



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 06:40 AM EDT

PDB ID : 6RNG
Title : Dipeptide Gly-Pro binds to a glycolytic enzyme fructose biphosphate aldolase
Authors : Shahar, A.; Zarivach, R.; Skirycz, A.; Wojciechowska, I.
Deposited on : 2019-05-08
Resolution : 2.15 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

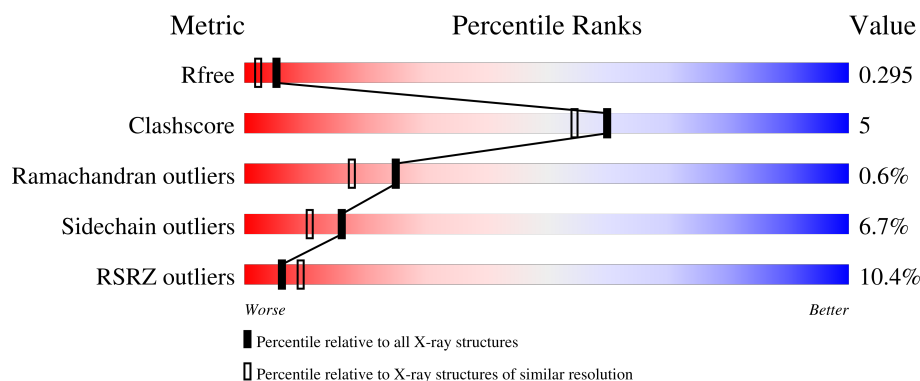
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	A	358	<div> <div>4%</div> <div>82%</div> <div>8%</div> <div>6%</div> </div>
1	B	358	<div> <div>17%</div> <div>81%</div> <div>10%</div> <div>7%</div> </div>
1	F	358	<div> <div>8%</div> <div>81%</div> <div>11%</div> <div>6%</div> </div>
1	G	358	<div> <div>10%</div> <div>78%</div> <div>13%</div> <div>7%</div> </div>

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	B	401	-	-	X	-
3	GLY	B	407	-	-	-	X

2 Entry composition [i](#)

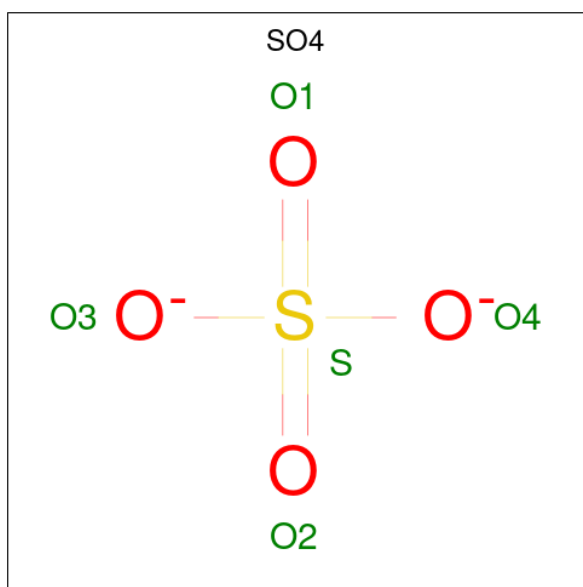
There are 5 unique types of molecules in this entry. The entry contains 10669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-bisphosphate aldolase 6, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2539	1600	441	489	9			
1	B	334	Total	C	N	O	S	0	2	0
			2530	1593	443	485	9			
1	F	337	Total	C	N	O	S	0	3	0
			2563	1615	450	489	9			
1	G	334	Total	C	N	O	S	0	1	0
			2517	1586	438	484	9			

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



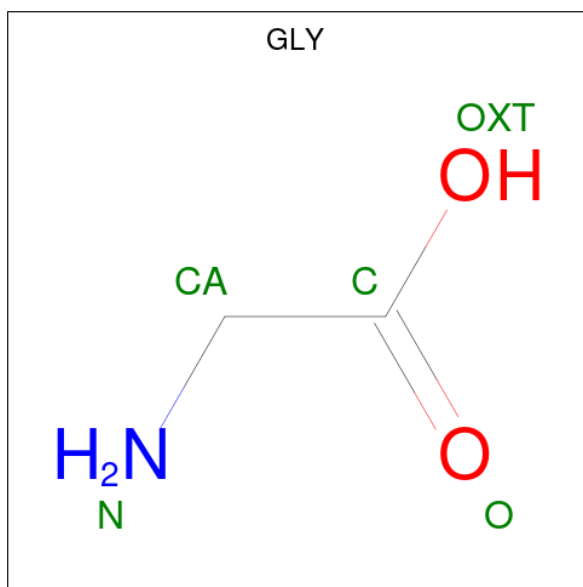
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

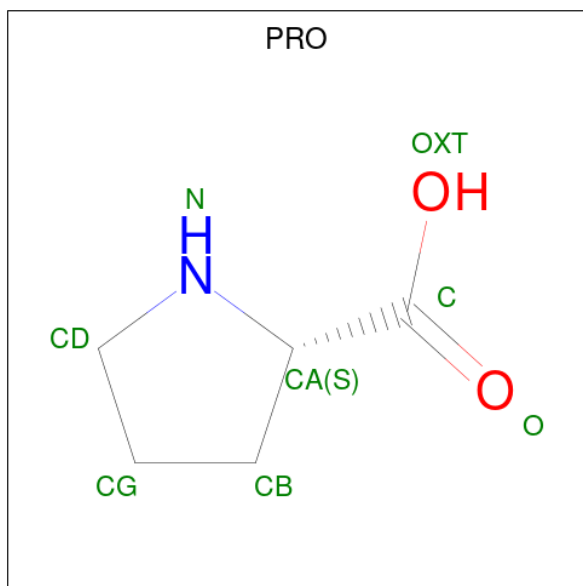
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			4	2	1	1		
3	G	1	Total	C	N	O	0	0
			4	2	1	1		
3	G	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 4 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	5	1	2		
4	G	1	Total	C	N	O	0	0
			8	5	1	2		
4	G	1	Total	C	N	O	0	0
			8	5	1	2		

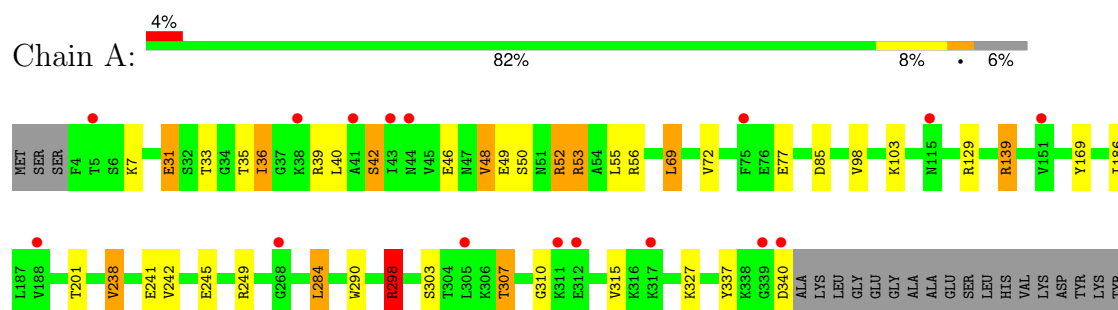
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	85	Total	O	0	0
			85	85		
5	F	120	Total	O	0	0
			120	120		
5	G	113	Total	O	0	0
			113	113		

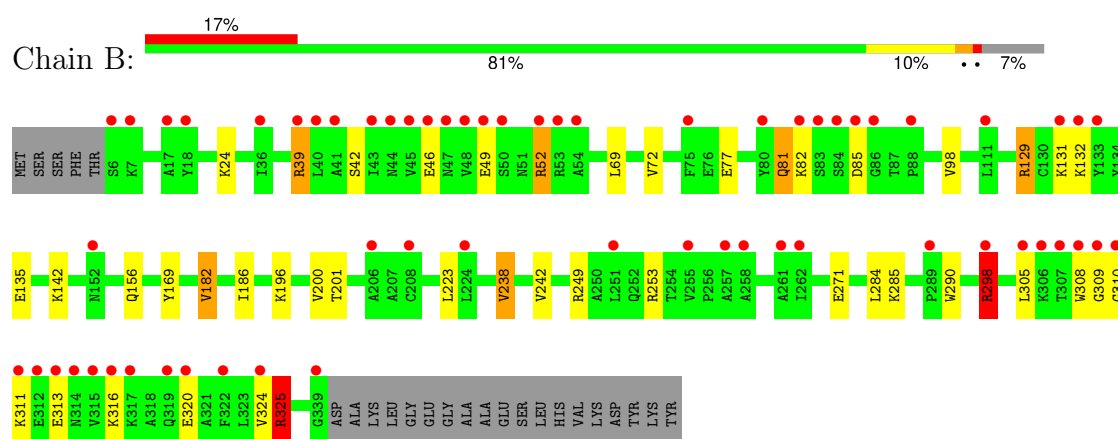
3 Residue-property plots [i](#)

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.

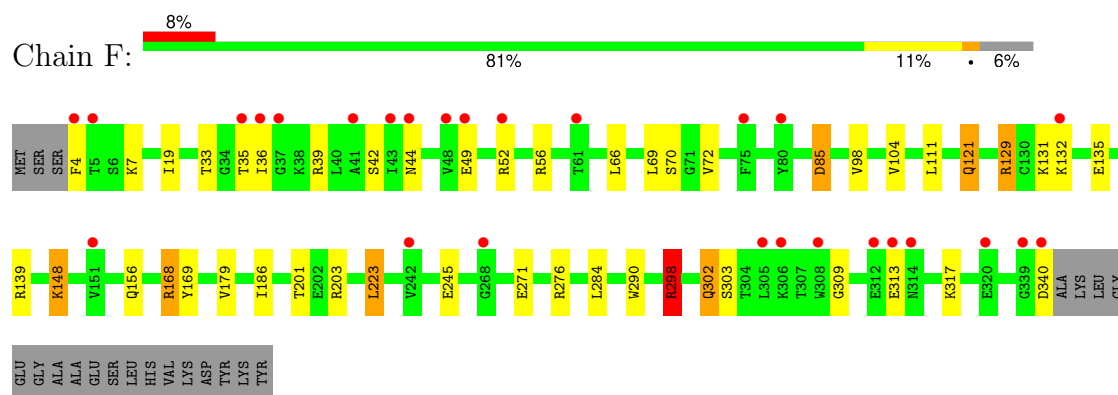
- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic



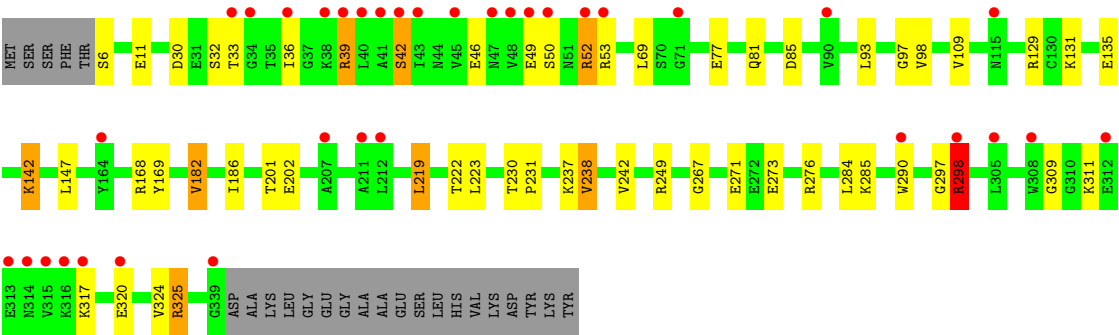
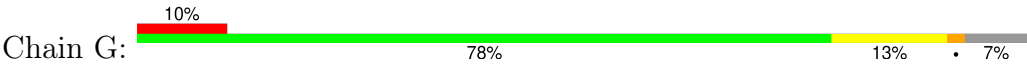
- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic



- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic



● Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.40Å 73.16Å 176.22Å 90.00° 106.52° 90.00°	Depositor
Resolution (Å)	46.23 – 2.15 46.23 – 2.18	Depositor EDS
% Data completeness (in resolution range)	81.8 (46.23-2.15) 92.0 (46.23-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.243 , 0.296 0.247 , 0.295	Depositor DCC
R_{free} test set	3335 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10669	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8062e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	1/2581 (0.0%)	0.79	3/3495 (0.1%)
1	B	0.59	0/2574	0.75	2/3484 (0.1%)
1	F	0.67	1/2614 (0.0%)	0.80	2/3537 (0.1%)
1	G	0.69	1/2561 (0.0%)	0.77	4/3468 (0.1%)
All	All	0.65	3/10330 (0.0%)	0.78	11/13984 (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	A	0	5
1	B	0	4
1	F	0	8
1	G	0	6
All	All	0	23

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	GLU	CD-OE1	-6.79	1.18	1.25
1	G	202	GLU	CD-OE1	6.48	1.32	1.25
1	F	245	GLU	CD-OE2	5.34	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	121	GLN	CB-CA-C	-6.92	96.56	110.40
1	A	139	ARG	NE-CZ-NH2	-6.42	117.09	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	F	121	GLN	CB-CG-CD	-6.36	95.08	111.60
1	B	325	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	G	249	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	31	GLU	CB-CA-C	5.73	121.86	110.40
1	G	129	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	G	249	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	249	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	G	129	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	56	ARG	Sidechain
1	B	129[A]	ARG	Sidechain
1	B	298	ARG	Sidechain
1	B	39	ARG	Sidechain
1	B	52	ARG	Sidechain
1	F	129[A]	ARG	Sidechain
1	F	129[B]	ARG	Sidechain
1	F	168[A]	ARG	Sidechain
1	F	168[B]	ARG	Sidechain
1	F	203	ARG	Sidechain
1	F	276	ARG	Sidechain
1	F	298	ARG	Sidechain
1	F	4	PHE	Peptide
1	G	168	ARG	Sidechain
1	G	276	ARG	Sidechain
1	G	298	ARG	Sidechain
1	G	325	ARG	Sidechain
1	G	39	ARG	Sidechain
1	G	52	ARG	Sidechain

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	A	2539	0	2574	20	0
1	B	2530	0	2574	23	0
1	F	2563	0	2613	24	1
1	G	2517	0	2561	28	1
2	A	5	0	0	0	0
2	B	30	0	0	3	0
2	F	10	0	0	0	0
2	G	20	0	0	0	0
3	B	4	0	2	0	0
3	G	8	0	4	2	0
4	B	8	0	7	3	0
4	G	16	0	14	2	0
5	A	101	0	0	1	0
5	B	85	0	0	3	0
5	F	120	0	0	4	0
5	G	113	0	0	1	0
All	All	10669	0	10349	95	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 5.

