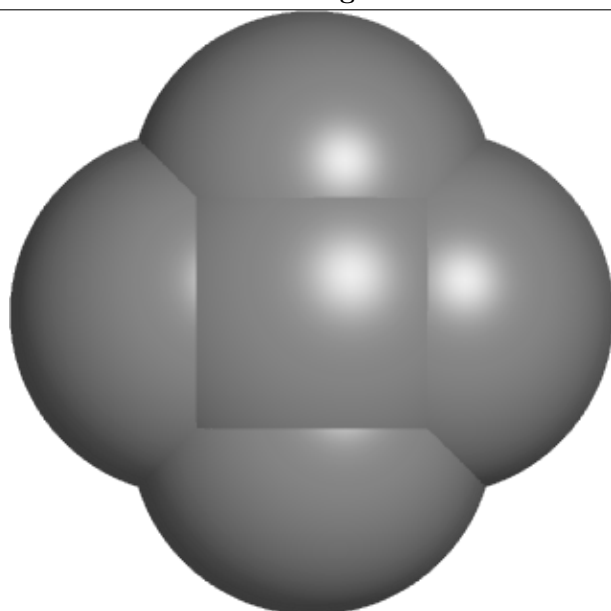
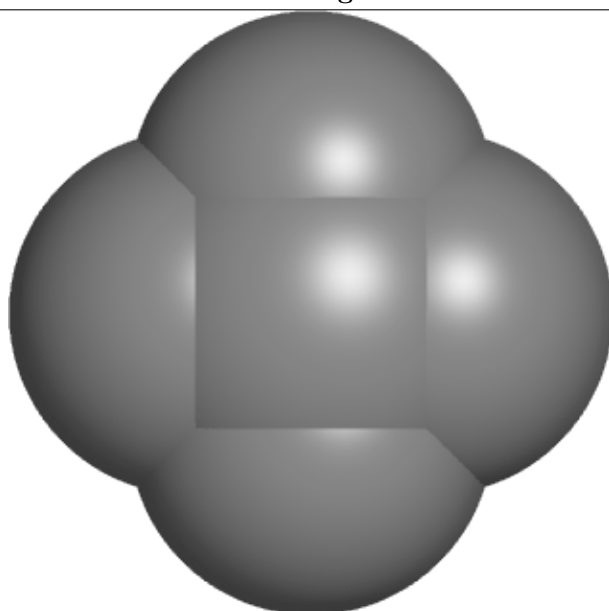
Ligand GOL AAA 302

