wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 07:51 PM EDT

PDB ID	:	6VVS
Title	:	Crystal structure of a Mycobacterium smegmatis RNA polymerase transcription initiation complex with antibiotic Sorangicin
Authors	:	Lilic, M.; Braffman, N.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2020-02-18
Resolution	:	3.11 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 (i) 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 (i)) were used in the production of this report:

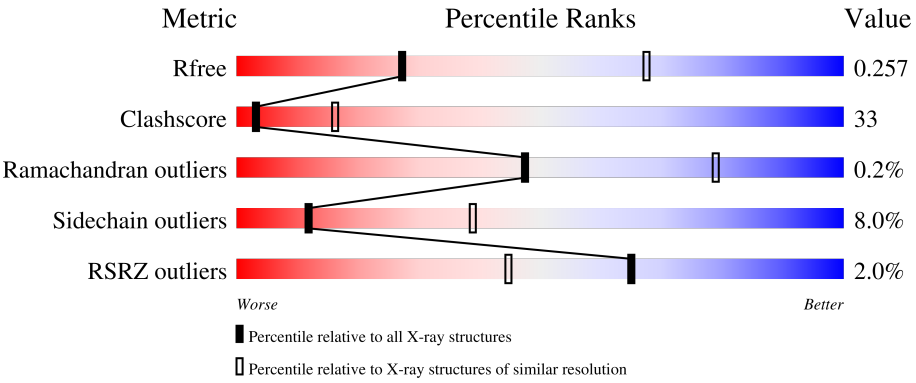
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 <=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	350	31% 29% 38%
1	B	350	2% 26% 35% 5% 33%
1	T	350	3% 12% 85%
2	C	1169	3% 43% 47% 6%
3	D	1317	50% 41% 5%

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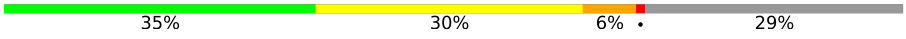
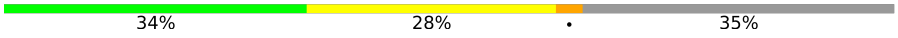
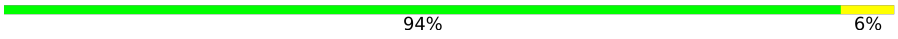
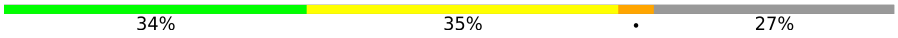
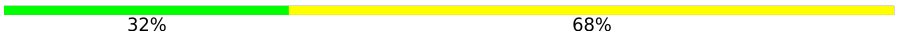
Mol	Chain	Length	Quality of chain
4	E	107	
5	F	466	
6	G	17	
7	J	114	
8	O	31	
9	P	26	

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
10	SO4	D	2004	-	-	X	-
11	EDO	D	2007	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26620 atoms, of which 56 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1605	1015	276	311	3			
1	B	233	Total	C	N	O	S	0	0	0
			1672	1056	289	325	2			
1	T	53	Total	C	N	O	S	0	0	0
			342	208	65	68	1			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1099	Total	C	N	O	S	0	0	0
			8275	5181	1453	1606	35			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1246	Total	C	N	O	S	0	0	0
			9555	5995	1720	1800	40			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			592	378	100	114			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	305	Total	C	N	O	S	0	0	0
			2407	1509	436	455	7			

- Molecule 6 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 7 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	83	Total	C	N	O	S	0	0	0
			671	422	119	128	2			

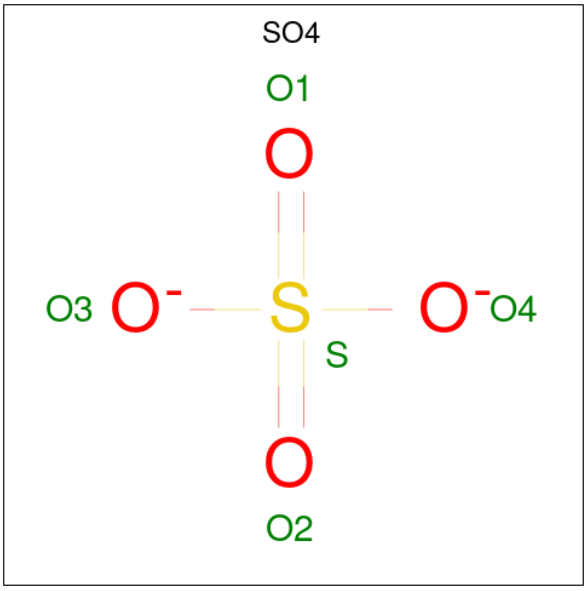
- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	O	31	Total	C	N	O	P	0	0	0
			633	305	114	184	30			

- Molecule 9 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

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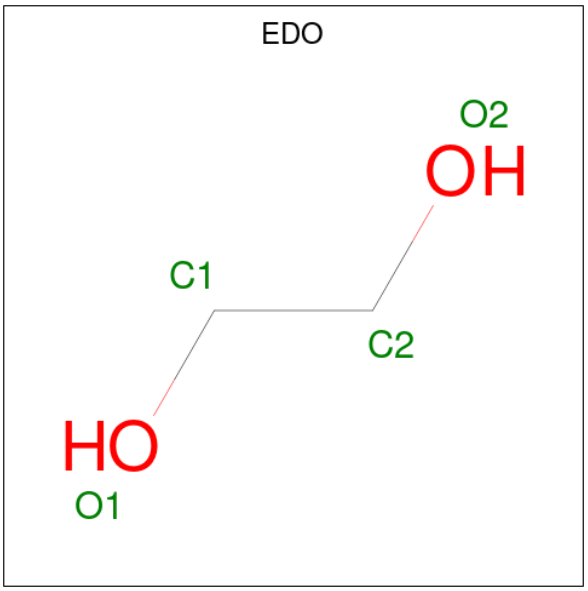
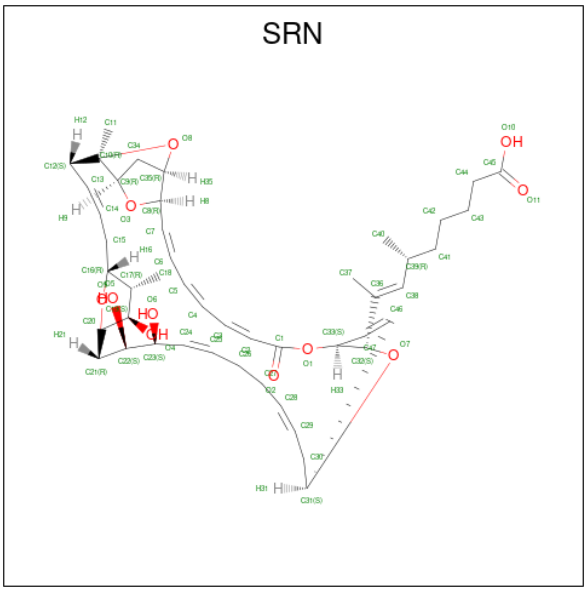
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C H O 10 2 6 2	0	0
11	C	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	F	1	Total C H O 10 2 6 2	0	0

- Molecule 12 is SORANGICIN A (three-letter code: SRN) (formula: $C_{47}H_{66}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C O 58 47 11	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	2	Total Zn 2 2	0	0

- Molecule 14 is water.