All (95) 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:F:298:ARG:NH2	5:F:501:HOH:O	1.99	0.94
1:B:156[A]:GLN:NE2	2:B:401:SO4:O3	2.10	0.84
1:F:49:GLU:HA	1:F:52:ARG:NH2	1.95	0.80
1:G:219:LEU:O	1:G:222[A]:THR:HG22	1.85	0.77
1:G:298:ARG:NE	1:G:298:ARG:HA	2.00	0.76
1:B:49:GLU:HG3	1:B:52:ARG:HH21	1.55	0.70
1:G:93:LEU:HB3	1:G:98:VAL:HG22	1.74	0.70
1:B:298:ARG:HB2	4:B:408:PRO:HD2	1.76	0.67
1:F:52:ARG:O	1:F:56:ARG:HG2	1.96	0.66
1:B:129[B]:ARG:HH11	1:B:129[B]:ARG:HG3	1.61	0.65
1:G:36:ILE:HG21	1:G:52:ARG:HD2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:GLU:HB3	1:G:325:ARG:HD2	1.79	0.64
1:A:103:LYS:HE2	5:A:525:HOH:O	1.98	0.63
1:B:308:TRP:HE1	1:B:311:LYS:HG2	1.63	0.63
1:F:139[B]:ARG:NH2	5:F:506:HOH:O	2.34	0.60
1:B:298:ARG:H	4:B:408:PRO:HD2	1.66	0.60
1:F:131:LYS:O	1:F:135:GLU:HG2	2.02	0.59
1:G:131:LYS:O	1:G:135:GLU:HG3	2.08	0.54
1:G:267:GLY:O	3:G:405:GLY:N	2.41	0.54
1:A:53:ARG:HG3	1:F:85:ASP:O	2.08	0.53
1:B:52:ARG:NH2	1:B:81:GLN:HE22	2.06	0.53
1:F:49:GLU:HA	1:F:52:ARG:HH22	1.72	0.53
1:A:69:LEU:O	1:A:98:VAL:HG22	2.09	0.52
1:A:36:ILE:HD13	1:A:40:LEU:HG	1.90	0.52
1:B:271:GLU:HB3	1:B:325:ARG:HD2	1.92	0.52
1:F:69:LEU:O	1:F:98:VAL:HG22	2.09	0.52
1:F:129[B]:ARG:HA	1:F:132:LYS:HE2	1.90	0.52
1:F:129[A]:ARG:HA	1:F:132:LYS:HE2	1.90	0.52
1:A:49:GLU:OE1	1:A:77:GLU:HG3	2.10	0.52
1:A:298:ARG:HD3	1:A:298:ARG:H	1.75	0.51
1:B:69:LEU:O	1:B:98:VAL:HG22	2.10	0.51
1:B:131:LYS:O	1:B:135:GLU:HG3	2.11	0.50
1:G:297:GLY:HA3	4:G:406:PRO:HG2	1.93	0.50
1:B:72:VAL:HG23	1:B:98:VAL:HG11	1.93	0.50
1:G:36:ILE:HG21	1:G:52:ARG:CD	2.41	0.50
1:G:93:LEU:HD22	1:G:98:VAL:HG21	1.94	0.50
1:A:238:VAL:HG13	1:A:242:VAL:HB	1.95	0.49
1:B:298:ARG:HB2	4:B:408:PRO:CD	2.40	0.49
1:B:238:VAL:HG13	1:B:242:VAL:HB	1.94	0.48
1:B:52:ARG:NH2	1:B:77:GLU:OE2	2.46	0.48
1:G:238:VAL:HG13	1:G:242:VAL:HB	1.96	0.48
1:F:271:GLU:HG3	1:F:302:GLN:HE21	1.78	0.48
1:F:36:ILE:HG21	1:F:52:ARG:HD3	1.96	0.48
1:F:139[B]:ARG:NH1	5:F:510:HOH:O	2.45	0.48
1:F:179:VAL:HG11	1:F:223:LEU:HD22	1.96	0.48
1:B:253:ARG:NH2	2:B:402:SO4:O2	2.40	0.47
1:A:303:SER:O	1:A:307:THR:HG23	2.14	0.47
1:G:33:THR:OG1	1:G:52:ARG:NH2	2.47	0.47
1:A:36:ILE:HD11	1:A:55:LEU:HD23	1.96	0.47
1:G:52:ARG:HH11	1:G:52:ARG:HG3	1.79	0.47
1:F:36:ILE:CG2	1:F:52:ARG:HD3	2.46	0.46
1:A:337:TYR:OH	1:A:340:ASP:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG23	1:A:98:VAL:HG11	1.98	0.46
1:F:104:VAL:O	1:F:129[A]:ARG:NH1	2.41	0.45
1:G:93:LEU:O	1:G:98:VAL:HG13	2.16	0.45
1:G:97:GLY:HA2	4:G:408:PRO:HG3	1.99	0.45
1:G:53:ARG:HG3	1:G:81:GLN:NE2	2.31	0.45
1:G:49:GLU:HG3	1:G:77:GLU:OE2	2.16	0.45
1:G:237:LYS:NZ	1:G:273:GLU:OE1	2.36	0.45
1:A:49:GLU:HA	1:A:52:ARG:NH1	2.32	0.45
2:B:401:SO4:O1	5:B:501:HOH:O	2.17	0.45
1:A:35:THR:O	1:A:39:ARG:HG2	2.17	0.44
1:F:72:VAL:HG23	1:F:98:VAL:HG11	1.99	0.44
1:A:48:VAL:HG12	5:F:516:HOH:O	2.18	0.44
1:F:35:THR:O	1:F:39:ARG:HG2	2.17	0.44
1:F:284:LEU:HD23	1:F:284:LEU:HA	1.90	0.44
1:G:298:ARG:NE	1:G:298:ARG:CA	2.78	0.44
1:F:148:LYS:HE3	1:F:148:LYS:HB3	1.74	0.43
1:A:186:ILE:CD1	1:A:201:THR:HA	2.48	0.43
1:B:24:LYS:NZ	5:B:508:HOH:O	2.51	0.43
1:B:142:LYS:NZ	5:B:507:HOH:O	2.48	0.43
1:G:298:ARG:HB2	3:G:405:GLY:HA2	2.00	0.43
1:G:36:ILE:CG2	1:G:52:ARG:HD2	2.46	0.43
1:F:186:ILE:CD1	1:F:201:THR:HA	2.49	0.42
1:B:186:ILE:CD1	1:B:201:THR:HA	2.50	0.42
1:B:310:GLY:O	1:B:311:LYS:CG	2.67	0.42
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.86	0.42
1:G:186:ILE:CD1	1:G:201:THR:HA	2.50	0.42
1:G:30:ASP:OD2	1:G:142:LYS:NZ	2.36	0.42
1:G:32:SER:O	1:G:36:ILE:HG22	2.19	0.42
1:A:49:GLU:HB2	1:A:52:ARG:HH12	1.85	0.42
1:B:320:GLU:O	1:B:324:VAL:HG23	2.20	0.42
1:F:19:ILE:HA	1:F:70:SER:HB2	2.01	0.41
1:B:196:LYS:HE2	1:B:200:VAL:HG23	2.03	0.41
1:F:33:THR:HG23	1:F:52:ARG:HE	1.85	0.41
1:G:320:GLU:O	1:G:324:VAL:HG23	2.20	0.41
1:A:337:TYR:OH	1:A:340:ASP:HB2	2.21	0.41
1:B:182:VAL:HG13	1:B:223:LEU:O	2.20	0.41
1:F:104:VAL:O	1:F:129[B]:ARG:NH2	2.54	0.41
1:G:11:GLU:HG2	5:G:545:HOH:O	2.20	0.41
1:A:245:GLU:HA	1:A:284:LEU:HD11	2.03	0.41
1:A:337:TYR:OH	1:A:340:ASP:HB3	2.21	0.41
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:VAL:HG13	1:G:223:LEU:O	2.22	0.40
1:G:230:THR:HB	1:G:231:PRO:HD2	2.04	0.40

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:F:44:ASN:ND2	1:G:42:SER:OG[4_454]	1.93	0.27

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	335/358 (94%)	320 (96%)	13 (4%)	2 (1%)	25	18
1	B	334/358 (93%)	317 (95%)	15 (4%)	2 (1%)	25	18
1	F	338/358 (94%)	323 (96%)	13 (4%)	2 (1%)	25	18
1	G	333/358 (93%)	317 (95%)	14 (4%)	2 (1%)	25	18
All	All	1340/1432 (94%)	1277 (95%)	55 (4%)	8 (1%)	25	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	GLY
1	F	309	GLY
1	G	309	GLY
1	A	310	GLY
1	A	42	SER
1	B	42	SER
1	F	42	SER
1	G	42	SER

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	A	268/284 (94%)	248 (92%)	20 (8%)	13	8
1	B	267/284 (94%)	251 (94%)	16 (6%)	19	14
1	F	271/284 (95%)	253 (93%)	18 (7%)	16	11
1	G	266/284 (94%)	247 (93%)	19 (7%)	14	9
All	All	1072/1136 (94%)	999 (93%)	73 (7%)	16	10

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	31	GLU
1	A	33	THR
1	A	36	ILE
1	A	42	SER
1	A	46	GLU
1	A	48	VAL
1	A	50	SER
1	A	53	ARG
1	A	69	LEU
1	A	85	ASP
1	A	169	TYR
1	A	238	VAL
1	A	241	GLU
1	A	284	LEU
1	A	290	TRP
1	A	298	ARG
1	A	307	THR
1	A	315	VAL
1	A	327	LYS
1	B	39	ARG
1	B	46	GLU
1	B	81	GLN
1	B	82	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	85	ASP
1	B	132	LYS
1	B	169	TYR
1	B	182	VAL
1	B	238	VAL
1	B	285	LYS
1	B	290	TRP
1	B	298	ARG
1	B	305	LEU
1	B	313	GLU
1	B	316	LYS
1	B	325	ARG
1	F	7	LYS
1	F	66	LEU
1	F	85	ASP
1	F	111	LEU
1	F	121	GLN
1	F	148	LYS
1	F	156	GLN
1	F	168[A]	ARG
1	F	168[B]	ARG
1	F	169	TYR
1	F	223	LEU
1	F	290	TRP
1	F	298	ARG
1	F	302	GLN
1	F	303	SER
1	F	313	GLU
1	F	317	LYS
1	F	340	ASP
1	G	6	SER
1	G	39	ARG
1	G	46	GLU
1	G	50	SER
1	G	69	LEU
1	G	85	ASP
1	G	109	VAL
1	G	142	LYS
1	G	147	LEU
1	G	169	TYR
1	G	182	VAL
1	G	219	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	238	VAL
1	G	284	LEU
1	G	285	LYS
1	G	290	TRP
1	G	298	ARG
1	G	311	LYS
1	G	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	195	GLN
1	B	81	GLN
1	B	121	GLN
1	B	283	GLN
1	F	15	ASN
1	F	81	GLN
1	F	302	GLN
1	G	15	ASN
1	G	44	ASN
1	G	121	GLN
1	G	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	G	402	-	4,4,4	0.43	0	6,6,6	0.30	0
3	GLY	B	407	-	3,3,4	0.91	0	1,2,4	0.59	0
2	SO4	G	404	-	4,4,4	0.51	0	6,6,6	0.21	0
2	SO4	B	402	-	4,4,4	0.50	0	6,6,6	0.24	0
4	PRO	G	406	-	8,8,8	0.79	0	10,10,10	1.91	3 (30%)
2	SO4	G	403	-	4,4,4	0.50	0	6,6,6	0.43	0
4	PRO	G	408	-	8,8,8	0.89	0	10,10,10	1.09	1 (10%)
2	SO4	B	404	-	4,4,4	0.41	0	6,6,6	0.17	0
3	GLY	G	407	-	3,3,4	0.82	0	1,2,4	0.60	0
2	SO4	B	403	-	4,4,4	0.48	0	6,6,6	0.13	0
2	SO4	B	406	-	4,4,4	0.46	0	6,6,6	0.21	0
2	SO4	B	401	-	4,4,4	0.41	0	6,6,6	0.58	0
2	SO4	F	401	-	4,4,4	0.48	0	6,6,6	0.25	0
4	PRO	B	408	-	8,8,8	0.84	0	10,10,10	1.62	2 (20%)
2	SO4	A	401	-	4,4,4	0.59	0	6,6,6	0.21	0
2	SO4	B	405	-	4,4,4	0.48	0	6,6,6	0.13	0
3	GLY	G	405	-	3,3,4	0.87	0	1,2,4	0.57	0
2	SO4	F	402	-	4,4,4	0.49	0	6,6,6	0.17	0
2	SO4	G	401	-	4,4,4	0.54	0	6,6,6	0.24	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
3	GLY	G	407	-	-	0/0/1/2	-
3	GLY	B	407	-	-	0/0/1/2	-
4	PRO	G	406	-	-	2/4/11/11	0/1/1/1
3	GLY	G	405	-	-	0/0/1/2	-
4	PRO	B	408	-	-	4/4/11/11	0/1/1/1
4	PRO	G	408	-	-	4/4/11/11	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	406	PRO	OXT-C-CA	3.57	125.58	113.51
4	B	408	PRO	OXT-C-O	-3.28	116.64	124.08
4	G	406	PRO	OXT-C-O	-3.28	116.64	124.08
4	B	408	PRO	OXT-C-CA	2.79	122.94	113.51
4	G	408	PRO	OXT-C-O	-2.19	119.10	124.08
4	G	406	PRO	C-CA-N	2.13	115.16	106.84

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	408	PRO	O-C-CA-N
4	B	408	PRO	OXT-C-CA-N
4	B	408	PRO	O-C-CA-CB
4	B	408	PRO	OXT-C-CA-CB
4	G	408	PRO	O-C-CA-N
4	G	408	PRO	OXT-C-CA-N
4	G	406	PRO	OXT-C-CA-CB
4	G	408	PRO	O-C-CA-CB
4	G	408	PRO	OXT-C-CA-CB
4	G	406	PRO	O-C-CA-CB

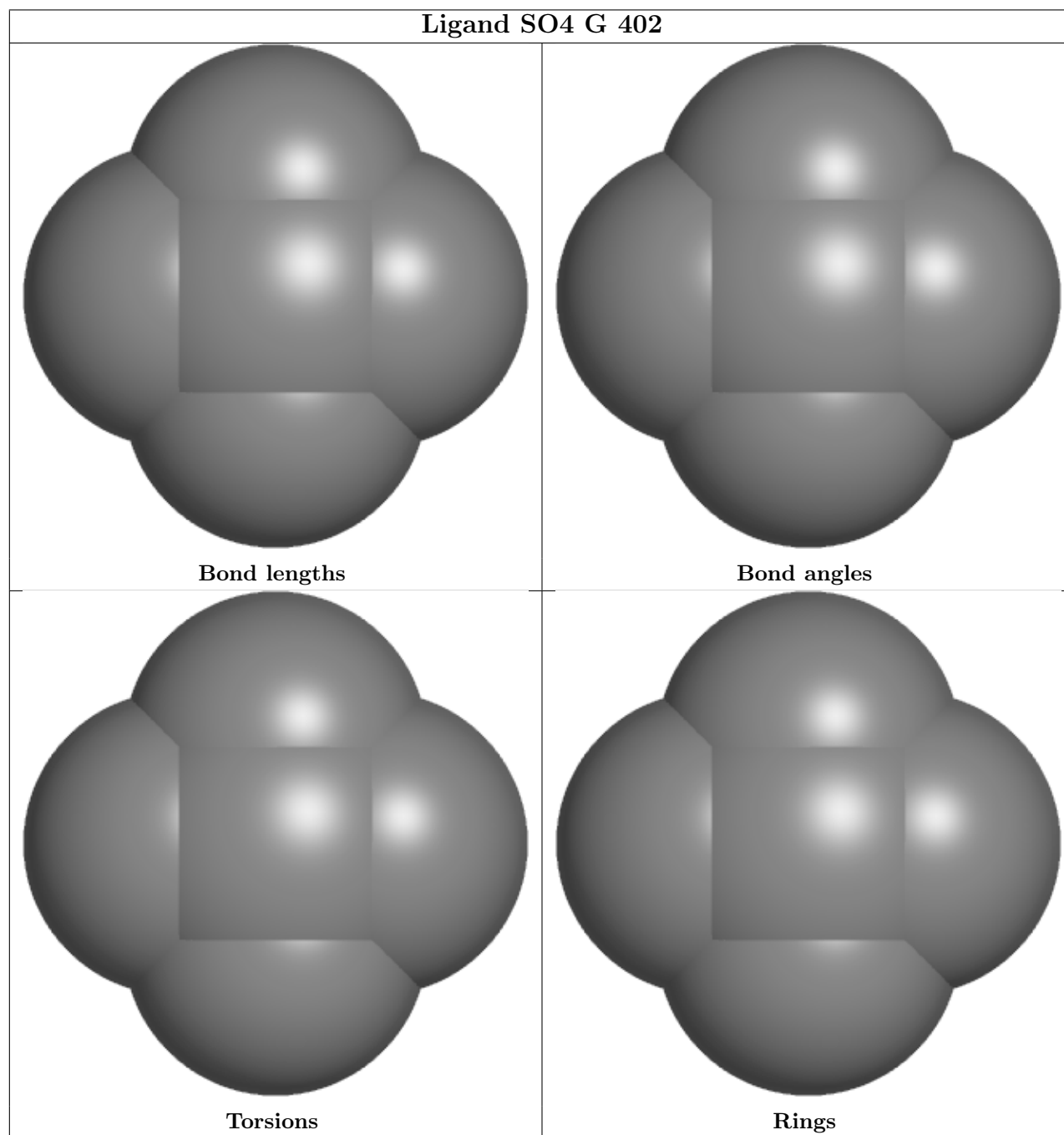
There are no ring outliers.