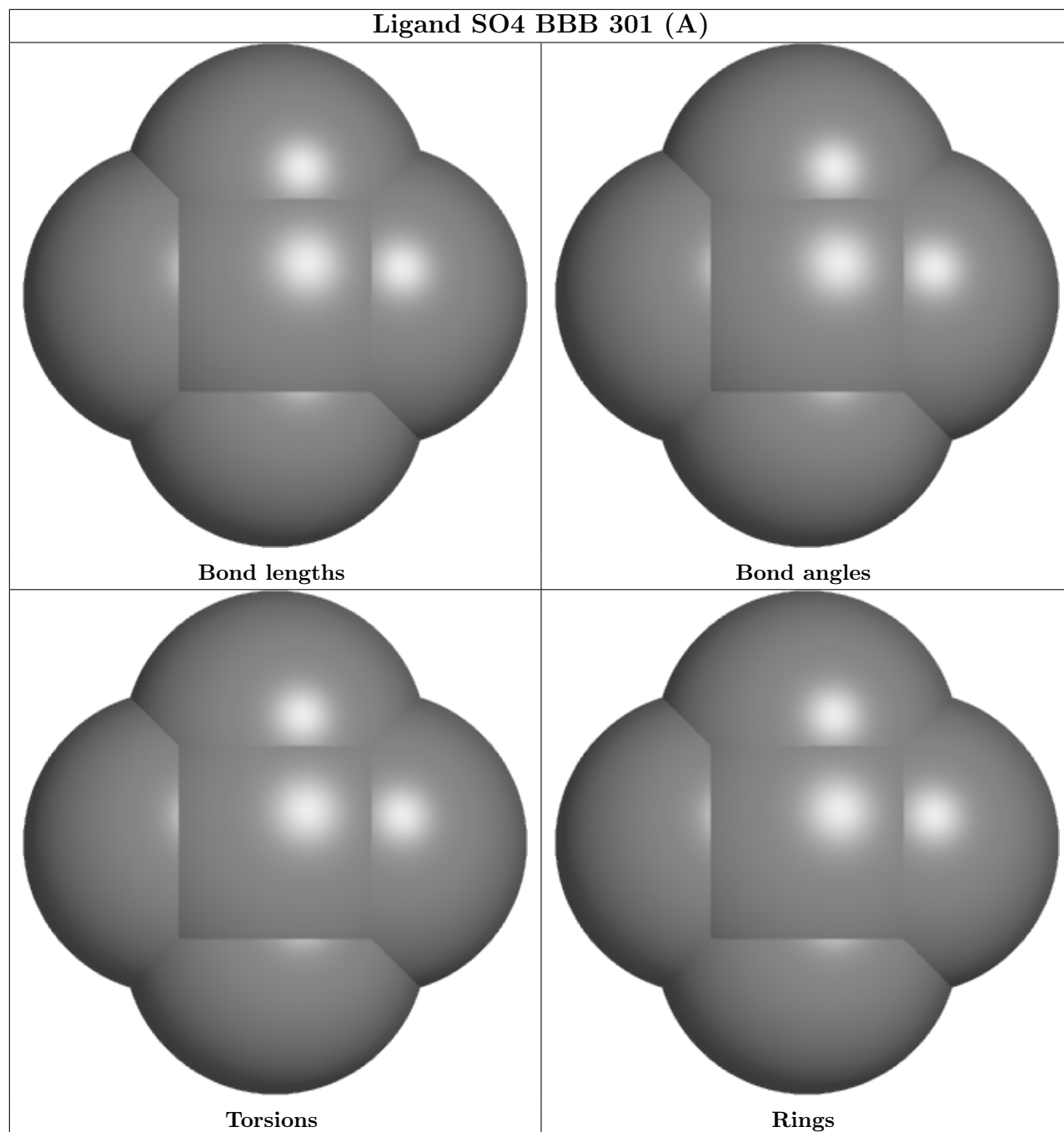


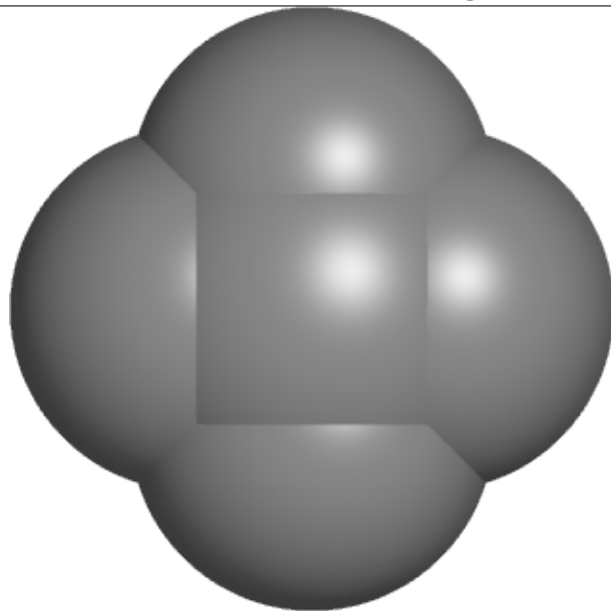
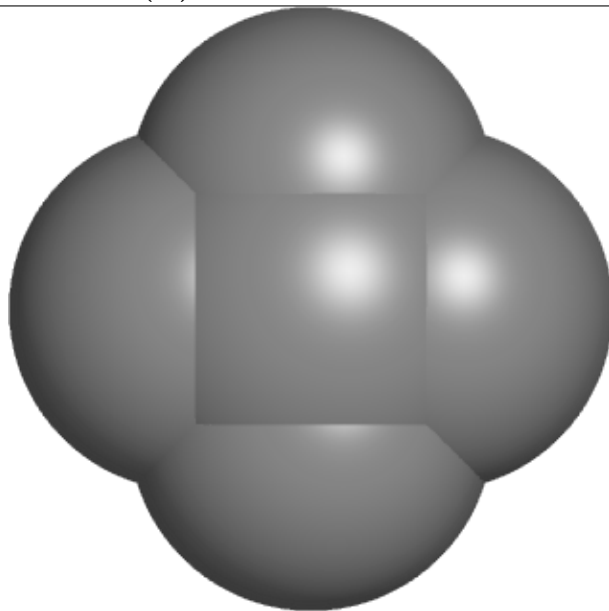
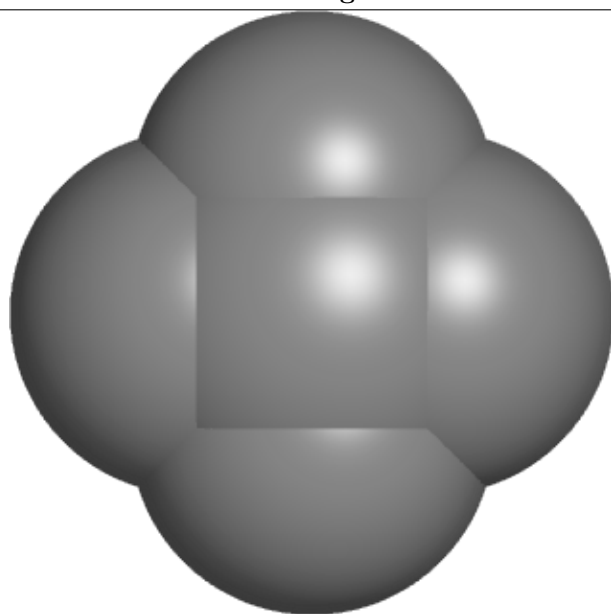
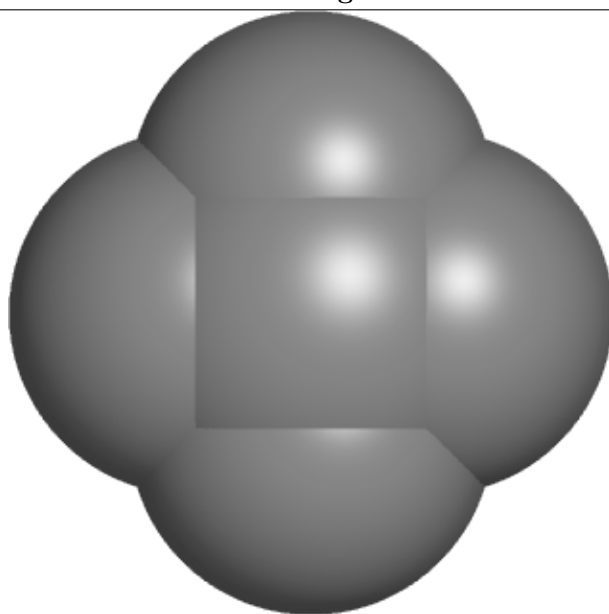
Ligand URA FFF 301