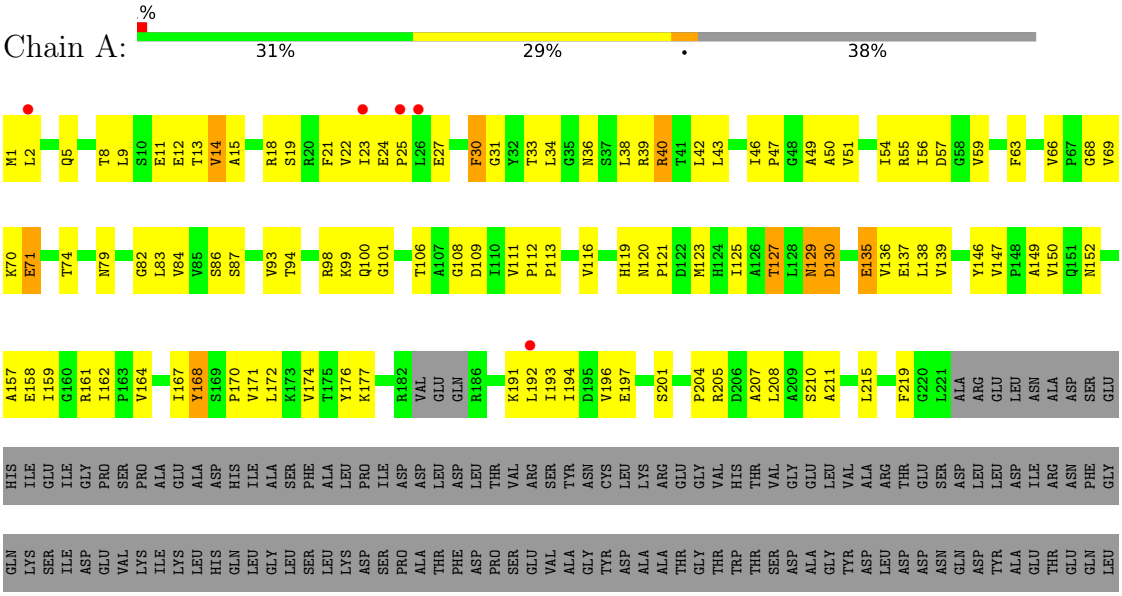
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	7	Total H O 11 4 7	0	0
14	D	21	Total H O 29 8 21	0	0
14	E	1	Total O 1 1	0	0
14	F	8	Total H O 10 2 8	0	0
14	J	1	Total O 1 1	0	0
14	O	3	Total O 3 3	0	0
14	P	2	Total O 2 2	0	0

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.

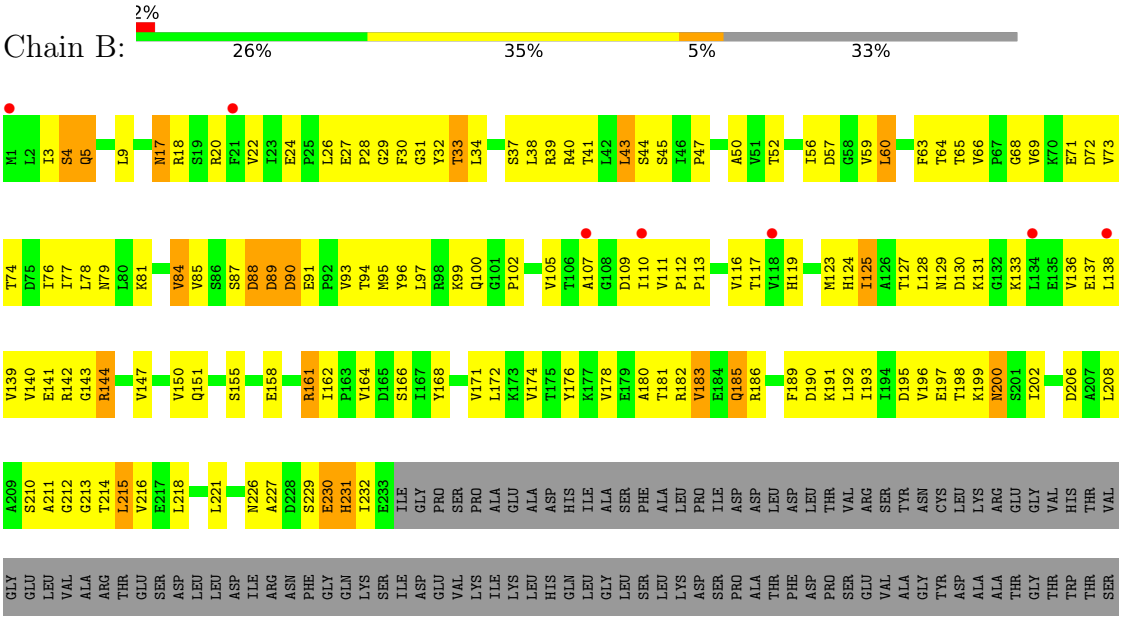
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:

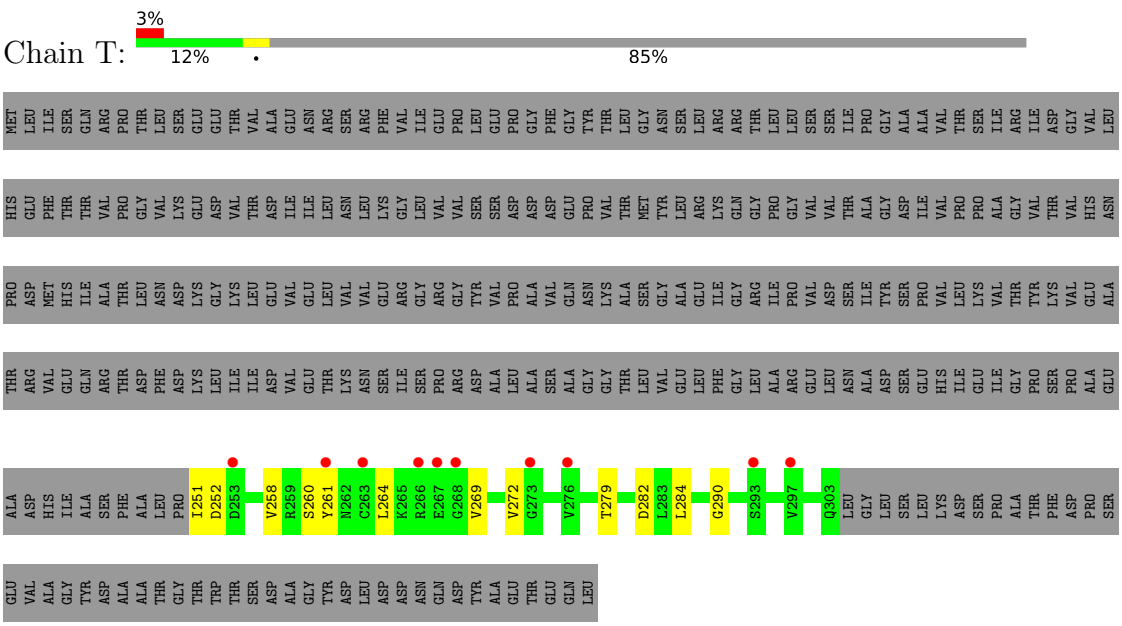


• Molecule 1: DNA-directed RNA polymerase subunit alpha

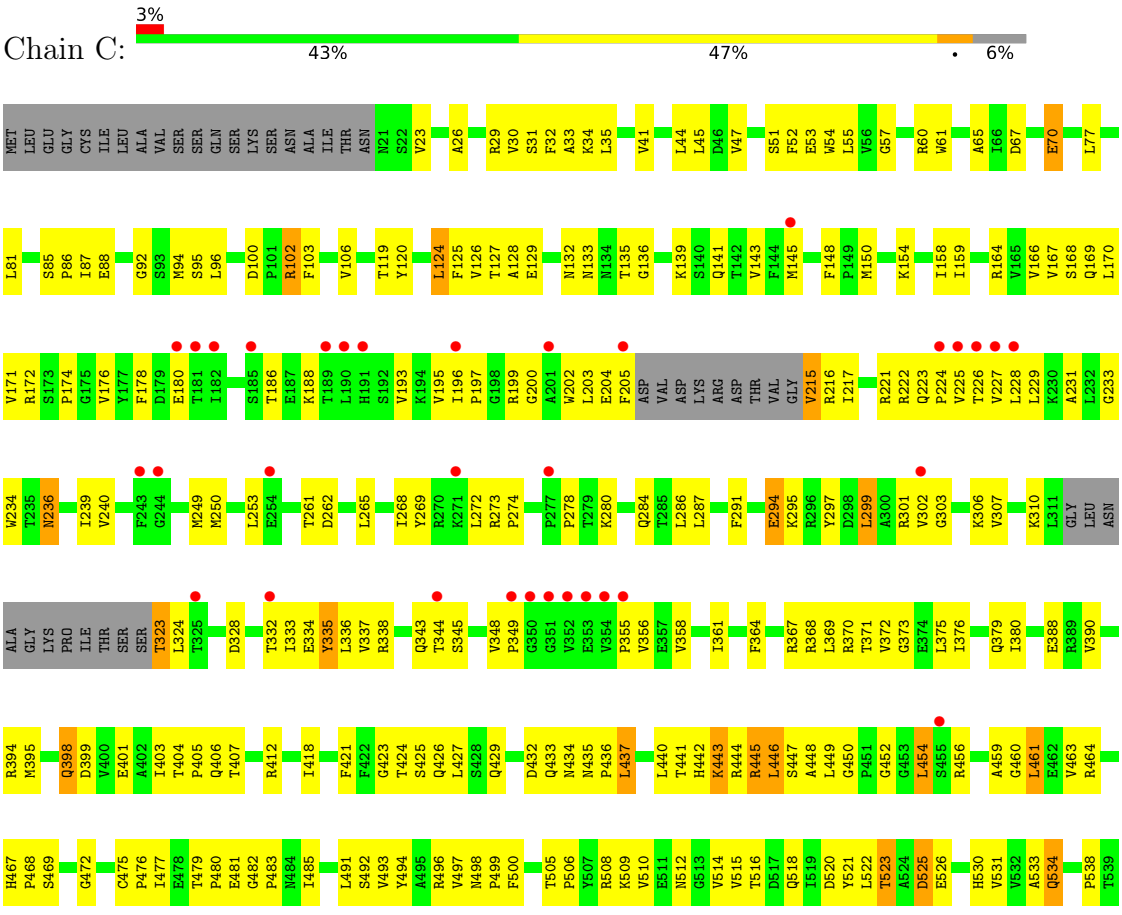
Chain B:

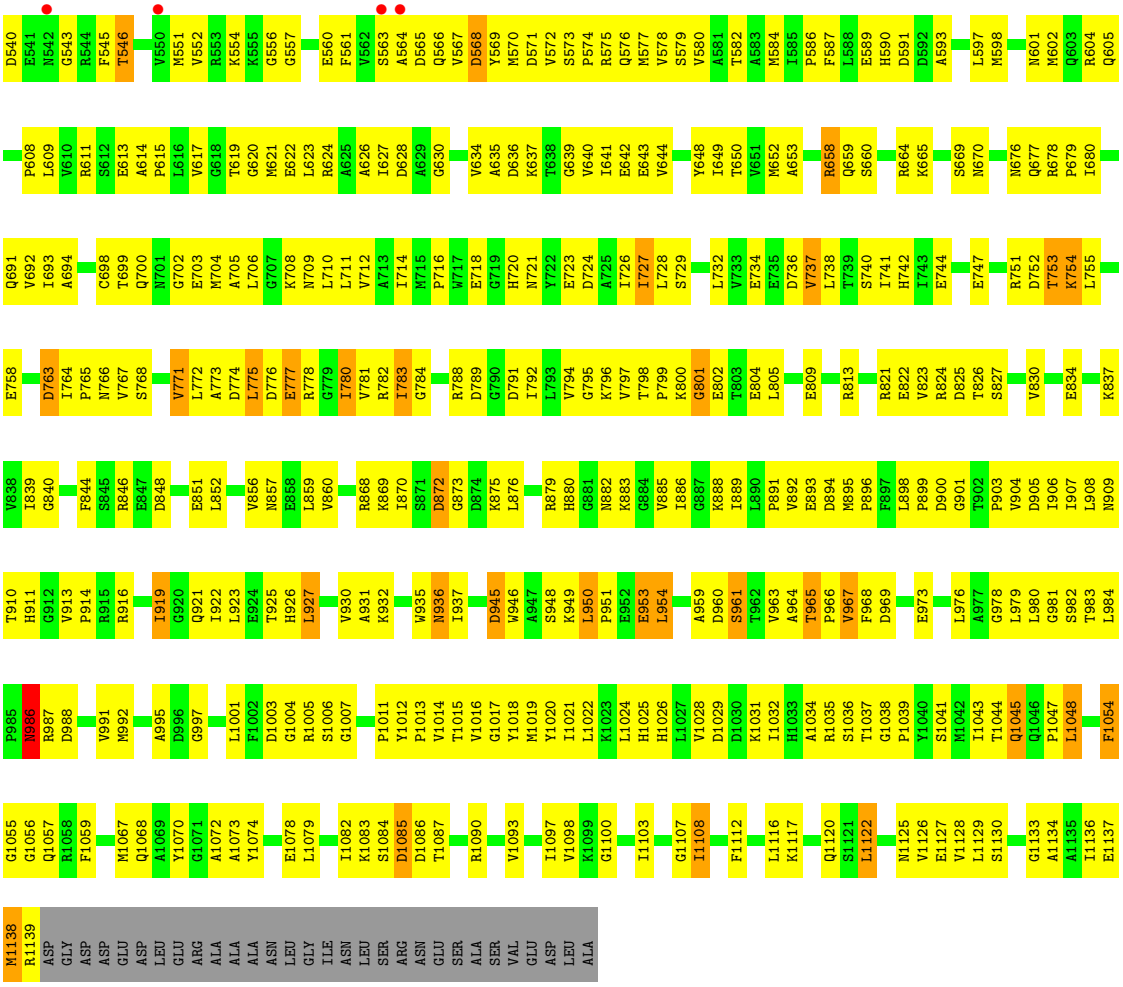


• Molecule 1: DNA-directed RNA polymerase subunit alpha



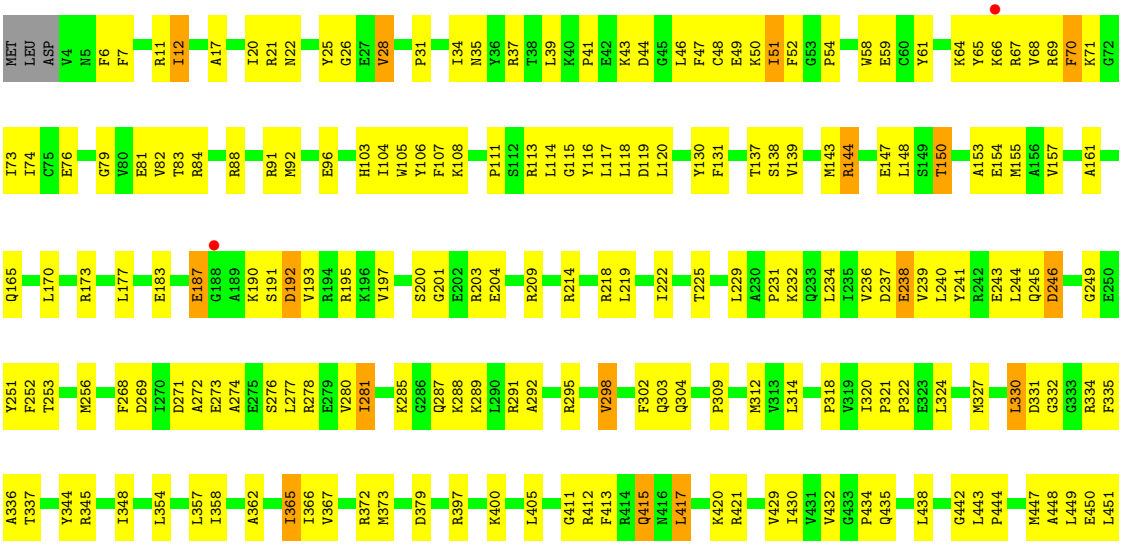
• Molecule 2: DNA-directed RNA polymerase subunit beta