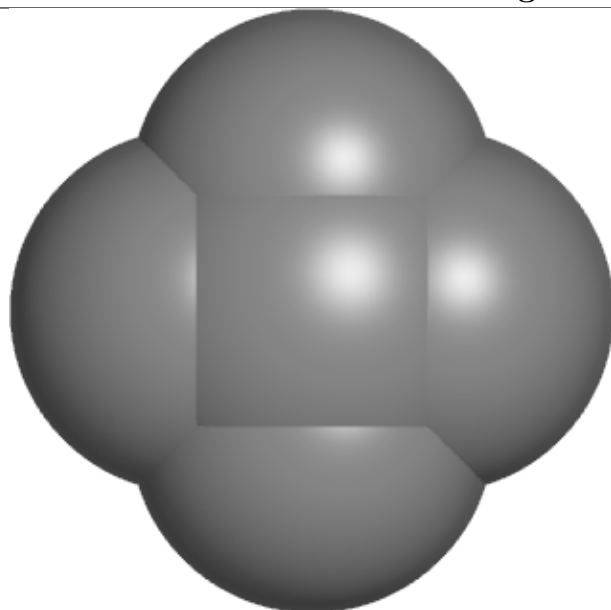
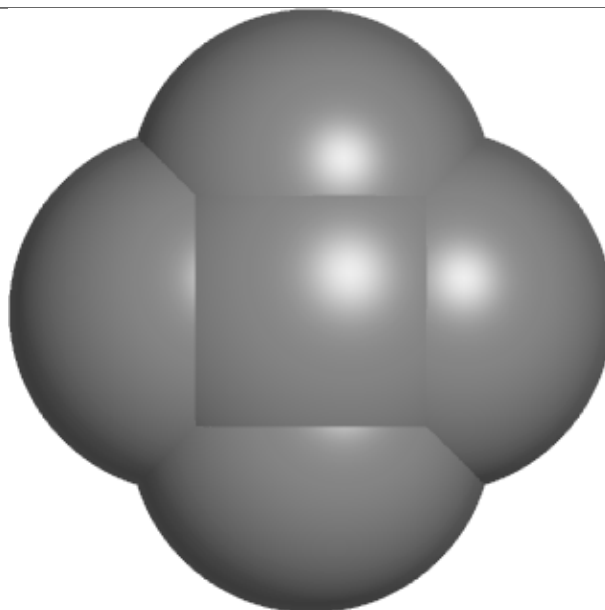
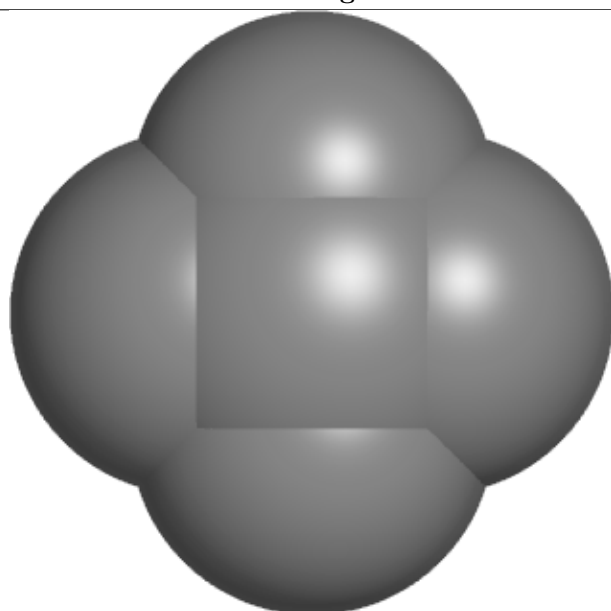
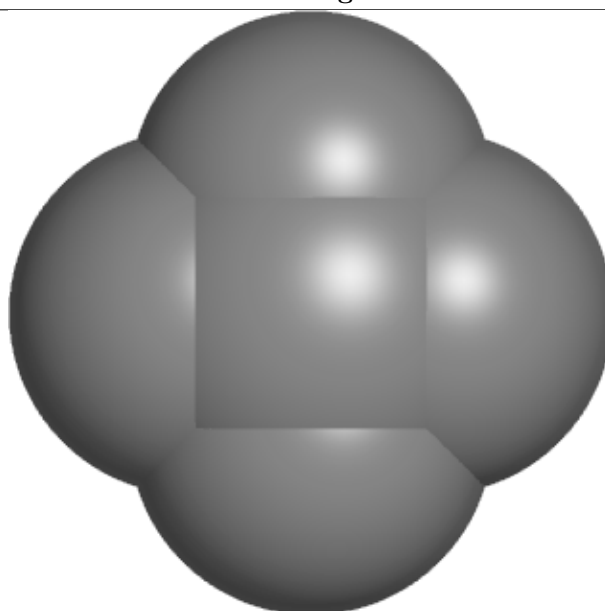
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SO4	1	0
4	G	406	PRO	1	0
4	G	408	PRO	1	0
2	B	401	SO4	2	0
4	B	408	PRO	3	0
3	G	405	GLY	2	0

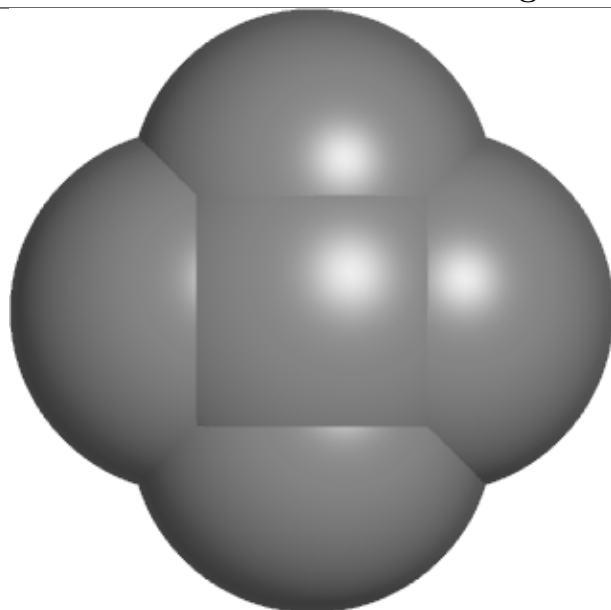
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

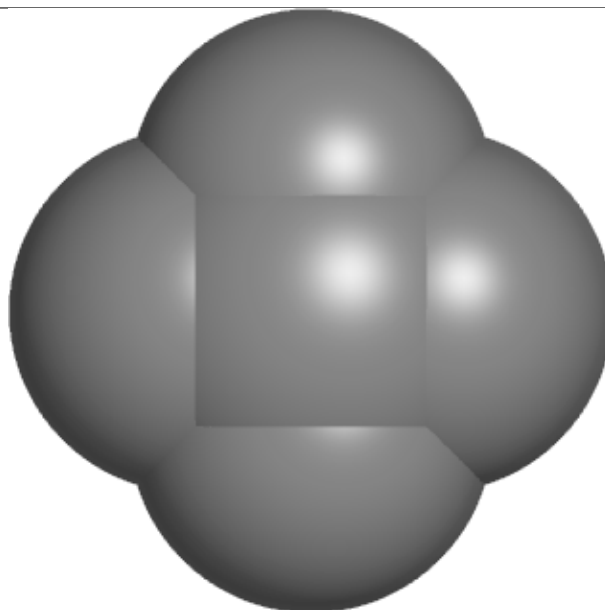


Ligand SO4 G 404**Bond lengths****Bond angles****Torsions****Rings**

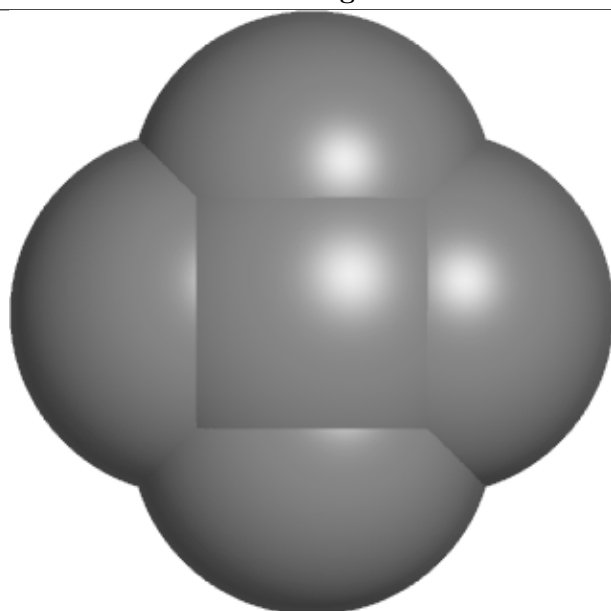
Ligand SO4 B 402



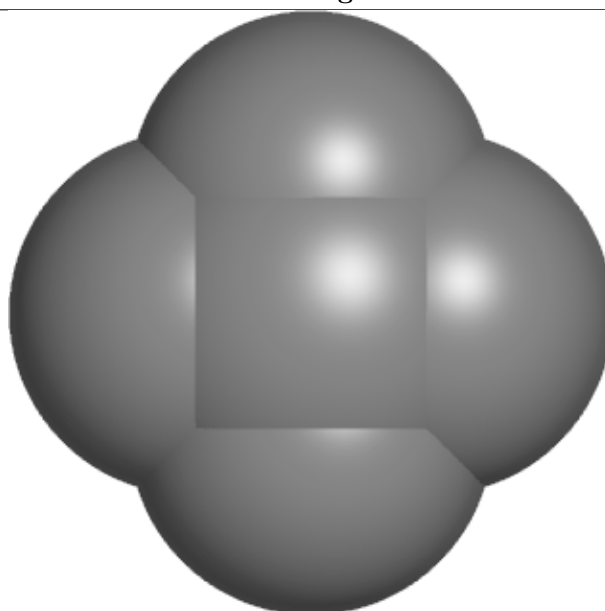
Bond lengths



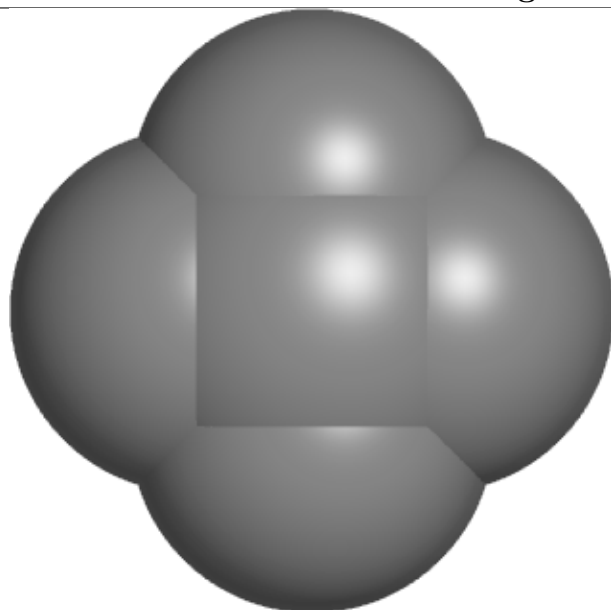
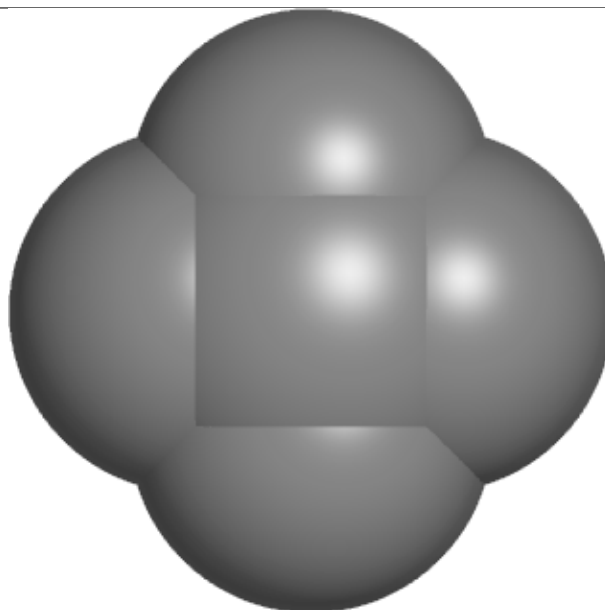
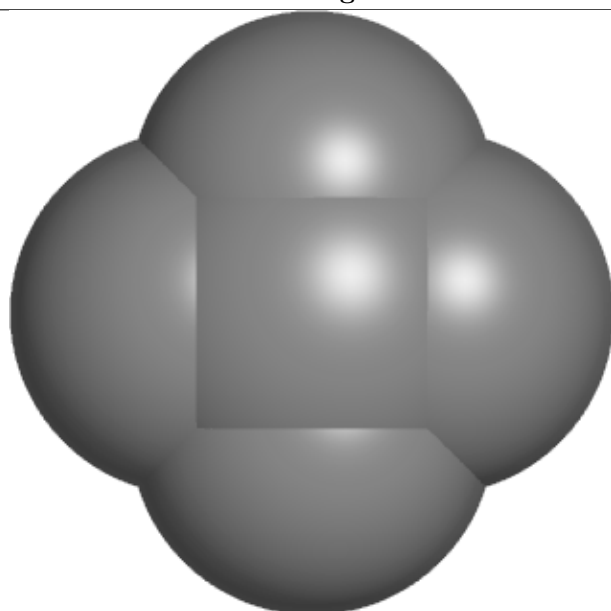
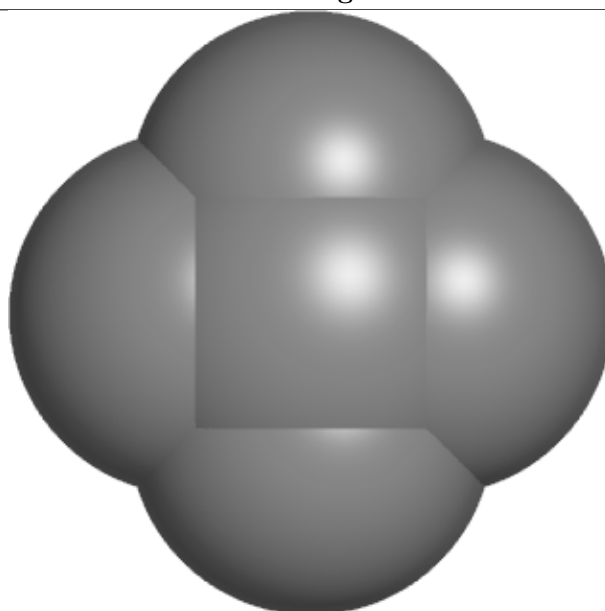
Bond angles