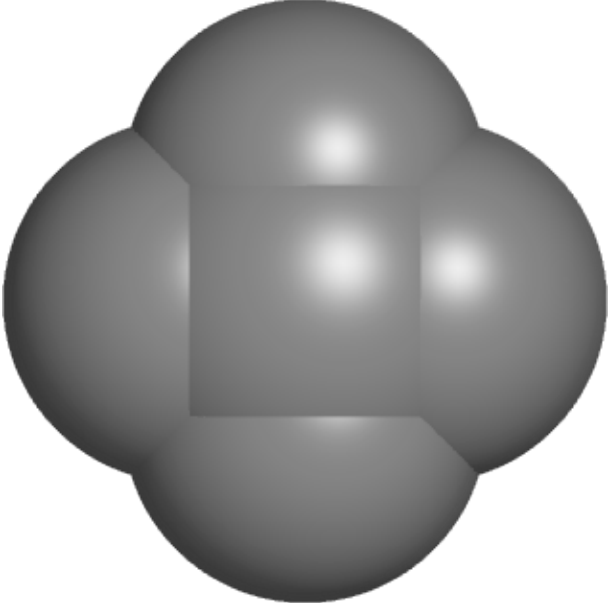
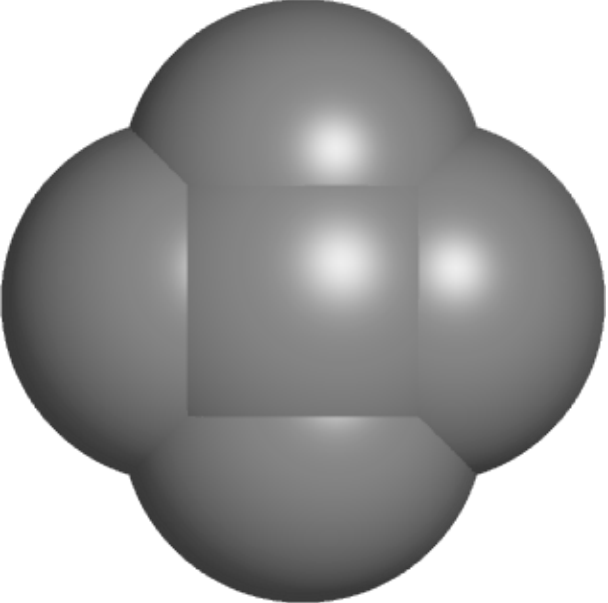
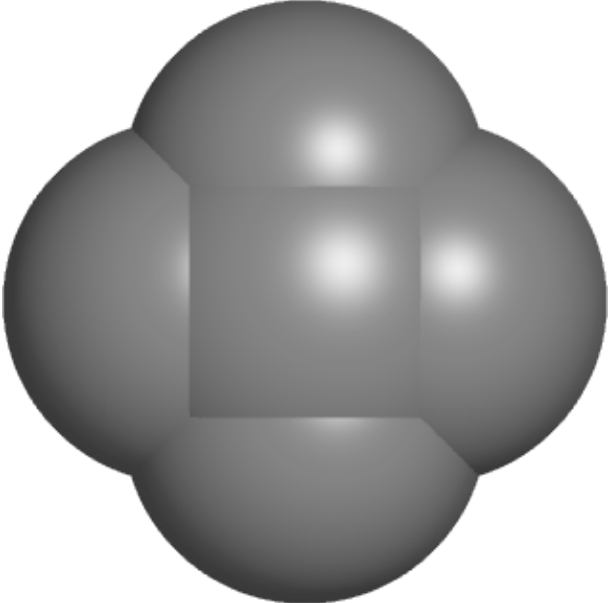
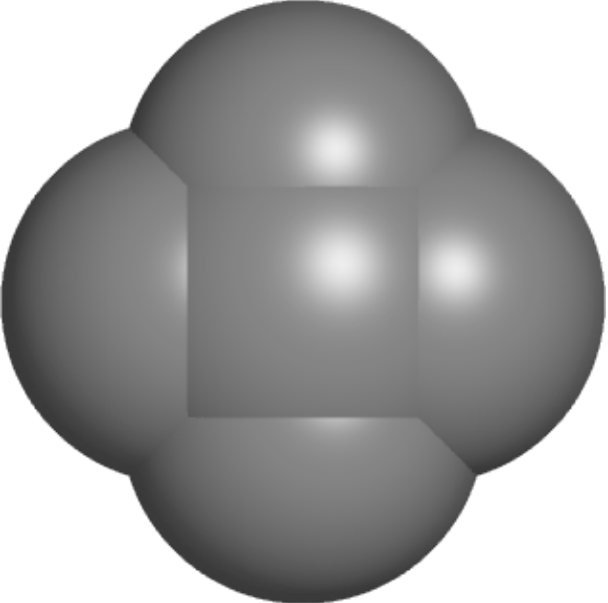


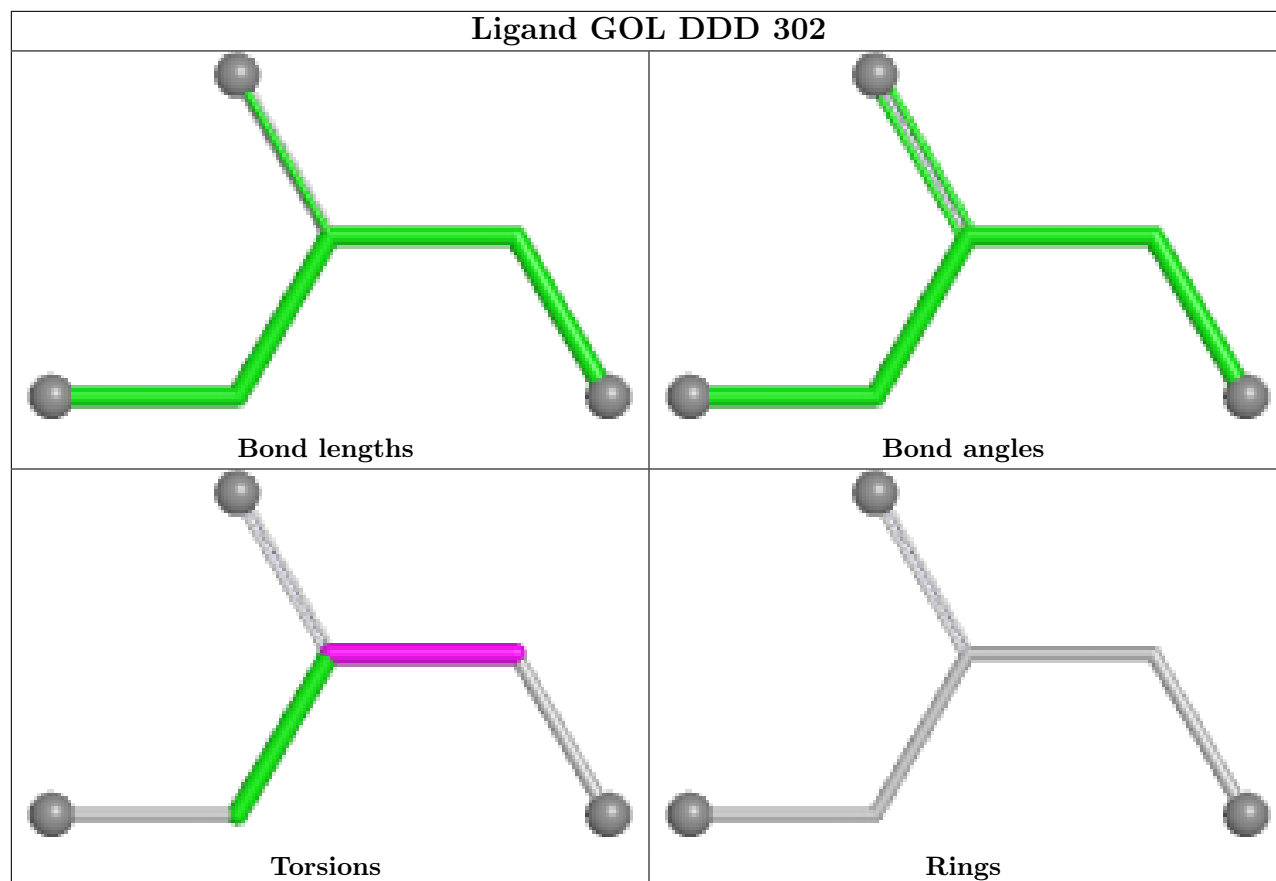
Ligand SO4 FFF 303**Bond lengths****Bond angles****Torsions****Rings**