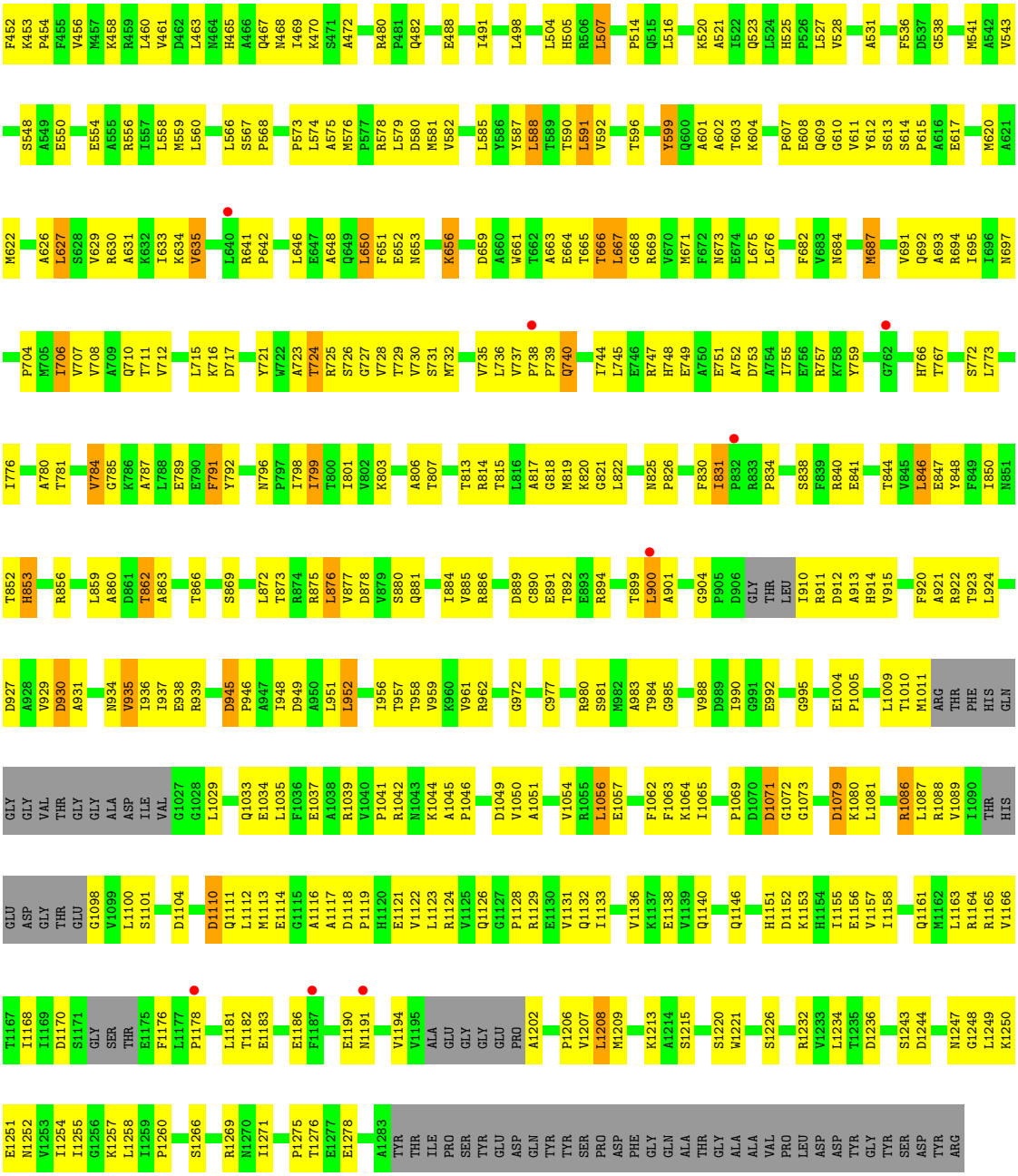




• Molecule 3: DNA-directed RNA polymerase subunit beta'

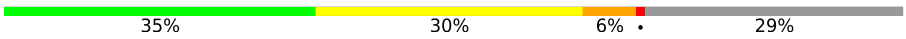
Chain D:

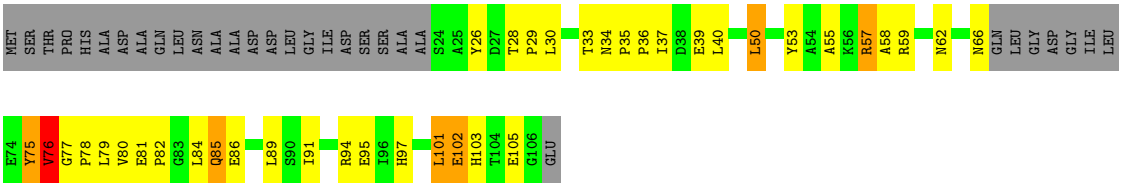




• Molecule 4: DNA-directed RNA polymerase subunit omega

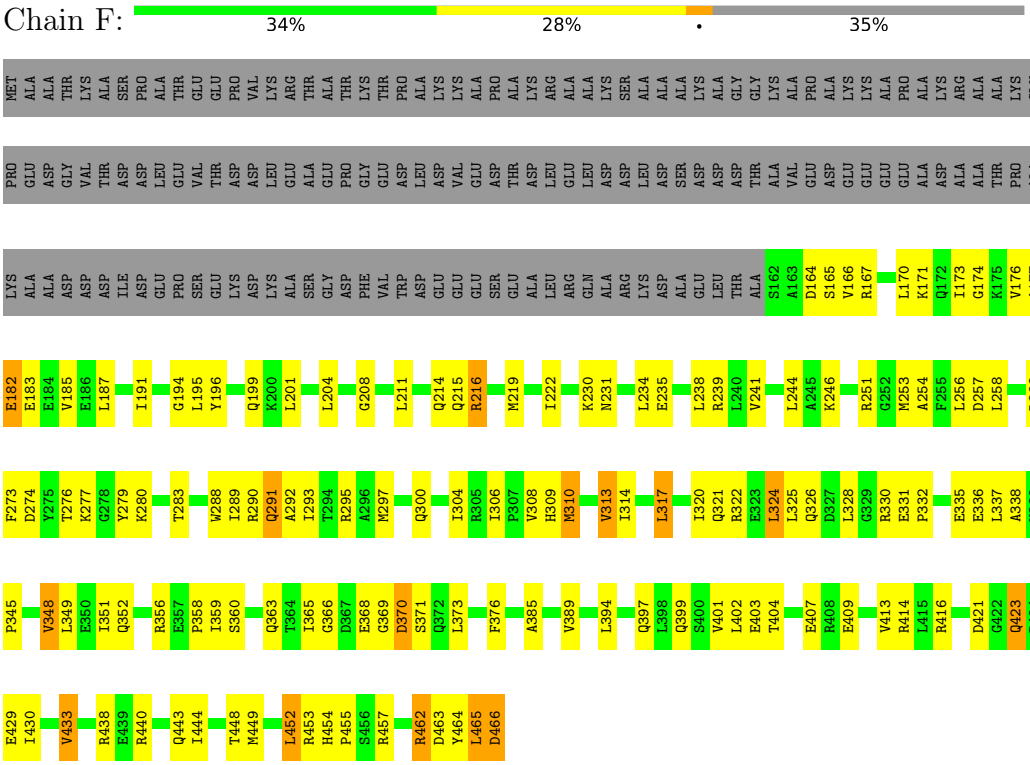
Chain E:





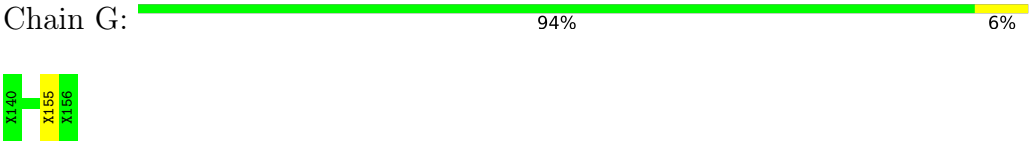
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



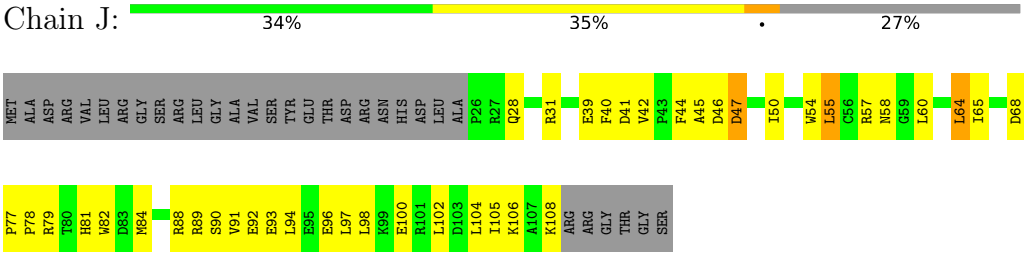
• Molecule 6: unknown

Chain G:



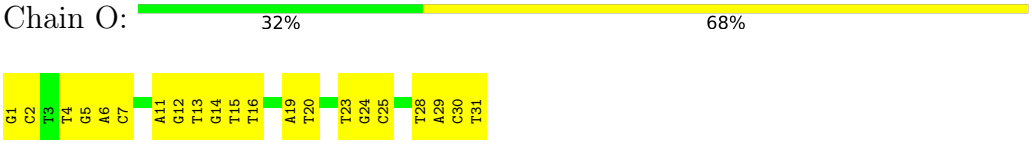
• Molecule 7: RNA polymerase-binding protein RbpA

Chain J:



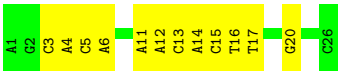
• Molecule 8: DNA (31-MER)

Chain O:



• Molecule 9: DNA (26-MER)

Chain P:


A1
G2
C3
A4
C5
A6
A11
A12
C13
A14
C15
T16
T17
G20
C26

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.46Å 162.91Å 139.32Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	54.66 – 3.11 54.66 – 3.11	Depositor EDS
% Data completeness (in resolution range)	96.7 (54.66-3.11) 96.7 (54.66-3.11)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.13Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.216 , 0.258 0.216 , 0.257	Depositor DCC
R_{free} test set	1997 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	94.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 72.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26620	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, SRN, EDO

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	0.24	0/1629	0.46	0/2220
1	B	0.24	0/1698	0.45	0/2322
1	T	0.23	0/343	0.37	0/468
2	C	0.26	0/8421	0.45	0/11444
3	D	0.26	0/9706	0.44	0/13140
4	E	0.25	0/604	0.42	0/822
5	F	0.25	0/2438	0.43	0/3291
7	J	0.25	0/685	0.43	0/927
8	O	0.56	0/710	0.93	0/1095
9	P	0.62	0/589	0.95	0/906
All	All	0.28	0/26823	0.49	0/36635

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
2	C	0	3
5	F	0	1
6	G	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	801	GLY	Peptide
2	C	950	LEU	Peptide
2	C	986	ASN	Peptide
5	F	368	GLU	Peptide
6	G	155	UNK	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1605	0	1623	141	0
1	B	1672	0	1643	177	0
1	T	342	0	275	14	0
2	C	8275	0	8025	681	1
3	D	9555	0	9509	574	1
4	E	592	0	583	41	0
5	F	2407	0	2428	155	0
6	G	85	0	19	0	0
7	J	671	0	660	48	0
8	O	633	0	350	38	0
9	P	526	0	296	14	0
10	C	20	0	0	3	0
10	D	25	0	0	2	0
10	F	25	0	0	2	0
11	C	8	12	12	1	0
11	D	16	24	24	3	0
11	F	4	6	6	1	0
12	C	58	0	64	14	0
13	D	2	0	0	0	0
14	C	7	4	0	1	0
14	D	21	8	0	2	0
14	E	1	0	0	0	0
14	F	8	2	0	1	0
14	J	1	0	0	0	0
14	O	3	0	0	0	0
14	P	2	0	0	0	0
All	All	26564	56	25517	1737	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 33.

The worst 5 of 1737 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)
12:C:1205:SRN:C12	12:C:1205:SRN:C10	1.77	1.57
12:C:1205:SRN:C8	12:C:1205:SRN:O3	1.80	1.28
12:C:1205:SRN:O3	12:C:1205:SRN:C9	1.80	1.28
3:D:922:ARG:HB3	3:D:961:VAL:HG21	1.31	1.13
2:C:203:LEU:HG	2:C:217:ILE:HG22	1.35	1.08

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)
2:C:658:ARG:NH1	3:D:147:GLU:OE1[2_356]	1.96	0.24

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	214/350 (61%)	202 (94%)	12 (6%)	0	100 100
1	B	231/350 (66%)	211 (91%)	19 (8%)	1 (0%)	34 68
1	T	51/350 (15%)	51 (100%)	0	0	100 100
2	C	1093/1169 (94%)	1040 (95%)	52 (5%)	1 (0%)	51 83
3	D	1234/1317 (94%)	1181 (96%)	51 (4%)	2 (0%)	47 79
4	E	72/107 (67%)	66 (92%)	4 (6%)	2 (3%)	5 24
5	F	303/466 (65%)	296 (98%)	7 (2%)	0	100 100
7	J	81/114 (71%)	76 (94%)	5 (6%)	0	100 100
All	All	3279/4223 (78%)	3123 (95%)	150 (5%)	6 (0%)	47 79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	76	VAL
3	D	1194	VAL
4	E	78	PRO
1	B	183	VAL
2	C	967	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	174/297 (59%)	161 (92%)	13 (8%)	13 41
1	B	173/297 (58%)	153 (88%)	20 (12%)	5 22
1	T	26/297 (9%)	25 (96%)	1 (4%)	33 65
2	C	862/984 (88%)	798 (93%)	64 (7%)	13 41
3	D	989/1095 (90%)	912 (92%)	77 (8%)	12 40
4	E	62/86 (72%)	52 (84%)	10 (16%)	2 10
5	F	251/379 (66%)	233 (93%)	18 (7%)	14 43
7	J	72/98 (74%)	66 (92%)	6 (8%)	11 37
All	All	2609/3533 (74%)	2400 (92%)	209 (8%)	12 39