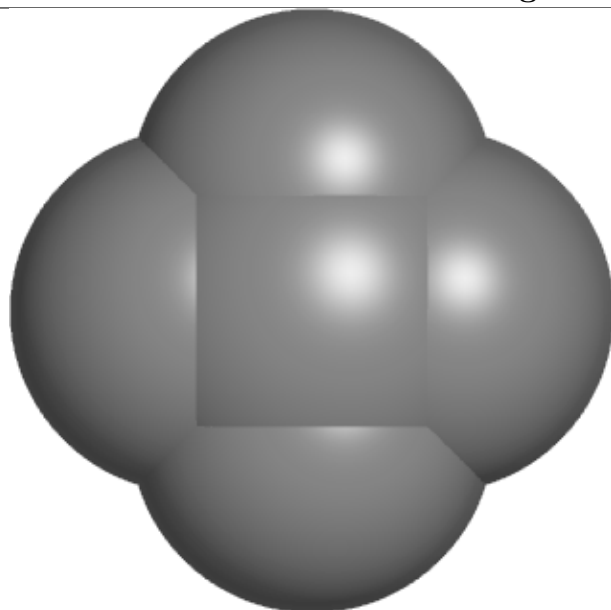
Torsions



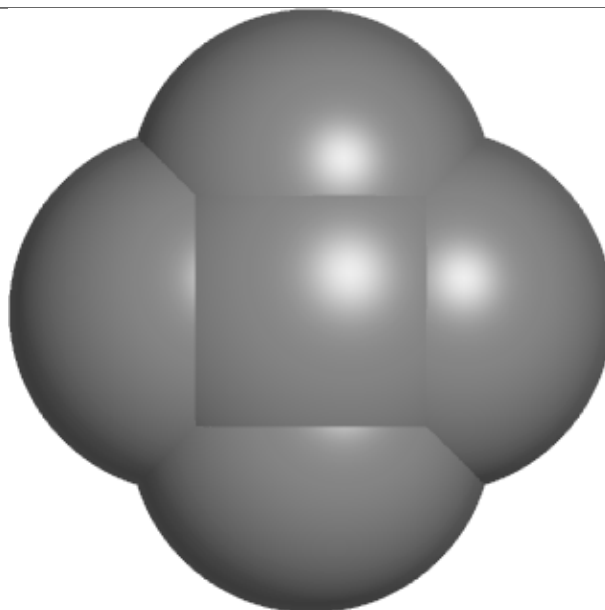
Rings

Ligand SO4 G 403**Bond lengths****Bond angles****Torsions****Rings**

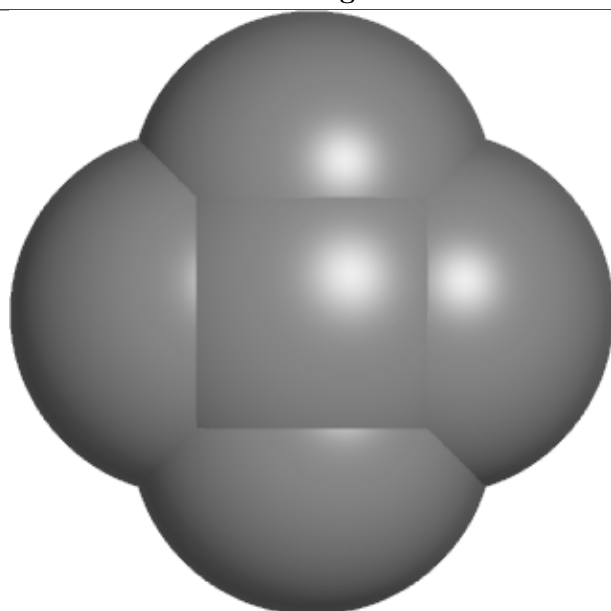
Ligand SO4 B 404



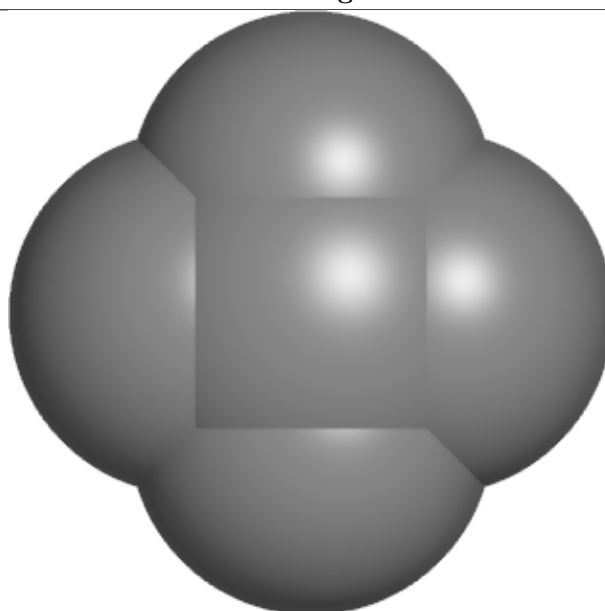
Bond lengths



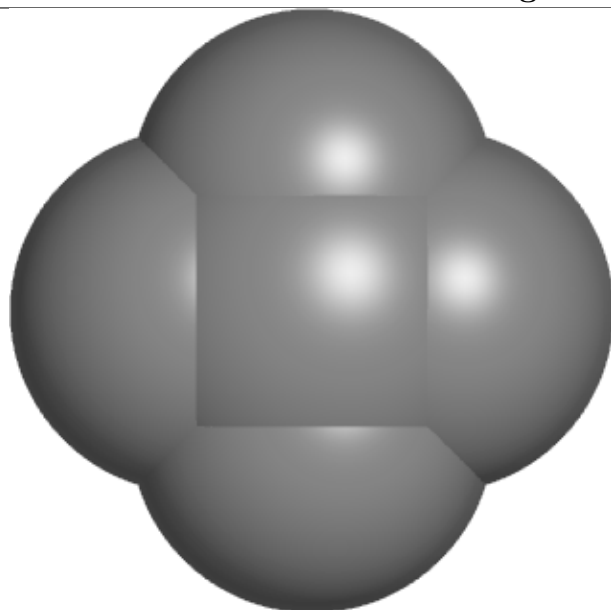
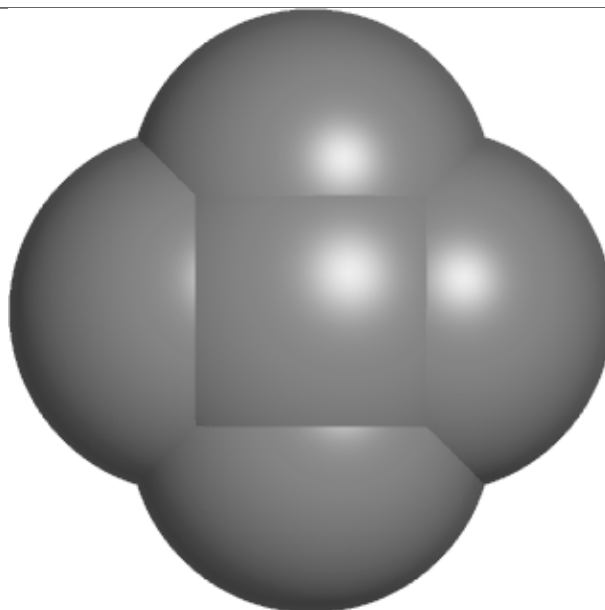
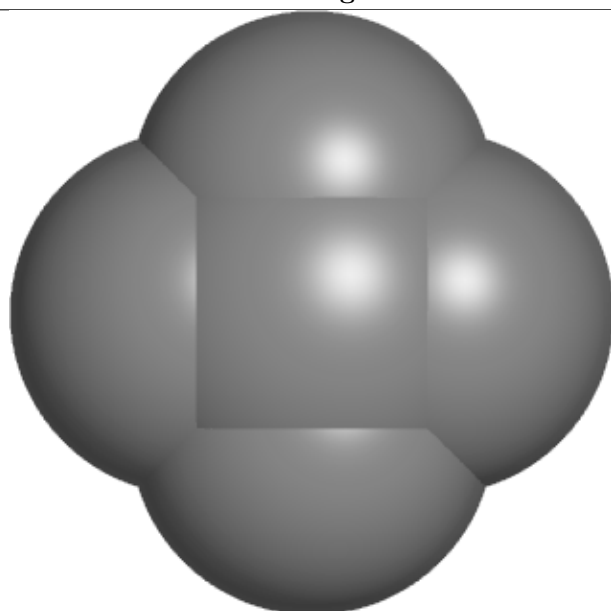
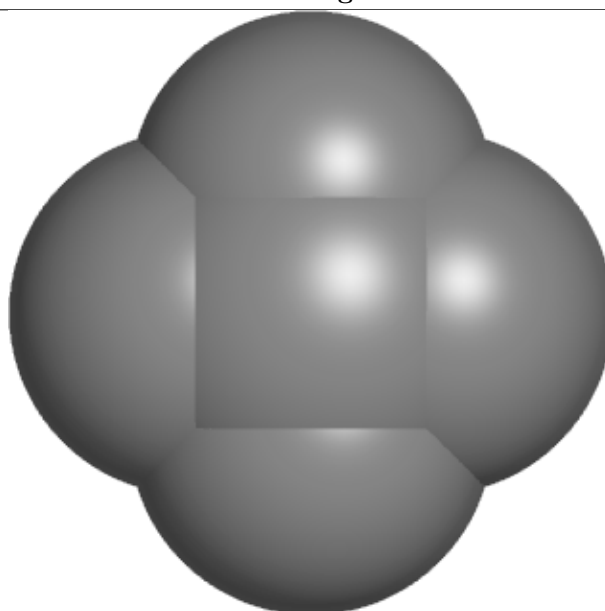
Bond angles

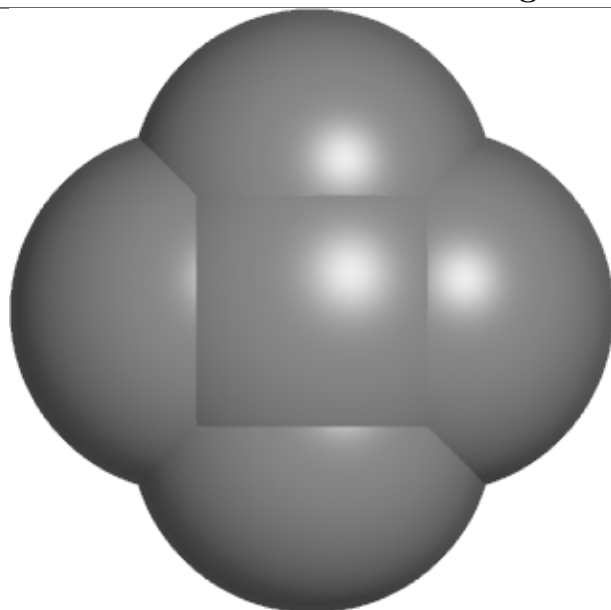
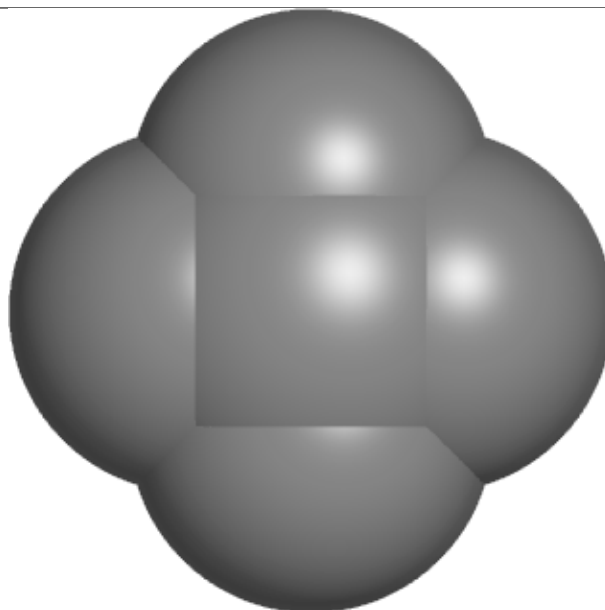
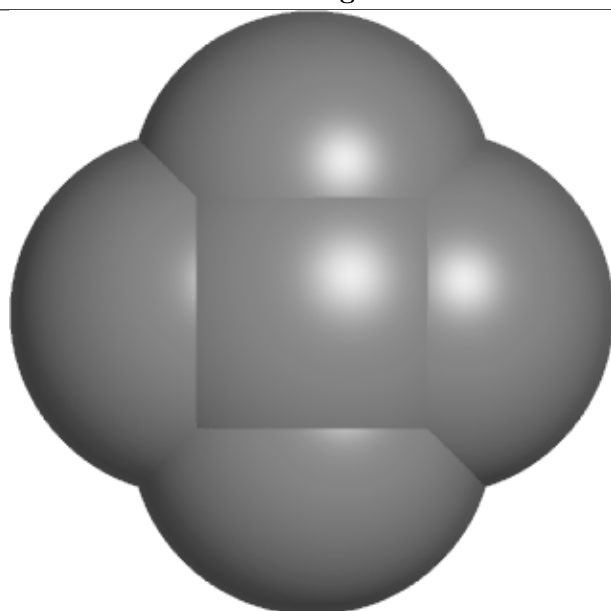
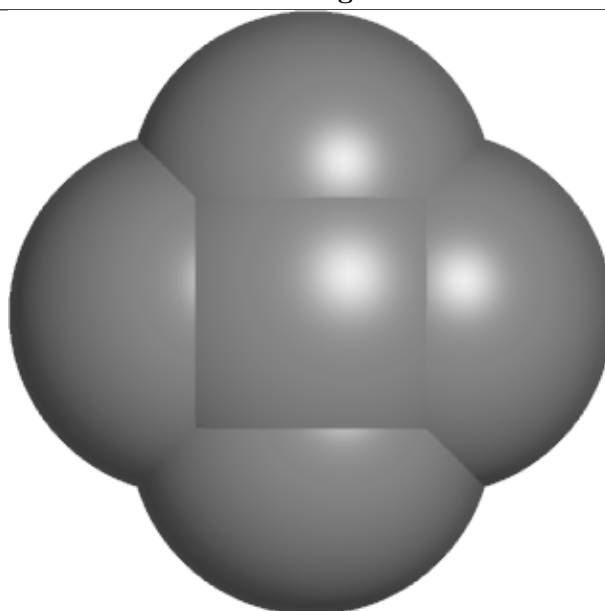


Torsions

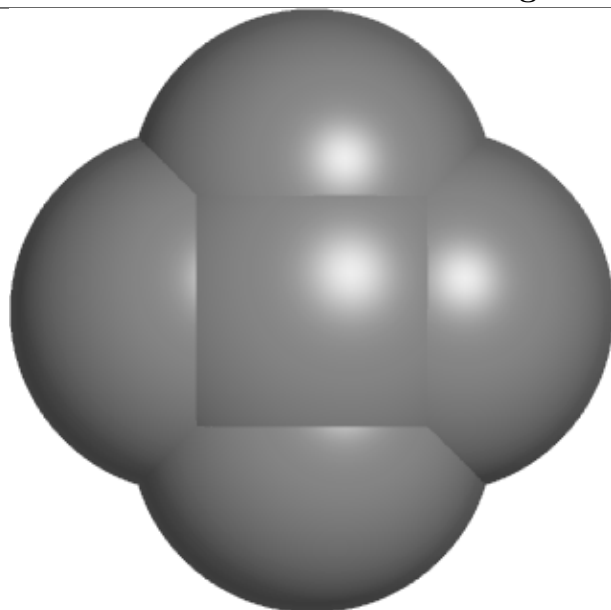


Rings

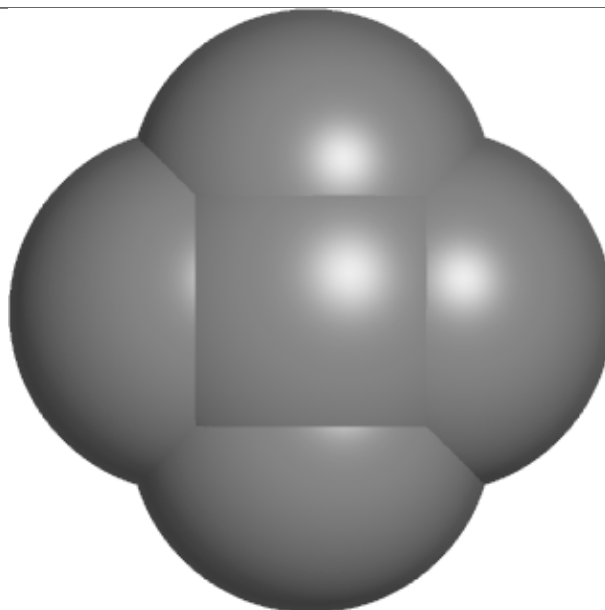
Ligand SO4 B 403**Bond lengths****Bond angles****Torsions****Rings**