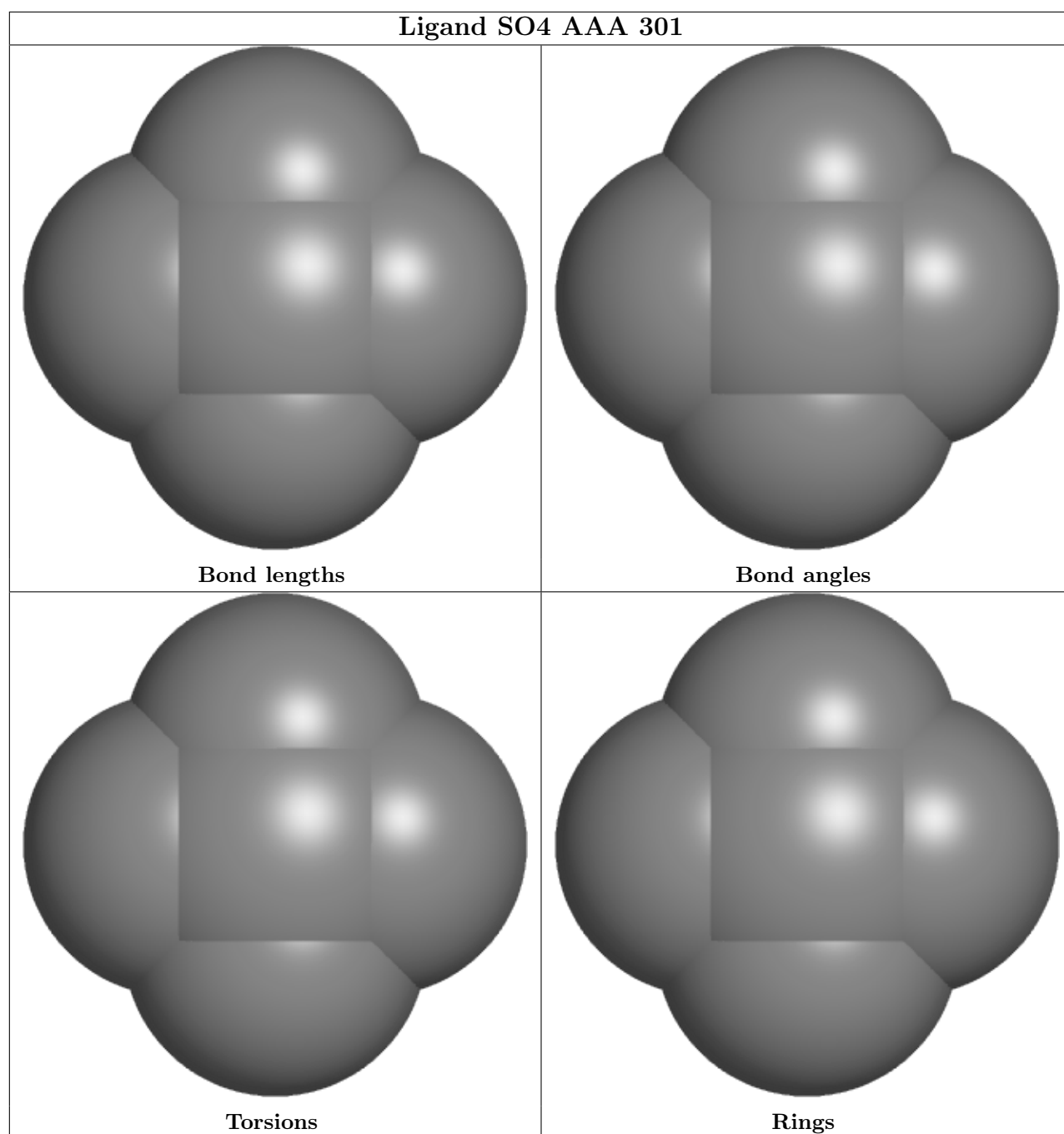
Ligand SO4 BBB 302**Bond lengths****Bond angles****Torsions****Rings**



Ligand SO4 BBB 301 (B)**Bond lengths****Bond angles****Torsions****Rings**

Ligand SO4 DDD 301	
	
Bond lengths	Bond angles
	
Torsions	Rings





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	245/251 (97%)	0.29	6 (2%) 59 59	10, 17, 30, 57	0
1	BBB	240/251 (95%)	0.22	0 100 100	11, 17, 28, 37	0
1	CCC	250/251 (99%)	0.14	2 (0%) 86 88	9, 16, 25, 46	0
1	DDD	251/251 (100%)	0.17	1 (0%) 92 93	10, 17, 28, 45	0
1	EEE	242/251 (96%)	0.13	1 (0%) 92 93	10, 17, 27, 40	0
1	FFF	244/251 (97%)	0.25	3 (1%) 79 81	9, 18, 31, 49	0
All	All	1472/1506 (97%)	0.20	13 (0%) 84 86	9, 17, 29, 57	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	236	VAL	6.0
1	AAA	228	GLU	4.0
1	AAA	229	ALA	3.5
1	FFF	91	SER	2.6
1	AAA	225	ILE	2.6