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	298	VAL
3	D	740	GLN
5	F	462	ARG
3	D	365	ILE
3	D	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	684	ASN
3	D	888	HIS
3	D	692	GLN
3	D	778	GLN
3	D	1126	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)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
11	EDO	D	2008	-	3,3,3	0.43	0	2,2,2	0.35	0
10	SO4	F	504	-	4,4,4	0.15	0	6,6,6	0.05	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.07	0
12	SRN	C	1205	-	60,62,62	5.09	32 (53%)	62,84,84	1.78	16 (25%)
10	SO4	C	1206	-	4,4,4	0.14	0	6,6,6	0.08	0
11	EDO	D	2009	-	3,3,3	0.48	0	2,2,2	0.25	0
10	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.11	0
10	SO4	C	1201	-	4,4,4	0.14	0	6,6,6	0.08	0
10	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.07	0
10	SO4	F	505	-	4,4,4	0.15	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	D	2011	-	3,3,3	0.46	0	2,2,2	0.27	0
10	SO4	C	1202	-	4,4,4	0.13	0	6,6,6	0.08	0
10	SO4	D	2003	-	4,4,4	0.13	0	6,6,6	0.15	0
11	EDO	F	506	-	3,3,3	0.48	0	2,2,2	0.26	0
10	SO4	D	2004	-	4,4,4	0.13	0	6,6,6	0.10	0
11	EDO	C	1207	-	3,3,3	0.49	0	2,2,2	0.26	0
10	SO4	F	503	-	4,4,4	0.13	0	6,6,6	0.10	0
11	EDO	C	1204	-	3,3,3	0.40	0	2,2,2	0.41	0
10	SO4	D	2010	-	4,4,4	0.14	0	6,6,6	0.08	0
10	SO4	D	2005	-	4,4,4	0.13	0	6,6,6	0.09	0
10	SO4	D	2006	-	4,4,4	0.15	0	6,6,6	0.09	0
11	EDO	D	2007	-	3,3,3	0.47	0	2,2,2	0.28	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
11	EDO	C	1207	-	-	0/1/1/1	-
11	EDO	D	2008	-	-	0/1/1/1	-
11	EDO	C	1204	-	-	1/1/1/1	-
11	EDO	D	2011	-	-	0/1/1/1	-
11	EDO	F	506	-	-	0/1/1/1	-
12	SRN	C	1205	-	-	5/52/105/105	0/4/5/5
11	EDO	D	2009	-	-	0/1/1/1	-
11	EDO	D	2007	-	-	0/1/1/1	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	SRN	O3-C8	19.79	1.80	1.44
12	C	1205	SRN	O3-C9	16.07	1.80	1.45
12	C	1205	SRN	C34-C9	-11.15	1.28	1.52
12	C	1205	SRN	C3-C2	9.74	1.59	1.34
12	C	1205	SRN	C34-C35	-8.88	1.33	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	1205	SRN	O9-C21-C20	5.19	115.31	109.94
12	C	1205	SRN	C8-C7-C6	-4.22	117.35	125.61

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	1205	SRN	C37-C36-C32	3.67	122.03	115.68
12	C	1205	SRN	C6-C5-C4	-3.66	116.66	124.81
12	C	1205	SRN	C9-C34-C35	3.28	113.21	103.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	1205	SRN	C25-C26-C27-C28
12	C	1205	SRN	C14-C15-C16-O9
12	C	1205	SRN	C42-C43-C44-C45
12	C	1205	SRN	C39-C41-C42-C43
12	C	1205	SRN	C14-C15-C16-C17

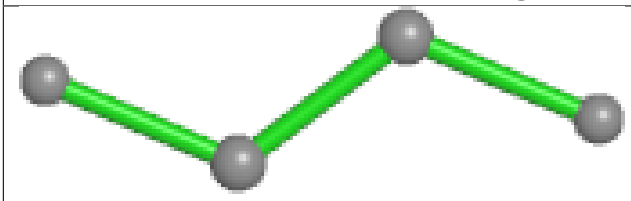
There are no ring outliers.

11 monomers are involved in 26 short contacts:

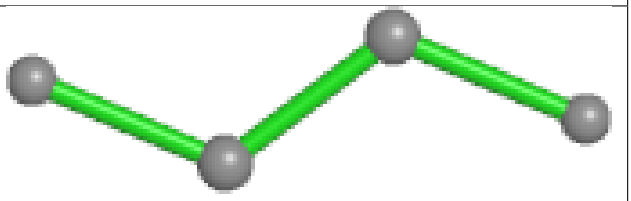
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1203	SO4	1	0
12	C	1205	SRN	14	0
10	C	1206	SO4	1	0
10	F	502	SO4	1	0
10	C	1201	SO4	1	0
10	F	505	SO4	1	0
11	D	2011	EDO	1	0
11	F	506	EDO	1	0
10	D	2004	SO4	2	0
11	C	1207	EDO	1	0
11	D	2007	EDO	2	0

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 then 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.