Ligand SO4 B 406**Bond lengths****Bond angles****Torsions****Rings**

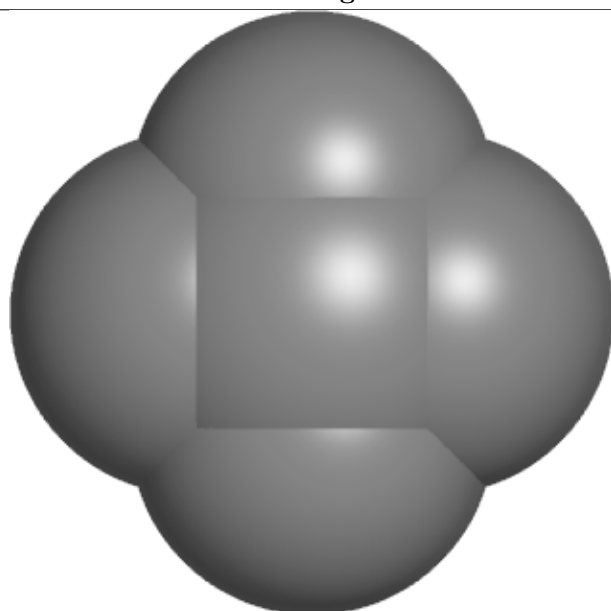
Ligand SO4 B 401



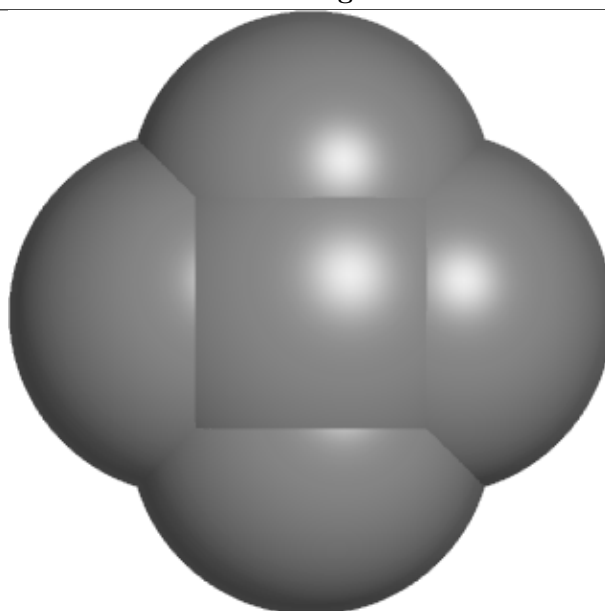
Bond lengths



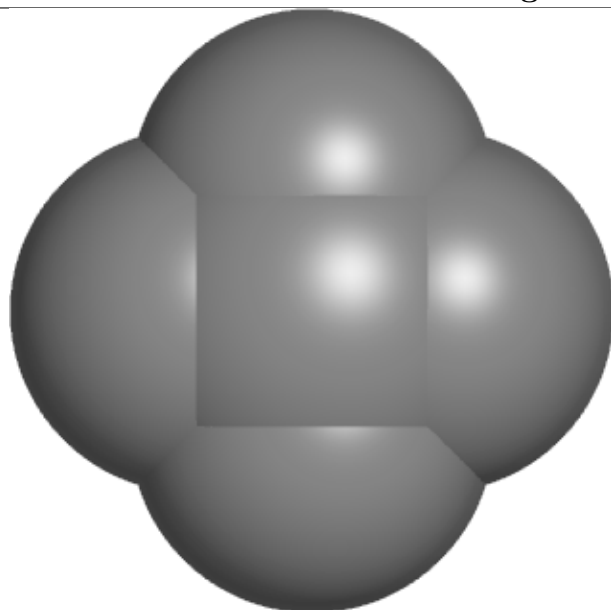
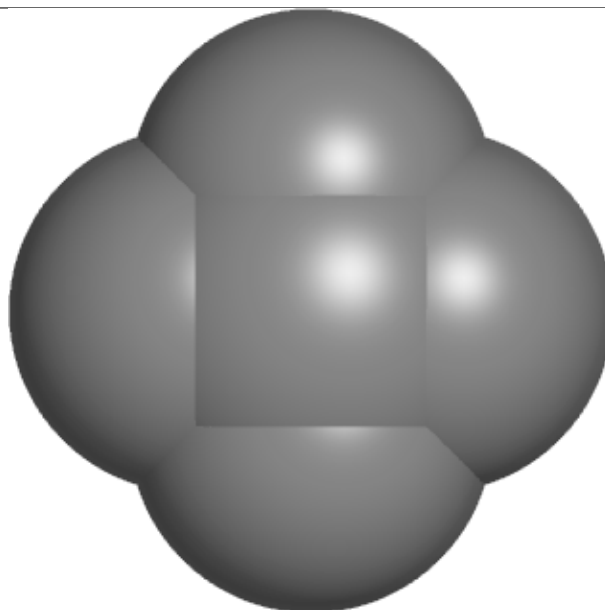
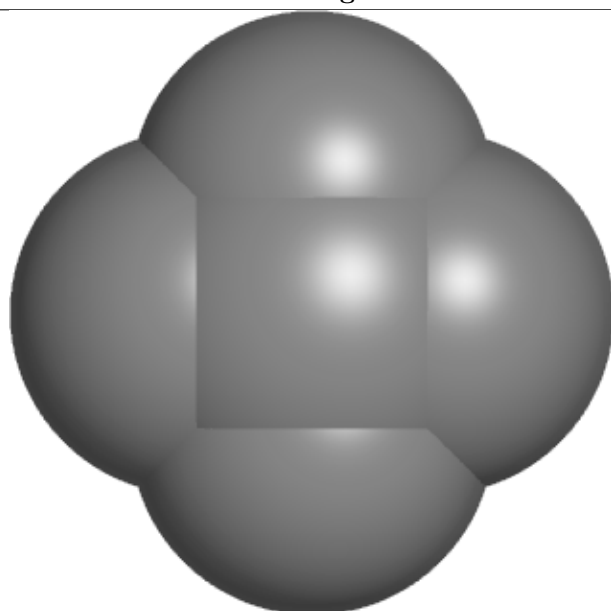
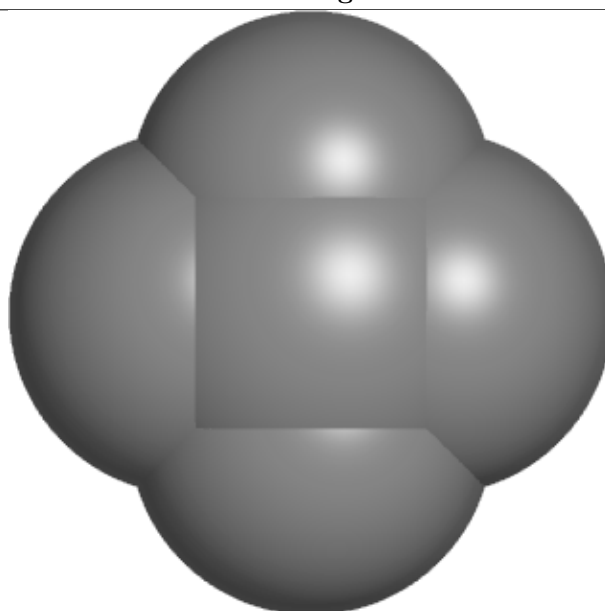
Bond angles

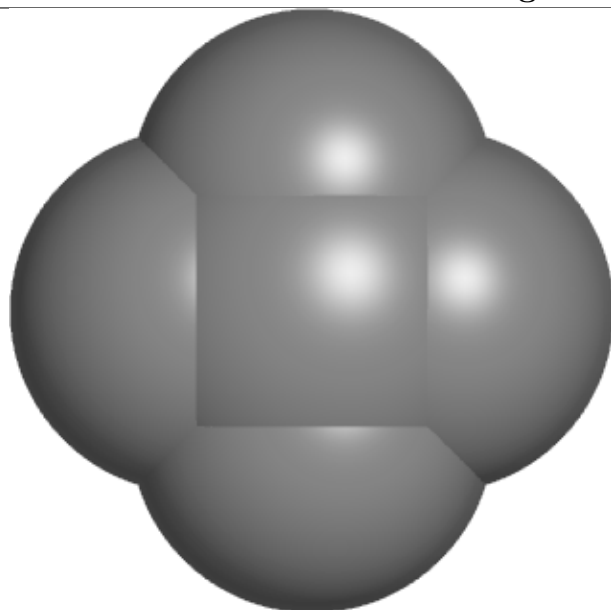
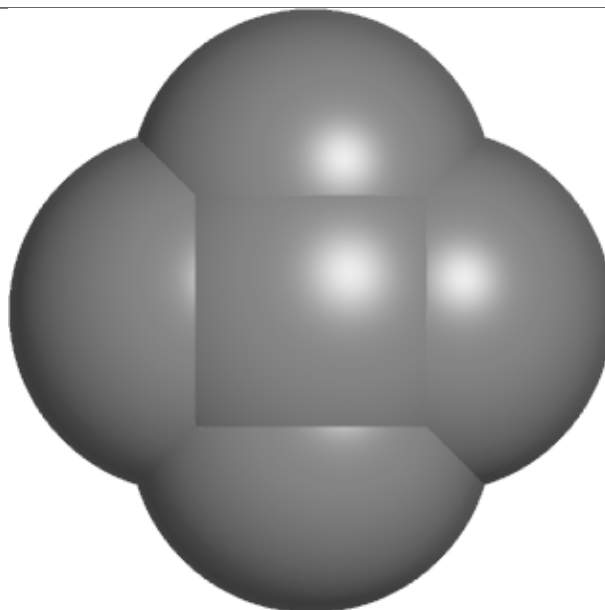
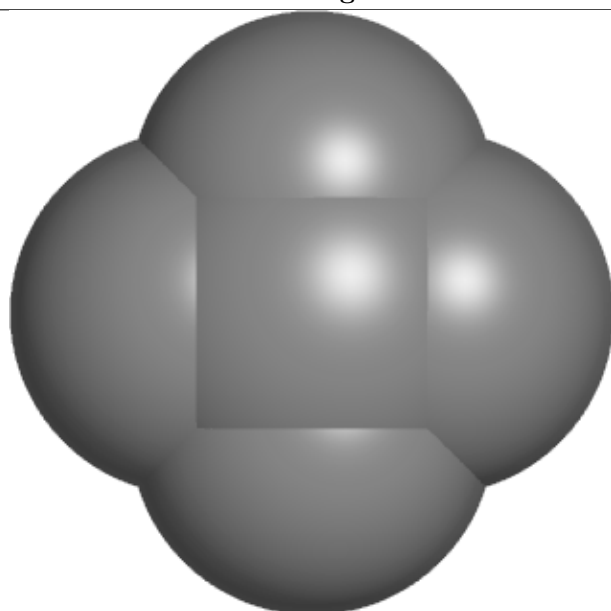
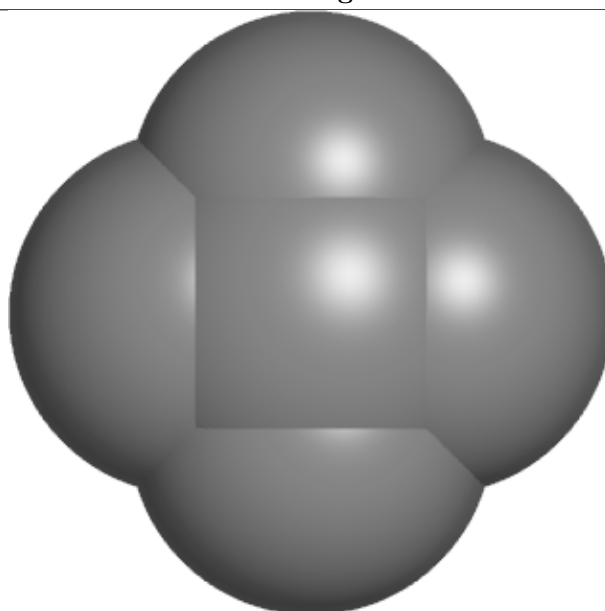


Torsions

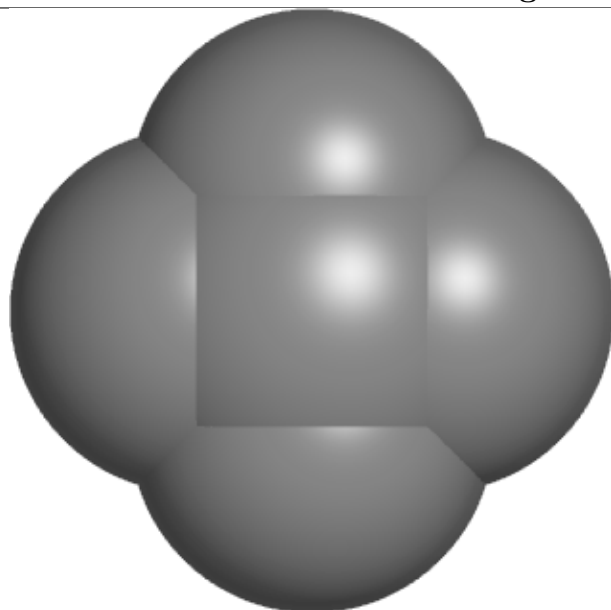


Rings

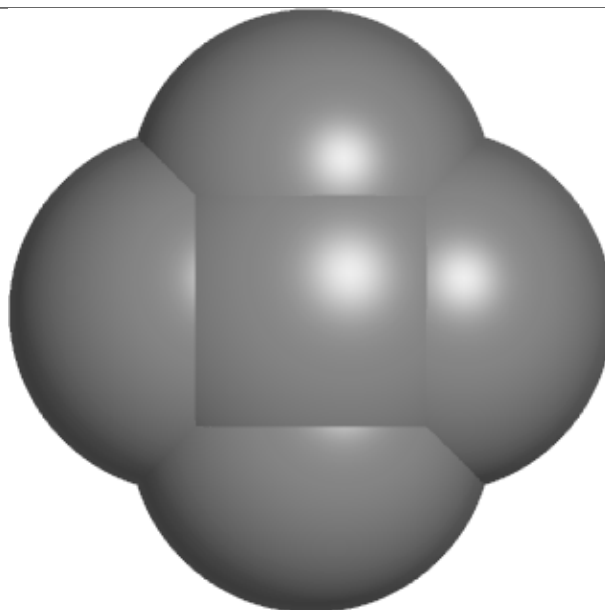
Ligand SO4 F 401**Bond lengths****Bond angles****Torsions****Rings**