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

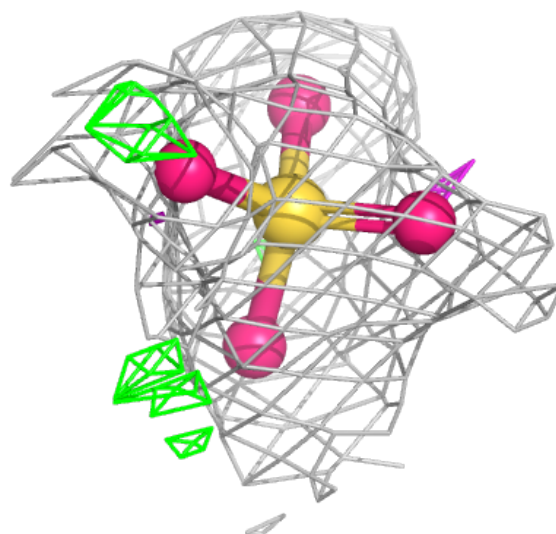
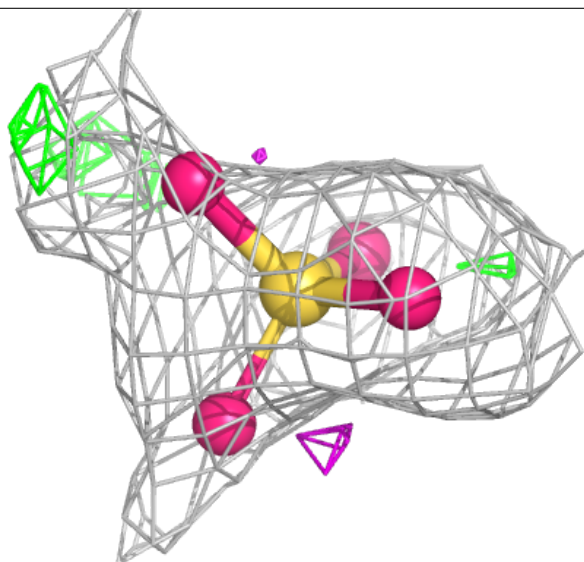
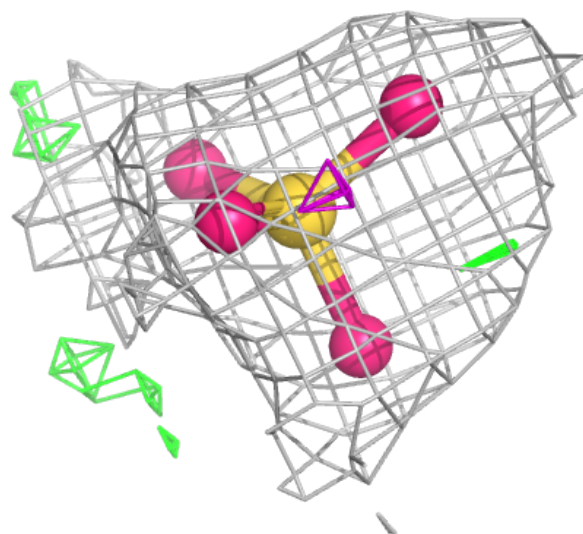
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	FFF	302[A]	5/5	0.81	0.27	21,22,23,30	5
2	SO4	AAA	301	5/5	0.86	0.17	35,40,46,52	0
4	URA	FFF	301	8/8	0.88	0.14	22,28,30,30	0
3	GOL	DDD	302	6/6	0.90	0.16	15,19,24,27	2
2	SO4	DDD	301	5/5	0.92	0.10	25,26,34,36	0
3	GOL	AAA	302	6/6	0.93	0.13	19,23,29,29	2
2	SO4	FFF	303	5/5	0.93	0.20	15,16,19,20	5
2	SO4	EEE	301	5/5	0.95	0.11	11,14,18,20	0
2	SO4	BBB	301[A]	5/5	0.95	0.11	8,9,10,11	5
2	SO4	BBB	301[B]	5/5	0.95	0.11	8,9,10,11	5
2	SO4	BBB	302	5/5	0.96	0.11	33,38,41,41	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.

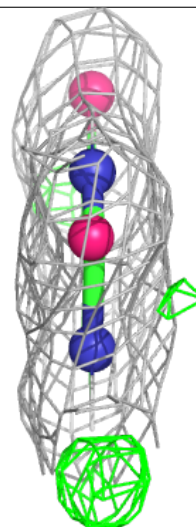
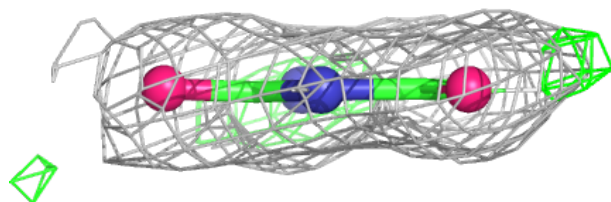
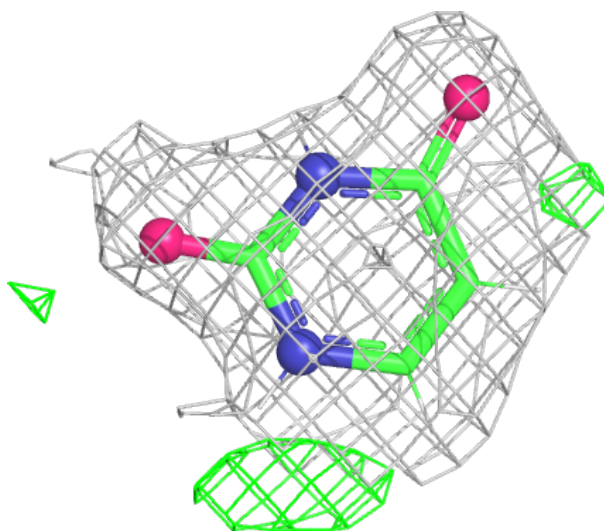
Electron density around SO4 AAA 301:

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



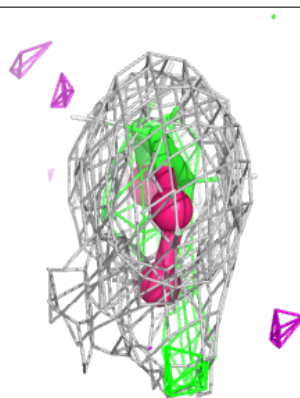
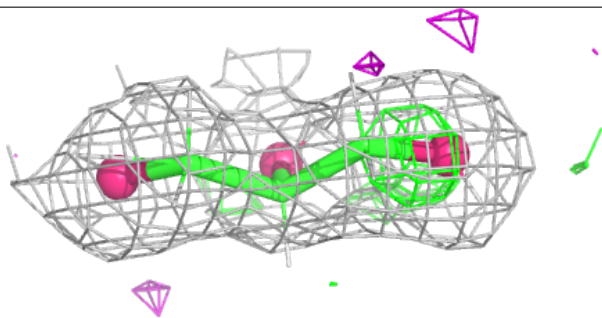
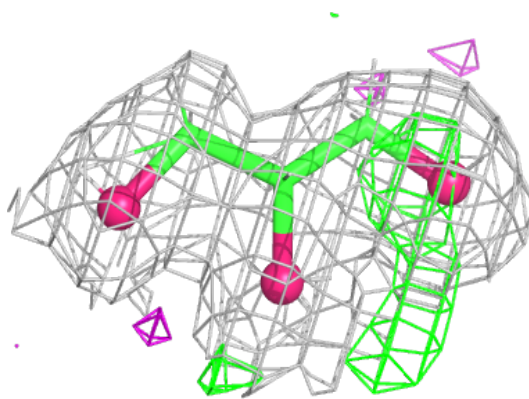
Electron density around URA FFF 301:

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



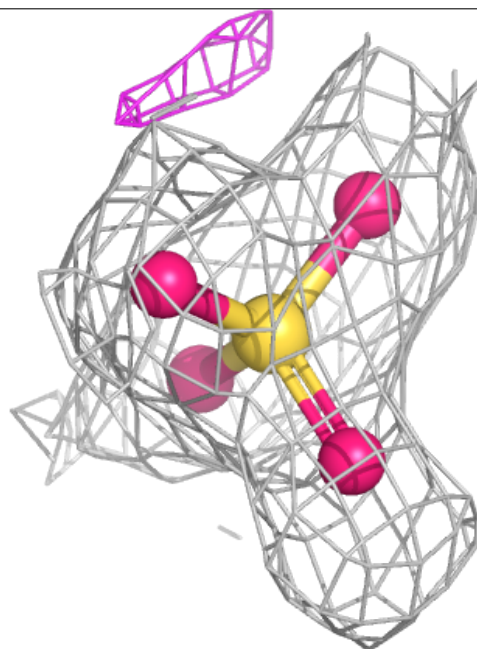
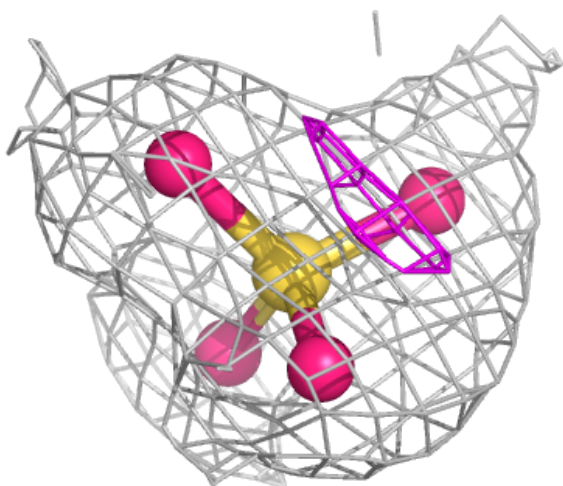
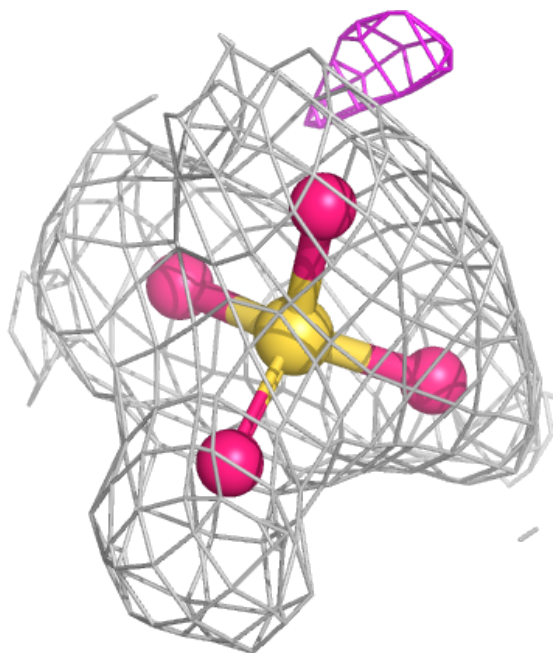
Electron density around GOL DDD 302:

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



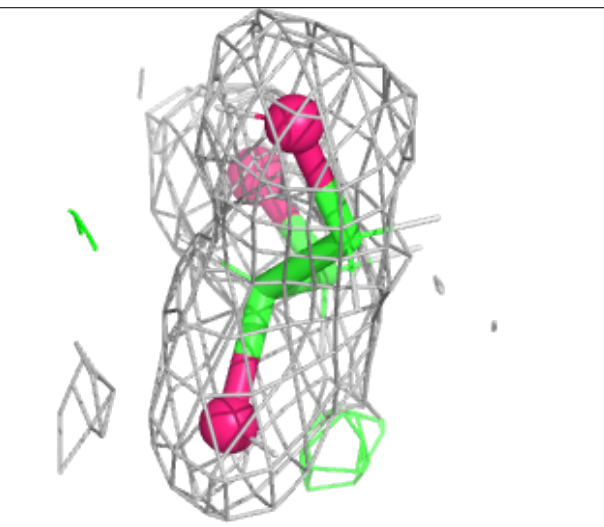
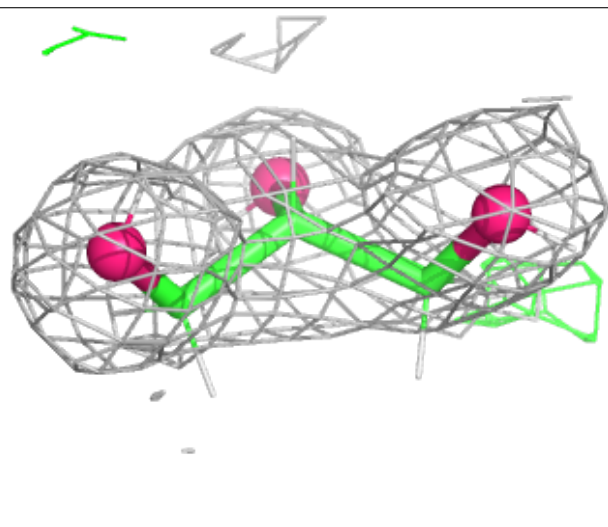
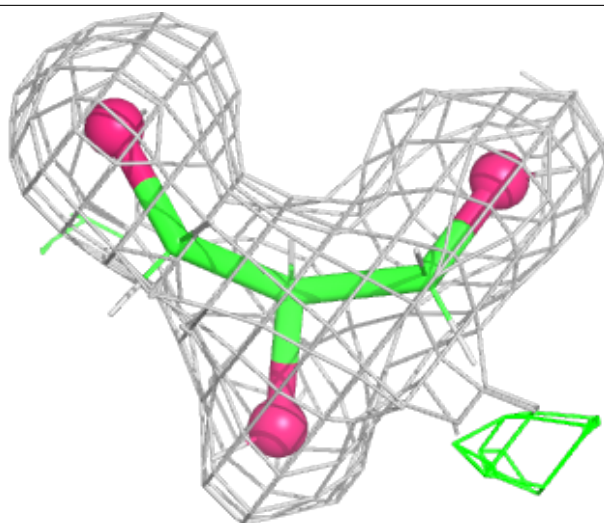
Electron density around SO4 DDD 301:

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



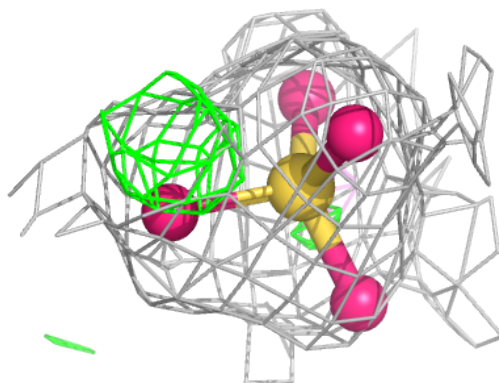
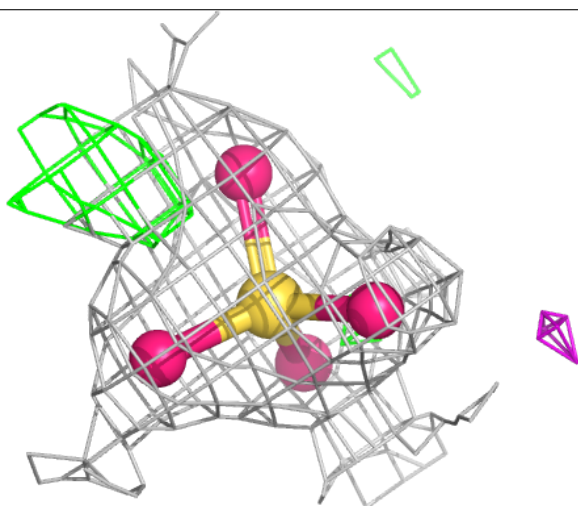
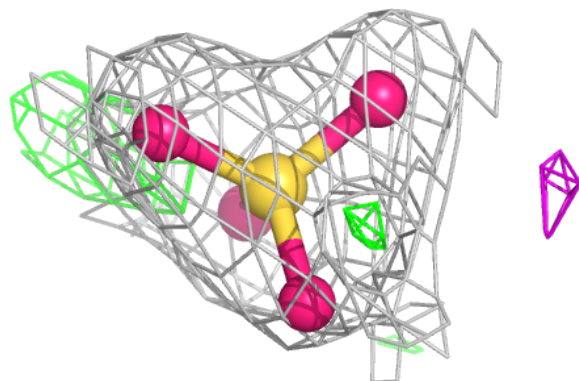
Electron density around GOL AAA 302:

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



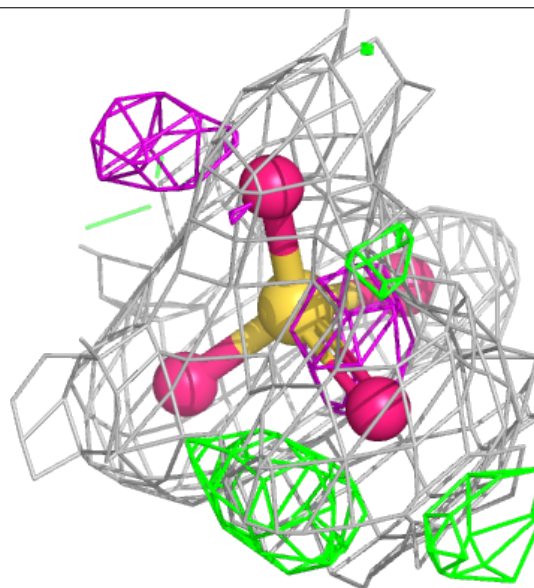
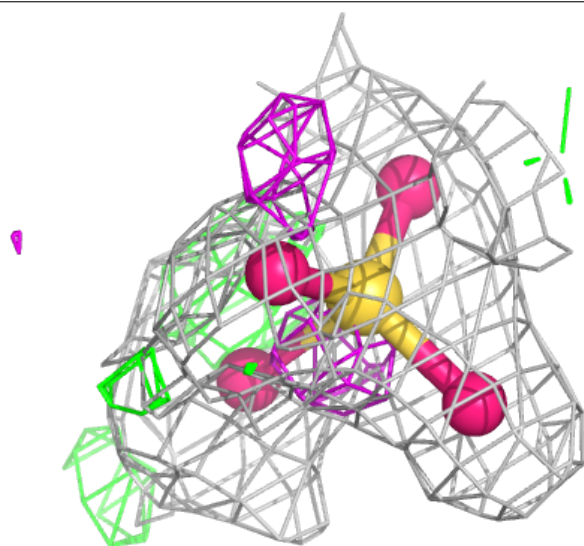
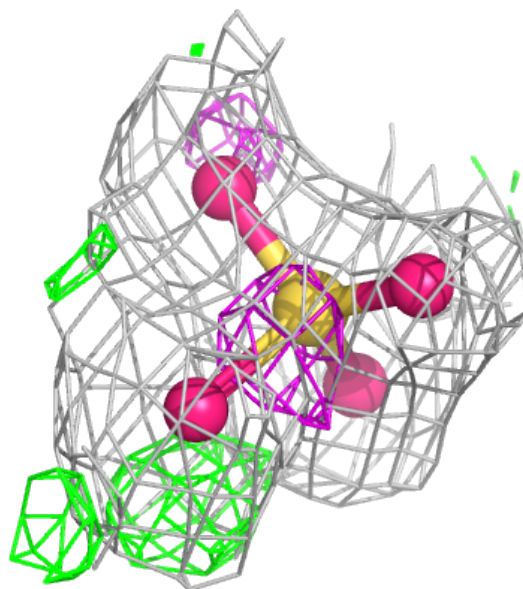
Electron density around SO4 FFF 303:

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



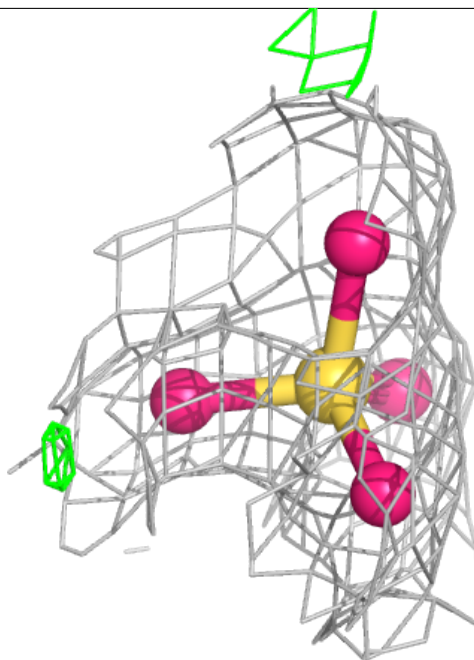
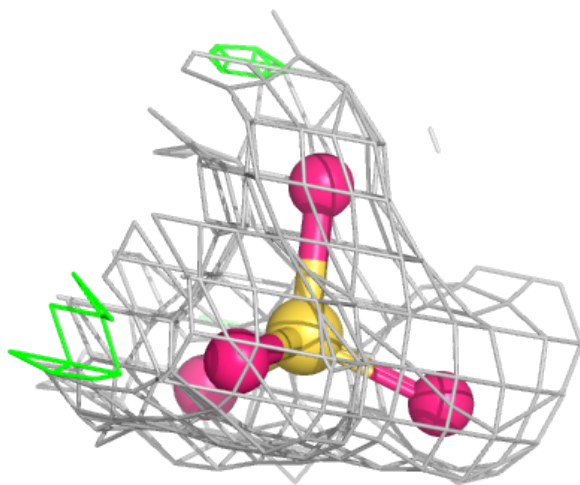
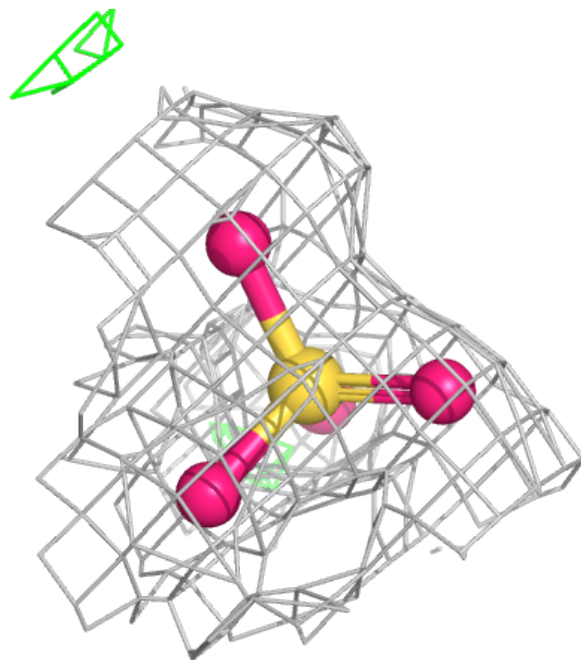
Electron density around SO4 EEE 301:

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



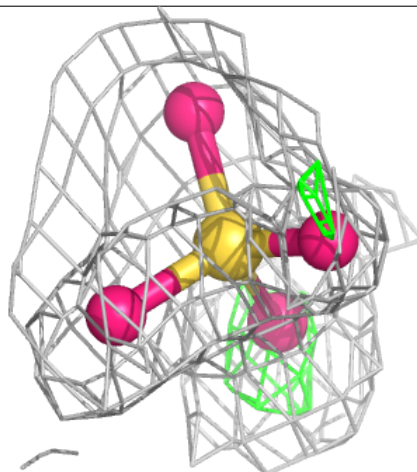
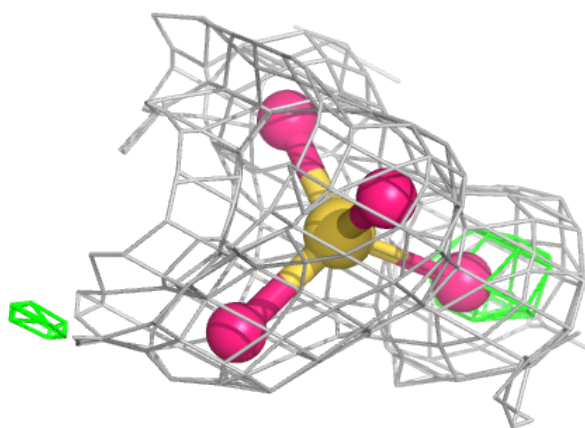
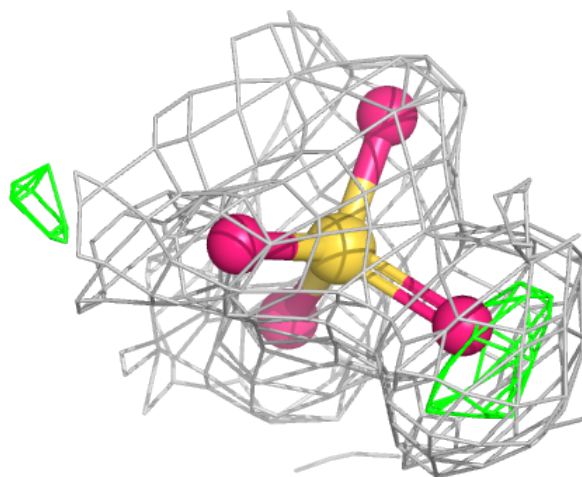
Electron density around SO4 BBB 301 (A):

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



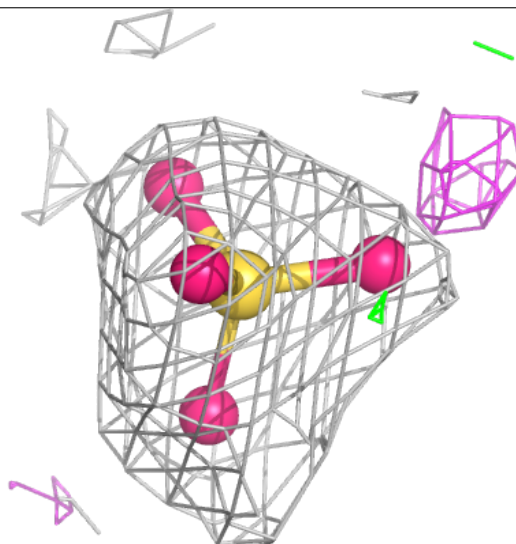
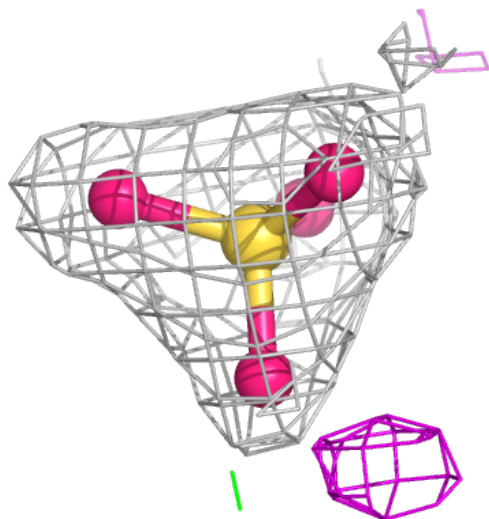
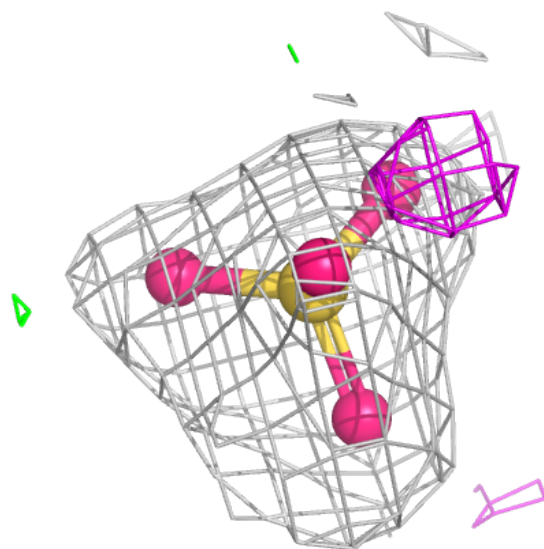
Electron density around SO4 BBB 301 (B):

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



Electron density around SO4 BBB 302:

$2mF_o-DF_c$ (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.