Ligand SO4 A 401**Bond lengths****Bond angles****Torsions****Rings**

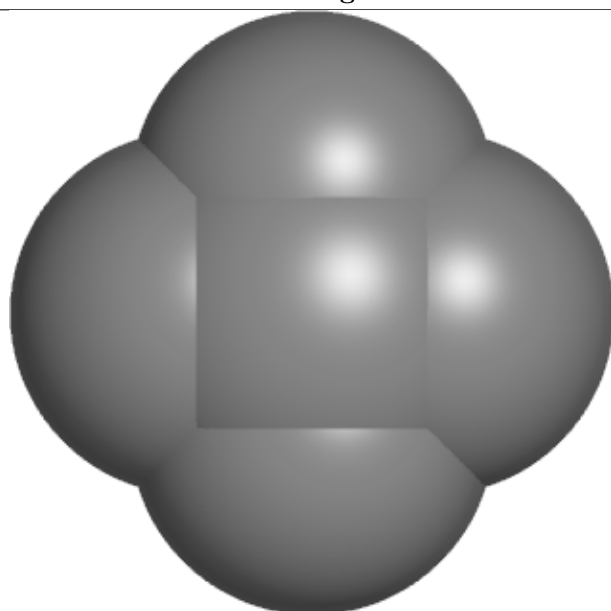
Ligand SO4 B 405



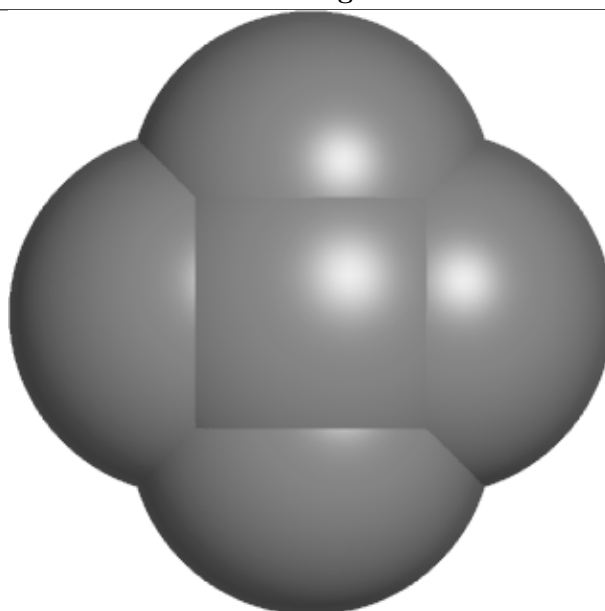
Bond lengths



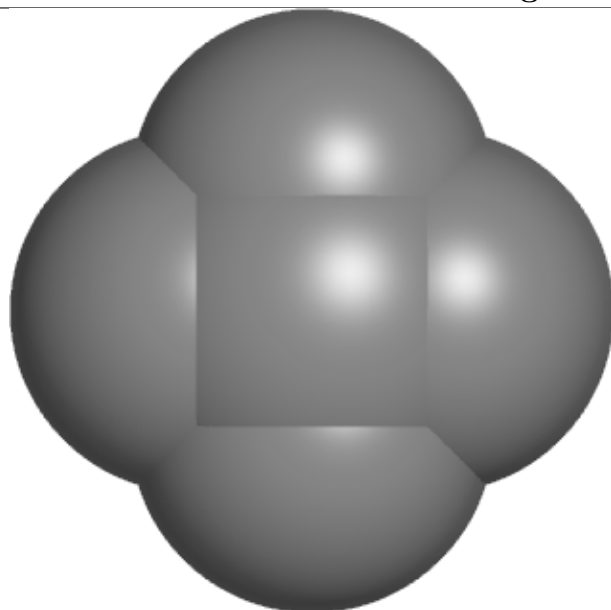
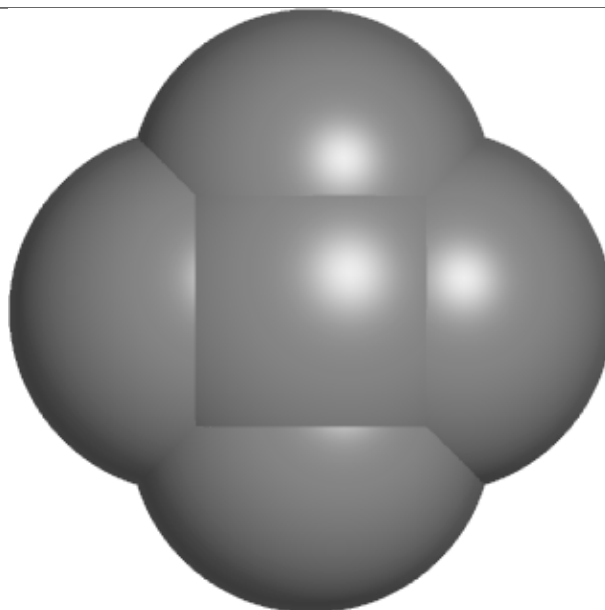
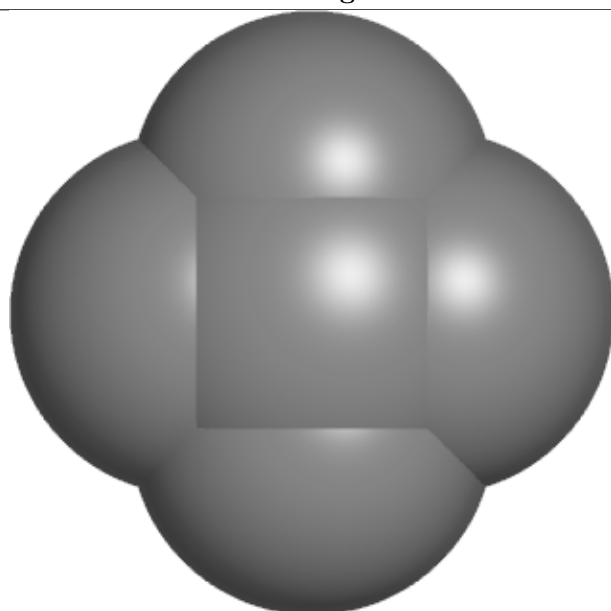
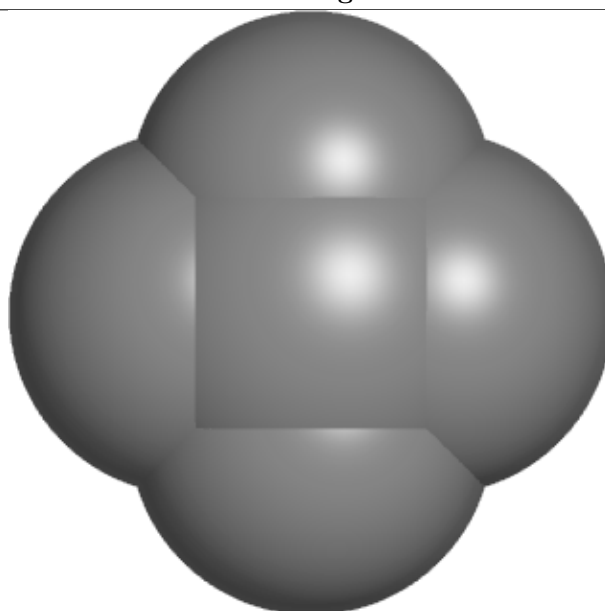
Bond angles

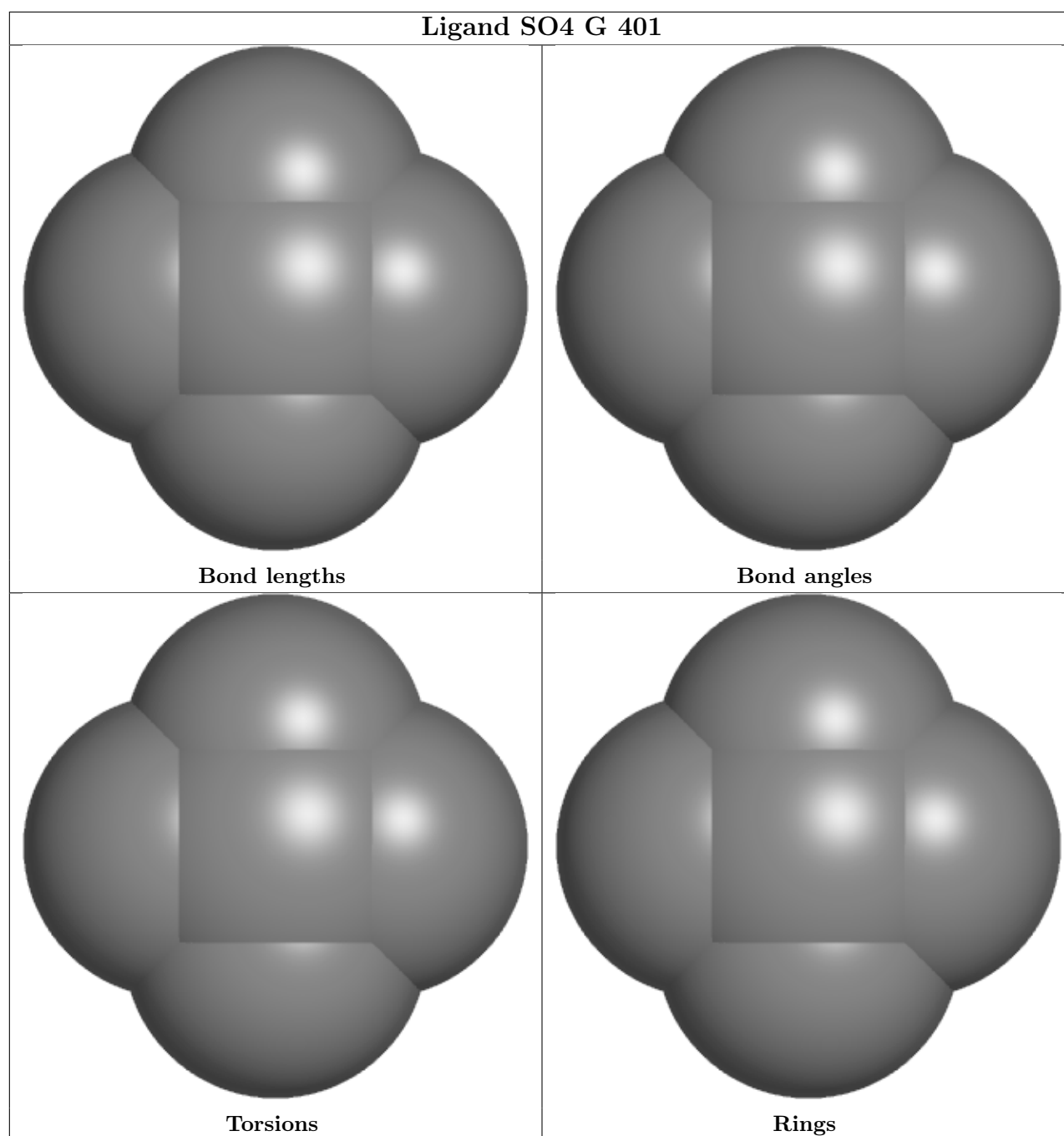


Torsions



Rings

Ligand SO4 F 402**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 ⓘ

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, 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	A	337/358 (94%)	0.62	16 (4%) 31 41	13, 21, 56, 87	0
1	B	334/358 (93%)	1.02	61 (18%) 1 1	11, 23, 69, 92	0
1	F	337/358 (94%)	0.64	27 (8%) 12 17	5, 14, 62, 79	0
1	G	334/358 (93%)	0.75	35 (10%) 6 9	6, 15, 64, 79	0
All	All	1342/1432 (93%)	0.76	139 (10%) 6 9	5, 19, 63, 92	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	48	VAL	7.2
1	B	305	LEU	6.1
1	F	305	LEU	5.9
1	B	48	VAL	5.8
1	B	40	LEU	5.6
1	F	41	ALA	5.3
1	B	314	ASN	5.1
1	B	45	VAL	4.8
1	A	151	VAL	4.8
1	B	312	GLU	4.5
1	A	5	THR	4.5
1	G	305	LEU	4.4
1	F	5	THR	4.2
1	B	43	ILE	4.2
1	B	306	LYS	4.1
1	F	36	ILE	4.1
1	A	41	ALA	4.1
1	B	310	GLY	4.0
1	B	84	SER	4.0
1	B	309	GLY	3.9
1	B	41	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	52	ARG	3.9
1	B	308	TRP	3.9
1	A	311	LYS	3.9
1	G	317	LYS	3.8
1	F	313	GLU	3.8
1	B	53	ARG	3.7
1	B	320	GLU	3.7
1	F	339	GLY	3.7
1	B	50	SER	3.6
1	F	44	ASN	3.6
1	G	207	ALA	3.6
1	G	41	ALA	3.5
1	B	85	ASP	3.4
1	F	268	GLY	3.4
1	B	313	GLU	3.4
1	G	308	TRP	3.4
1	B	52	ARG	3.4
1	B	262	ILE	3.4
1	B	307	THR	3.3
1	F	312	GLU	3.3
1	F	48	VAL	3.3
1	B	339	GLY	3.3
1	A	339	GLY	3.2
1	F	37	GLY	3.2
1	G	314	ASN	3.2
1	G	320	GLU	3.2
1	B	47	ASN	3.2
1	G	53	ARG	3.1
1	A	43	ILE	3.1
1	B	46	GLU	3.1
1	G	312	GLU	3.1
1	G	298	ARG	3.1
1	B	316	LYS	3.1
1	B	39	ARG	3.0
1	A	75	PHE	3.0
1	B	255	VAL	3.0
1	B	257	ALA	3.0
1	G	36	ILE	3.0
1	G	164	TYR	2.9
1	G	49	GLU	2.9
1	F	43	ILE	2.9
1	G	43	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	49	GLU	2.9
1	B	315	VAL	2.8
1	A	38	LYS	2.8
1	F	49	GLU	2.8
1	F	314	ASN	2.8
1	G	34	GLY	2.8
1	B	289	PRO	2.7
1	F	4	PHE	2.7
1	B	6	SER	2.7
1	G	33	THR	2.7
1	G	315	VAL	2.7
1	G	50	SER	2.7
1	B	131	LYS	2.6
1	B	80	TYR	2.6
1	A	305	LEU	2.6
1	F	132	LYS	2.6
1	A	115	ASN	2.6
1	B	17	ALA	2.5
1	B	83	SER	2.5
1	G	115	ASN	2.5
1	A	312	GLU	2.5
1	F	320	GLU	2.5
1	G	316	LYS	2.5
1	B	7	LYS	2.5
1	B	86	GLY	2.5
1	G	38	LYS	2.5
1	B	208	CYS	2.4
1	B	251	LEU	2.4
1	B	88	PRO	2.4
1	G	47	ASN	2.4
1	B	319	GLN	2.4
1	G	39	ARG	2.4
1	B	44	ASN	2.4
1	A	340	ASP	2.4
1	F	308	TRP	2.4
1	B	322	PHE	2.3
1	G	212	LEU	2.3
1	F	80	TYR	2.3
1	A	268	GLY	2.3
1	B	311	LYS	2.3
1	F	52	ARG	2.3
1	B	75	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	75	PHE	2.3
1	F	306	LYS	2.3
1	B	224	LEU	2.2
1	B	317	LYS	2.2
1	G	211	ALA	2.2
1	G	313	GLU	2.2
1	F	340	ASP	2.2
1	B	258	ALA	2.2
1	G	339	GLY	2.2
1	B	36	ILE	2.2
1	B	54	ALA	2.2
1	A	317	LYS	2.2
1	G	45	VAL	2.1
1	B	18	TYR	2.1
1	A	44	ASN	2.1
1	G	90	VAL	2.1
1	G	40	LEU	2.1
1	G	42	SER	2.1
1	G	290	TRP	2.1
1	B	206	ALA	2.1
1	B	132	LYS	2.1
1	F	35	THR	2.1
1	B	111	LEU	2.1
1	G	71	GLY	2.1
1	B	324	VAL	2.1
1	F	61	THR	2.1
1	F	151	VAL	2.1
1	F	242	VAL	2.1
1	B	133	TYR	2.1
1	B	298	ARG	2.0
1	B	82	LYS	2.0
1	B	261	ALA	2.0
1	B	152	ASN	2.0
1	A	188	VAL	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

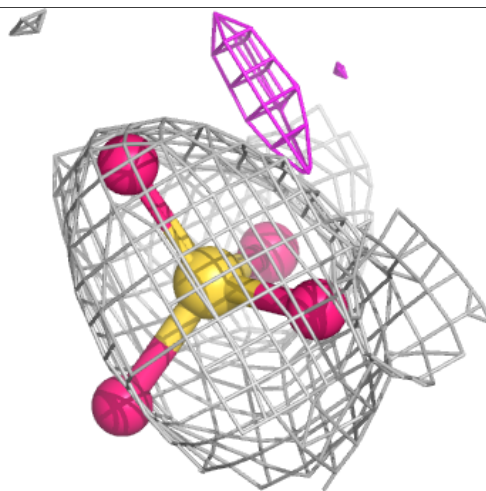
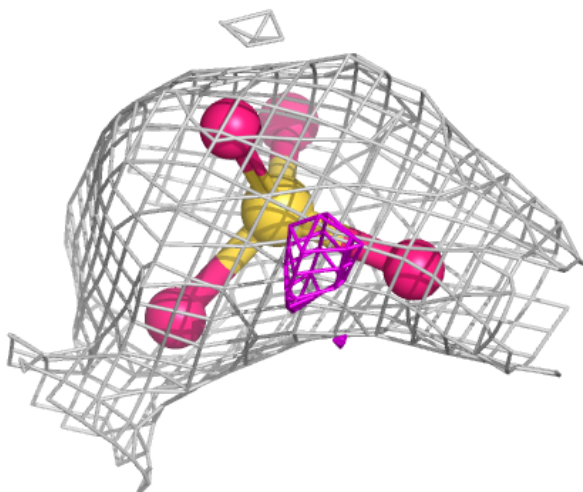
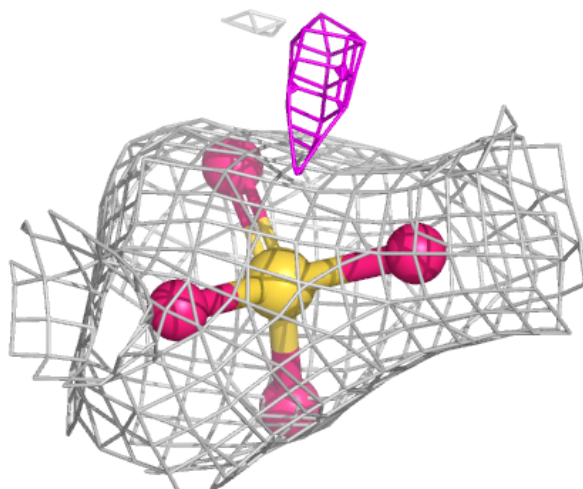
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PRO	G	406	8/8	0.47	0.38	53,57,59,65	0
3	GLY	G	405	4/5	0.52	0.37	54,57,57,58	0
4	PRO	B	408	8/8	0.57	0.33	48,53,54,56	0
4	PRO	G	408	8/8	0.66	0.23	53,59,60,61	0
3	GLY	B	407	4/5	0.70	0.57	57,57,58,61	0
2	SO4	B	402	5/5	0.76	0.27	67,68,73,74	0
3	GLY	G	407	4/5	0.79	0.29	53,57,58,58	0
2	SO4	F	402	5/5	0.81	0.32	70,70,74,78	0
2	SO4	B	405	5/5	0.85	0.18	68,72,73,75	0
2	SO4	B	404	5/5	0.86	0.24	71,73,76,76	0
2	SO4	G	402	5/5	0.86	0.23	53,56,60,64	0
2	SO4	G	404	5/5	0.88	0.15	59,60,64,65	0
2	SO4	B	406	5/5	0.89	0.15	66,69,71,71	0
2	SO4	G	403	5/5	0.90	0.16	40,44,49,54	0
2	SO4	B	403	5/5	0.92	0.16	61,64,66,66	0
2	SO4	B	401	5/5	0.94	0.15	52,55,55,56	0
2	SO4	F	401	5/5	0.95	0.13	41,42,46,47	0
2	SO4	G	401	5/5	0.96	0.12	39,40,43,45	0
2	SO4	A	401	5/5	0.97	0.10	43,45,47,48	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.

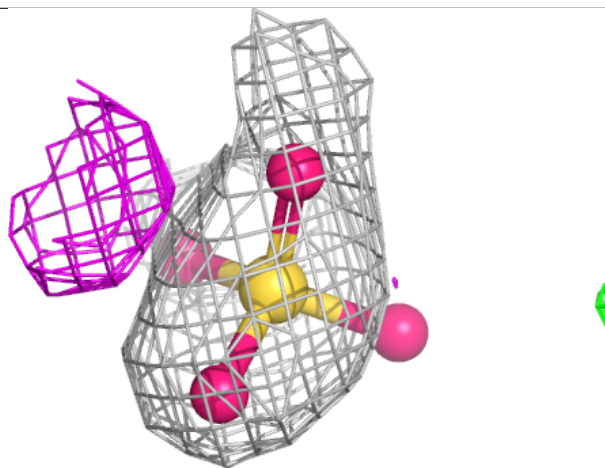
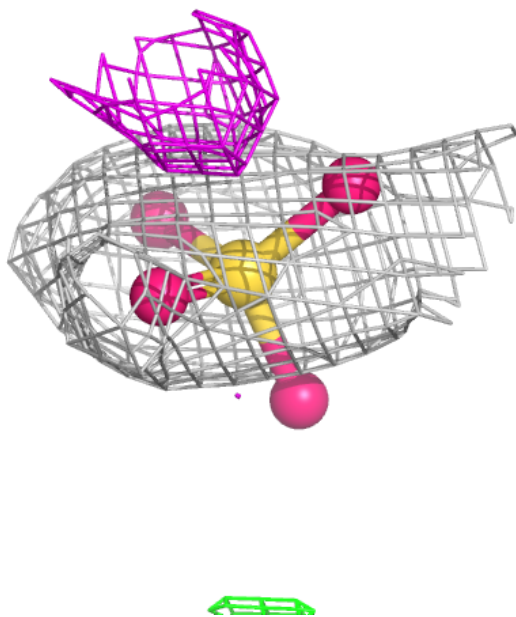
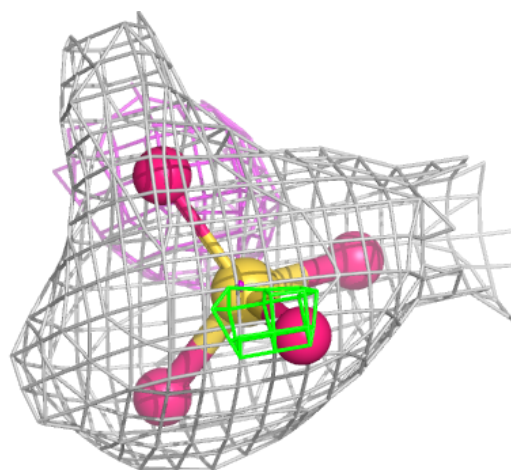
Electron density around SO4 B 402:

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



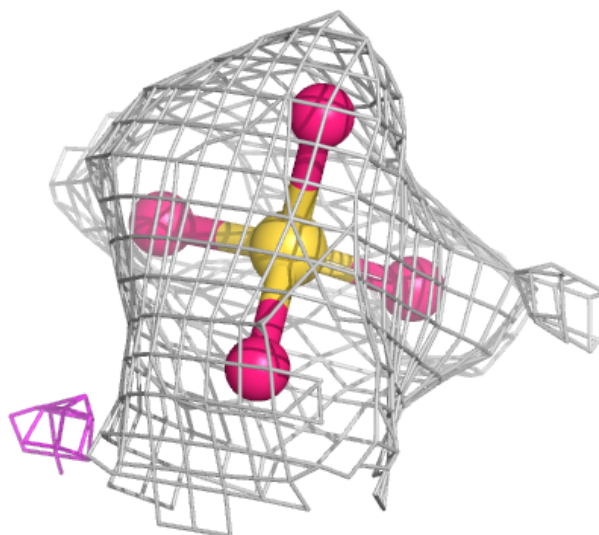
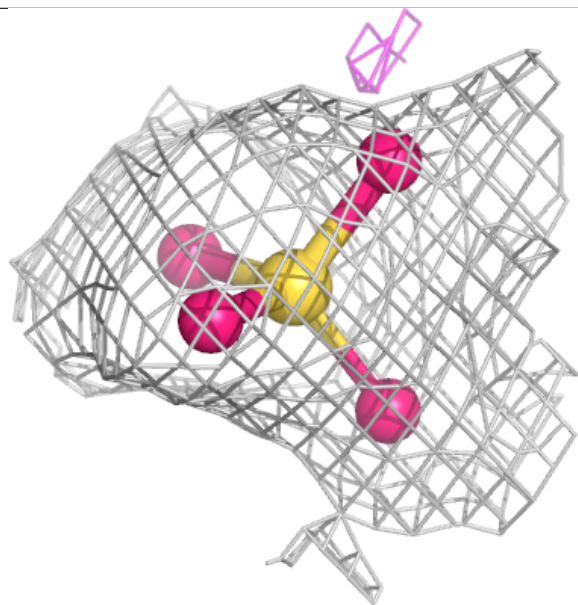
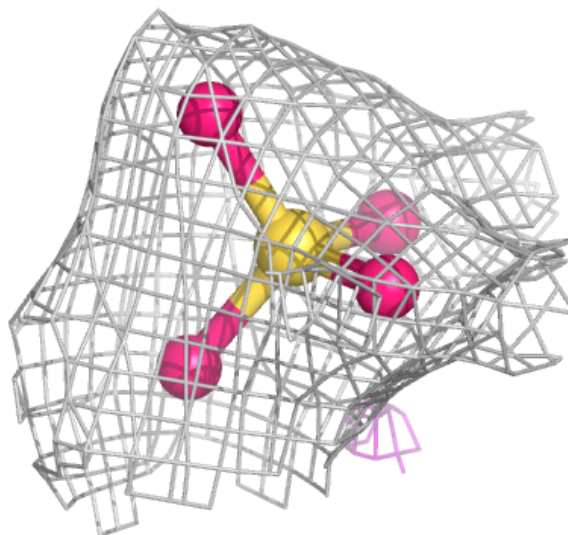
Electron density around SO4 F 402:

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



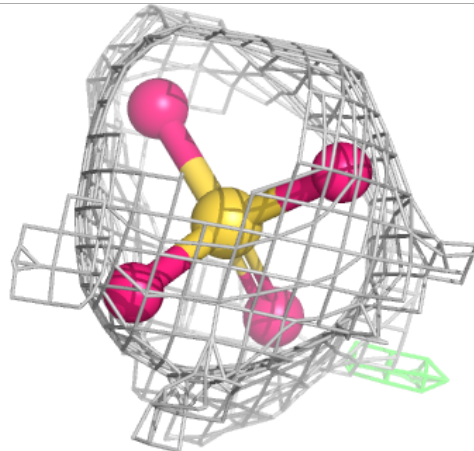
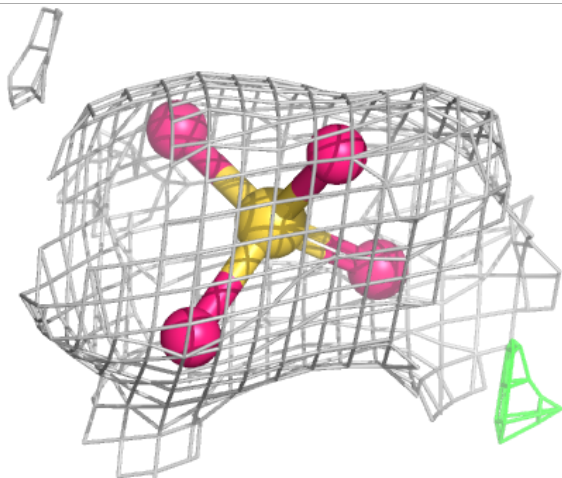
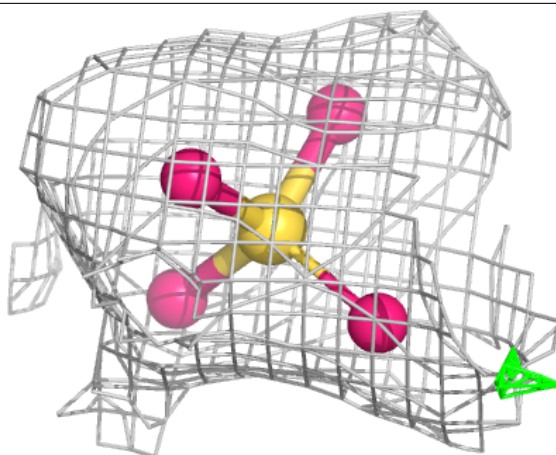
Electron density around SO4 B 405:

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



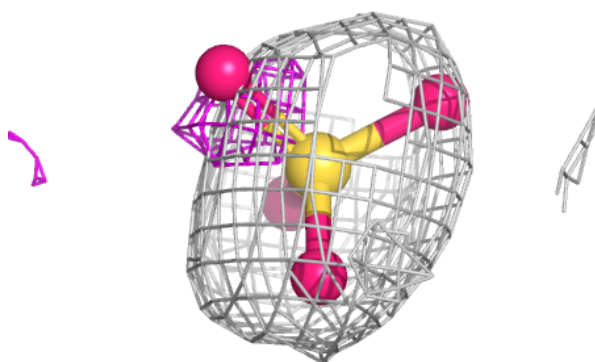
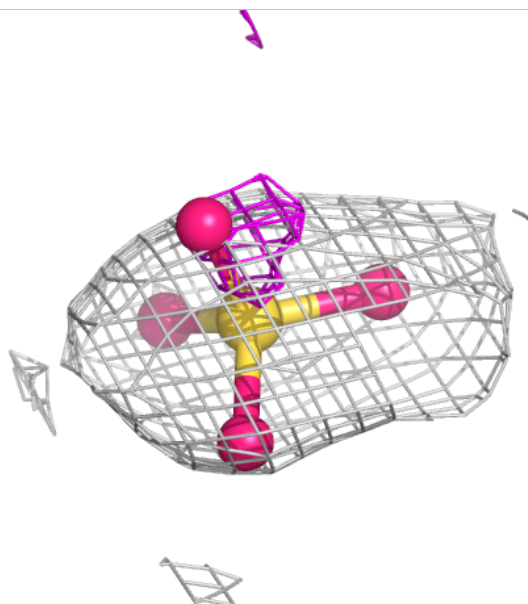
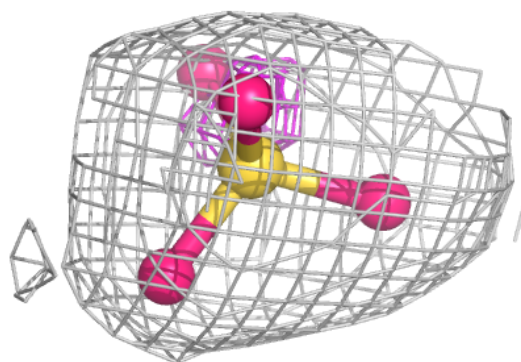
Electron density around SO4 B 404:

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



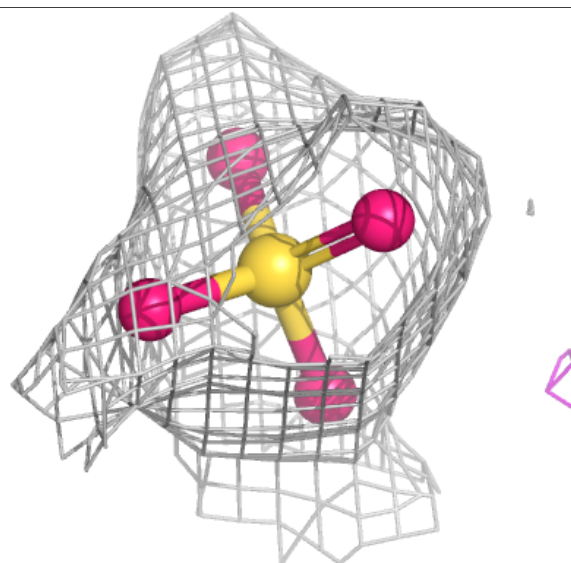
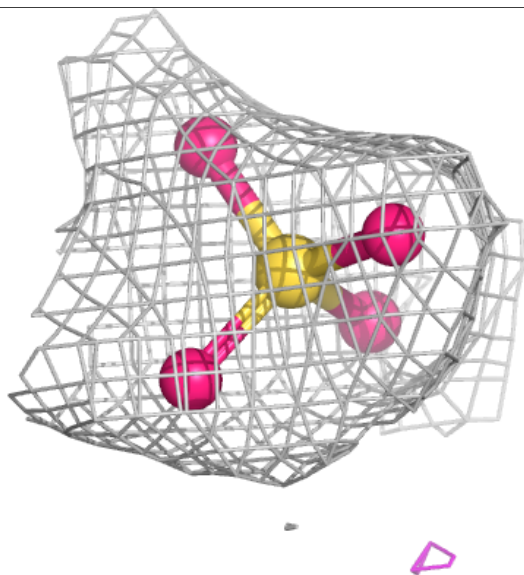
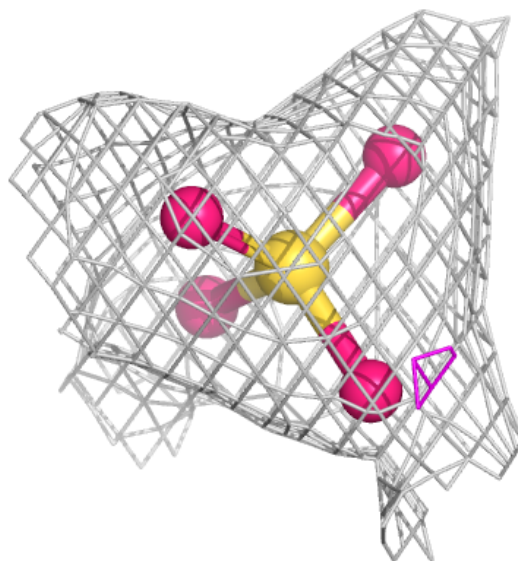
Electron density around SO4 G 402:

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



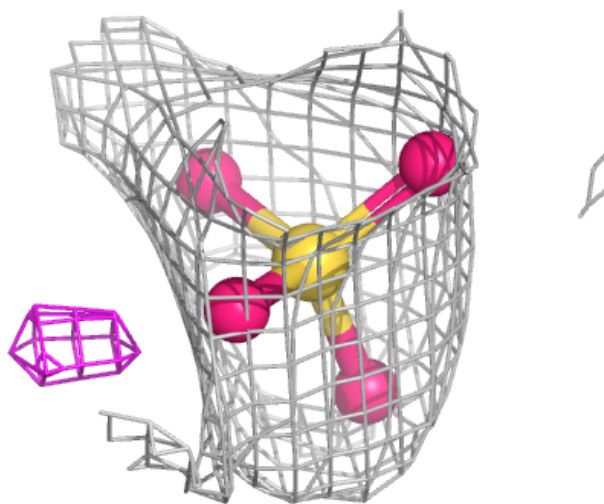
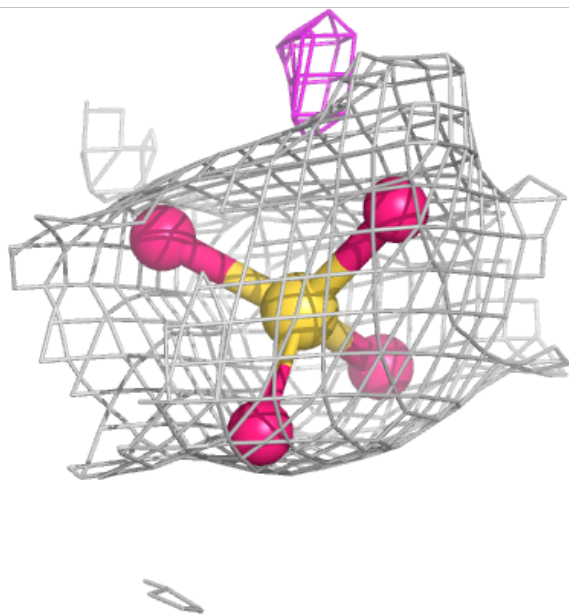
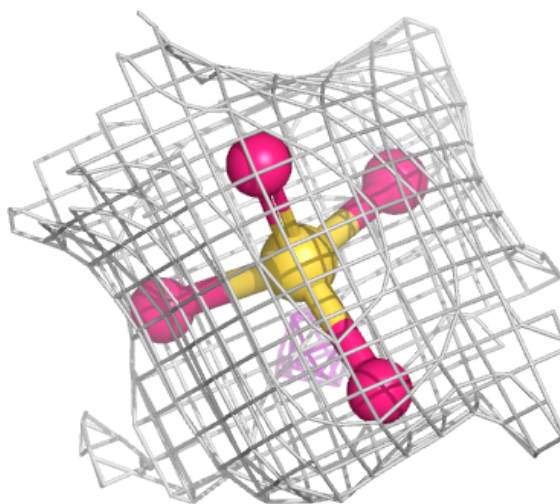
Electron density around SO4 G 404:

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



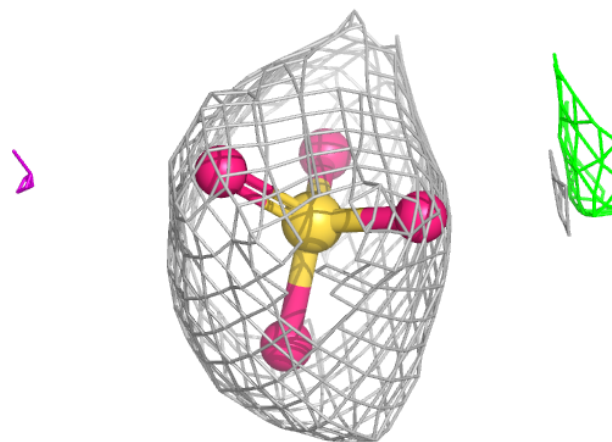
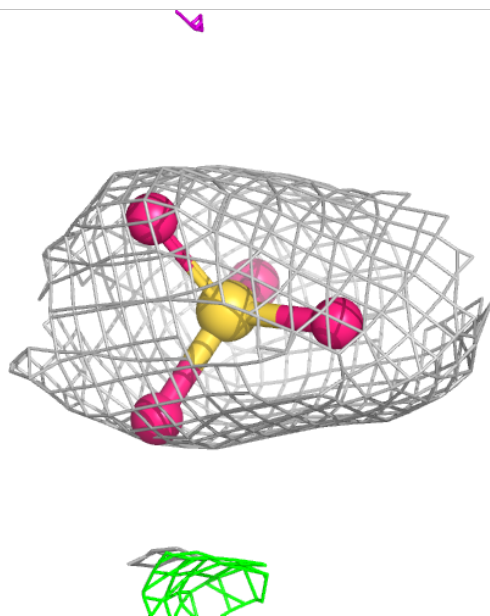
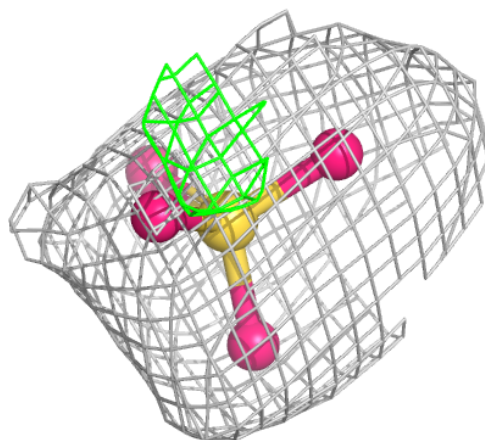
Electron density around SO4 B 406:

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



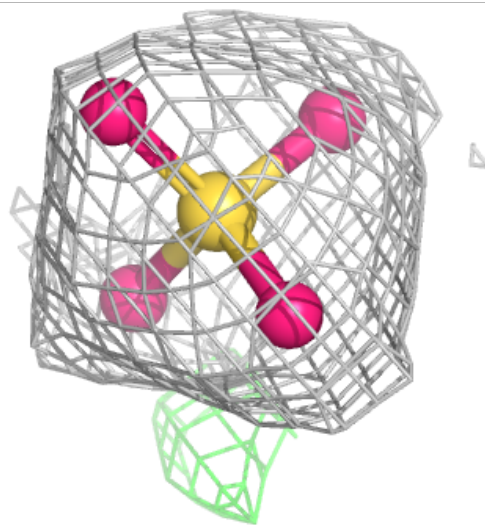
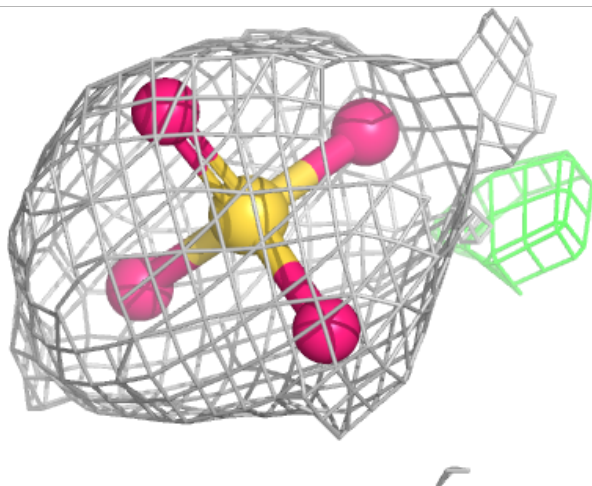
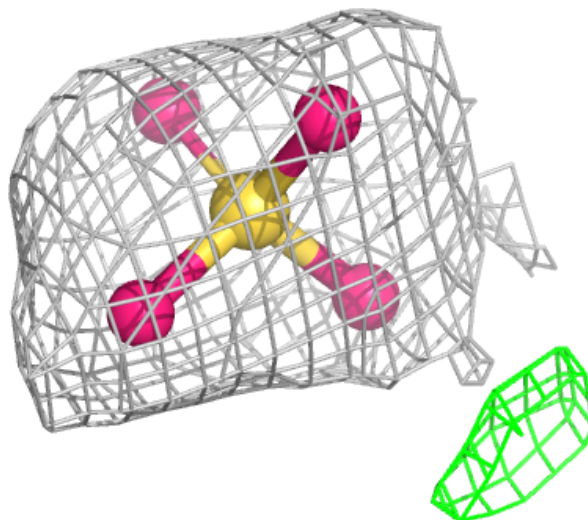
Electron density around SO4 G 403:

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



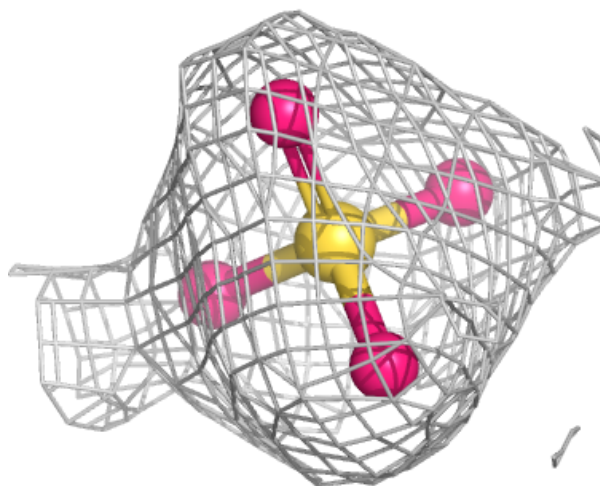
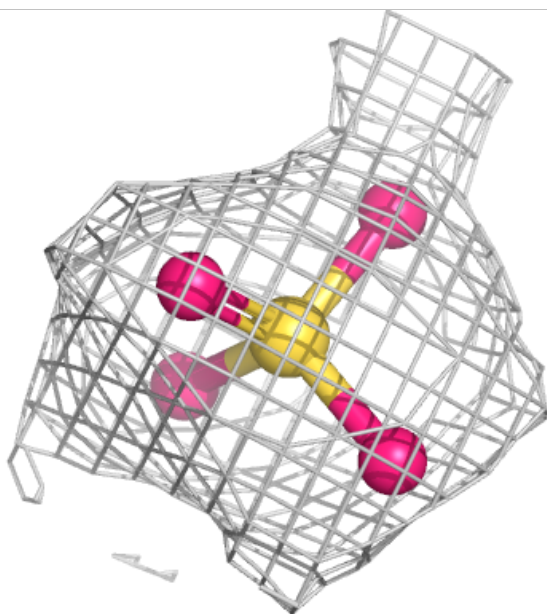
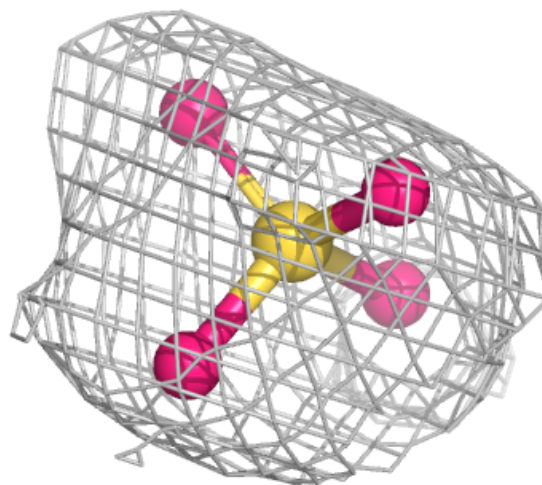
Electron density around SO4 B 403:

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



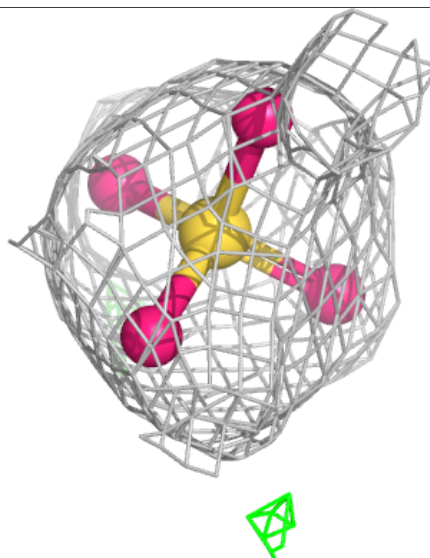
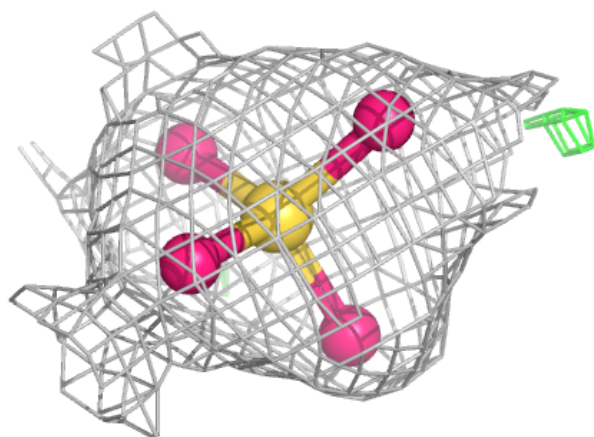
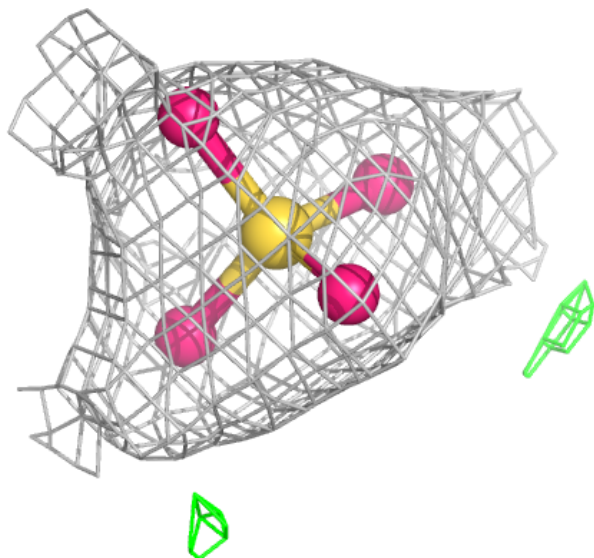
Electron density around SO4 B 401:

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



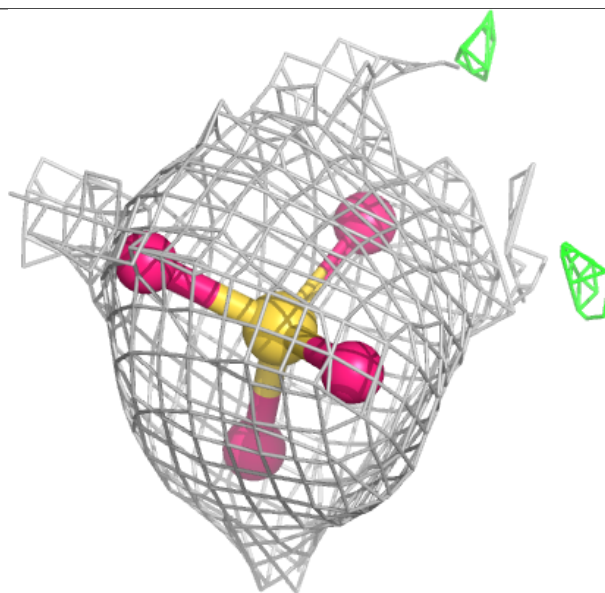
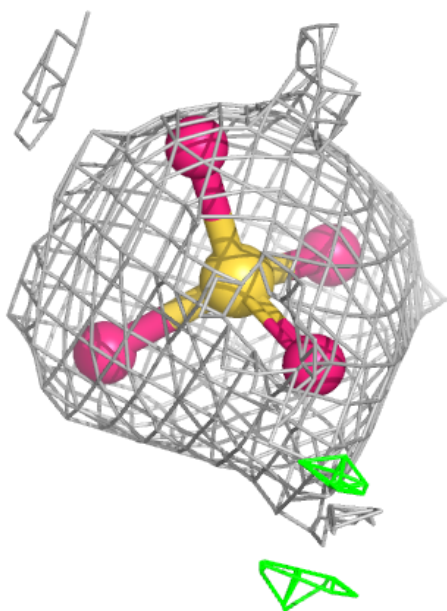
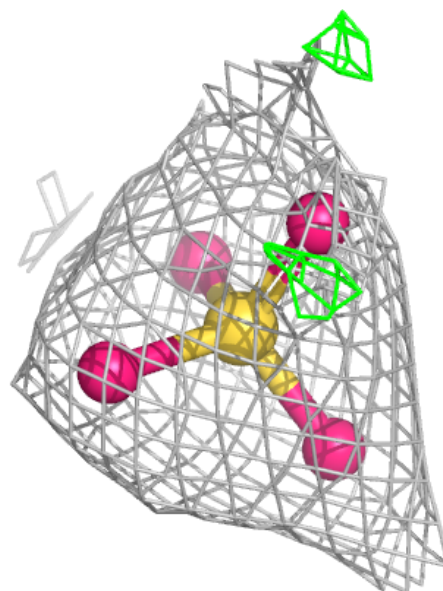
Electron density around SO4 F 401:

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



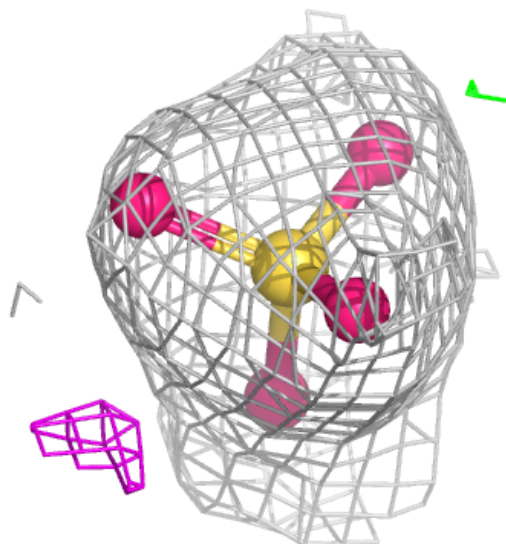
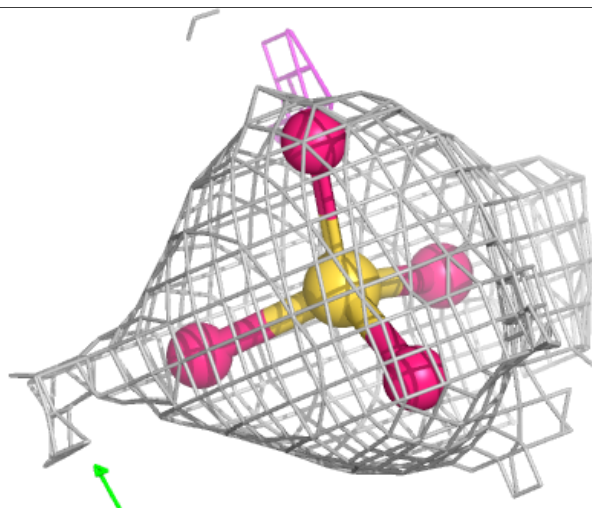
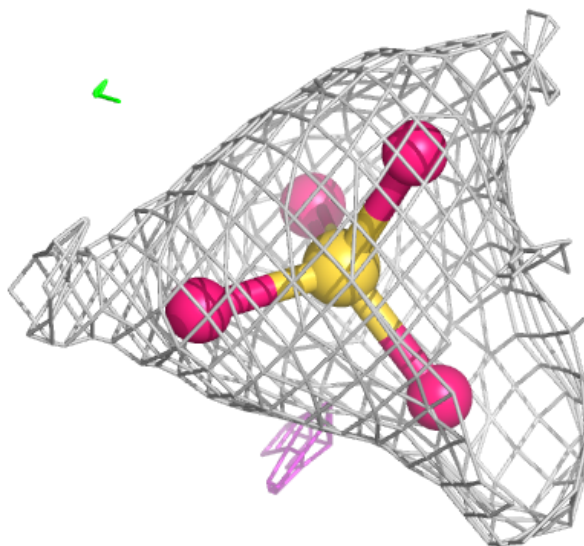
Electron density around SO4 G 401:

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



Electron density around SO4 A 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.