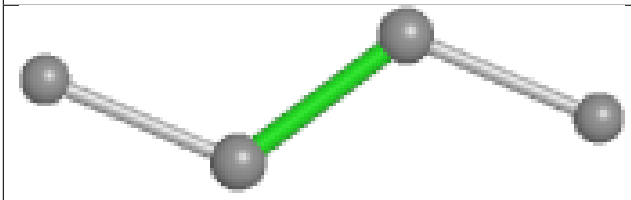
Ligand EDO D 2008



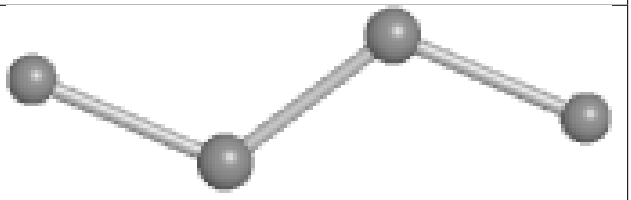
Bond lengths



Bond angles

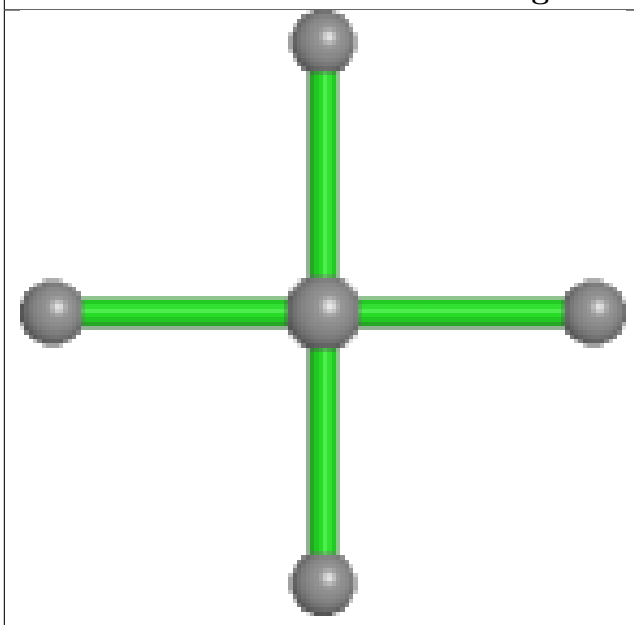


Torsions



Rings

Ligand SO4 F 504



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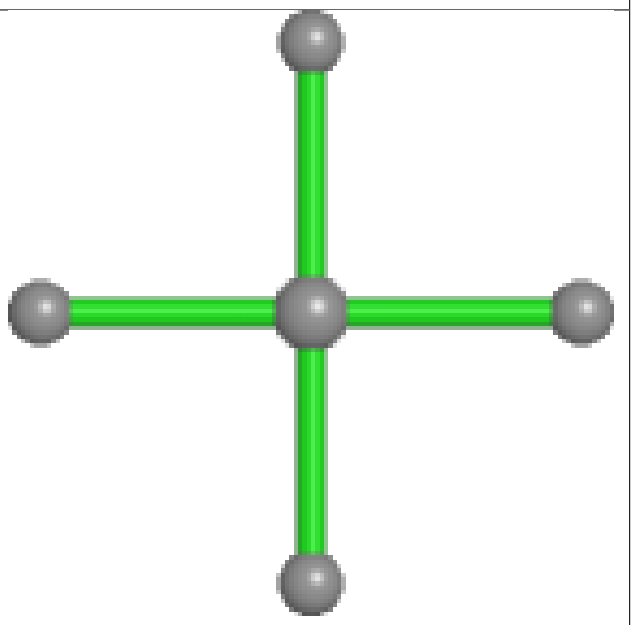

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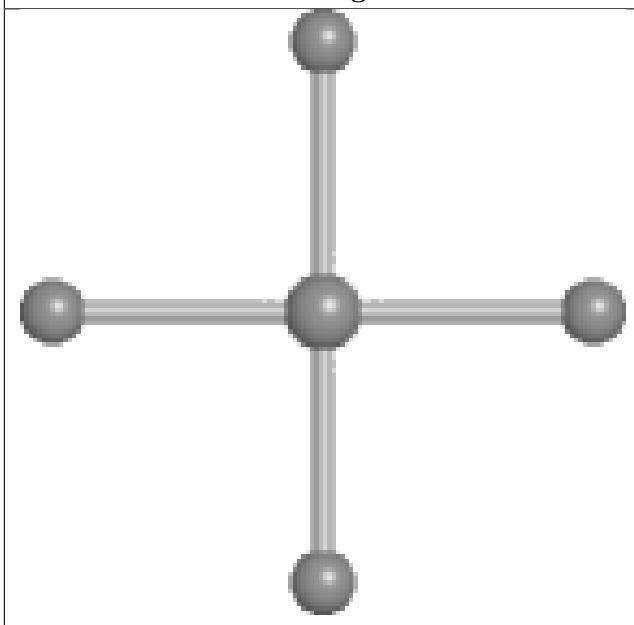

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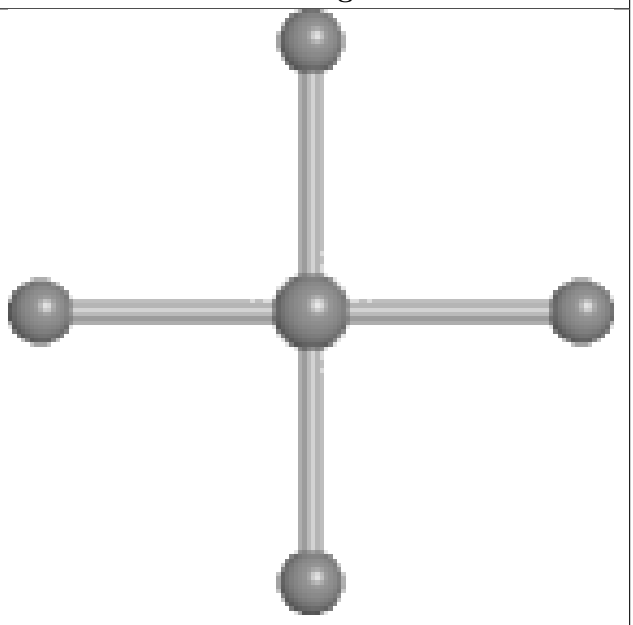
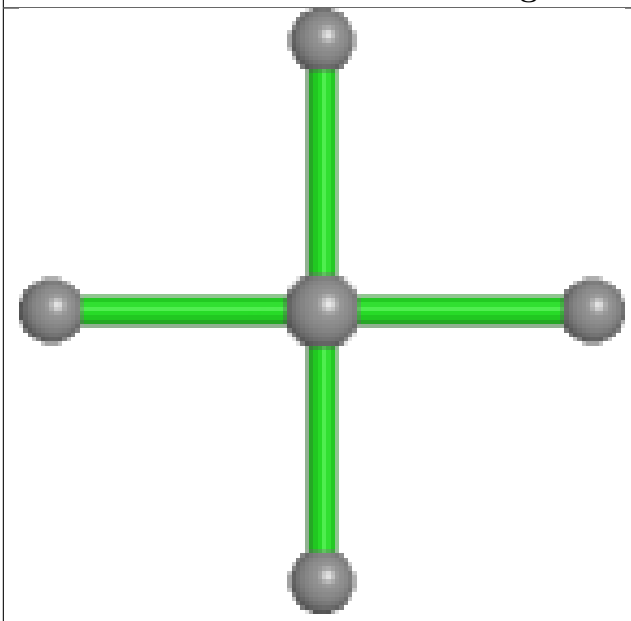


Rings

Ligand SO4 C 1203



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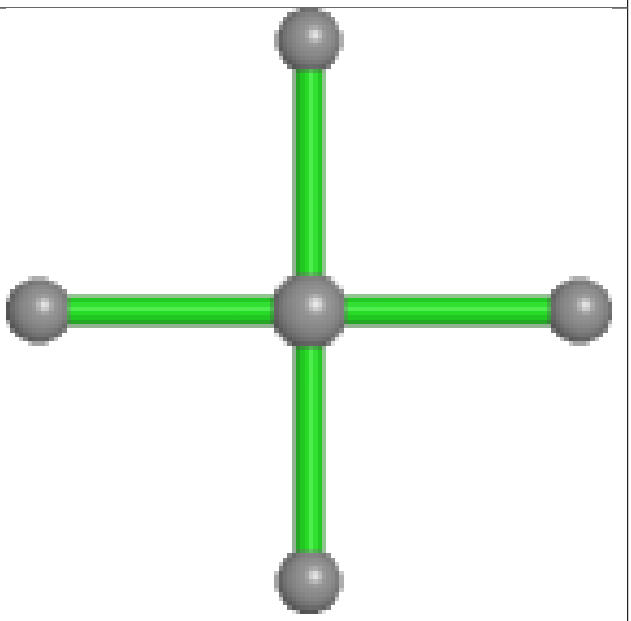

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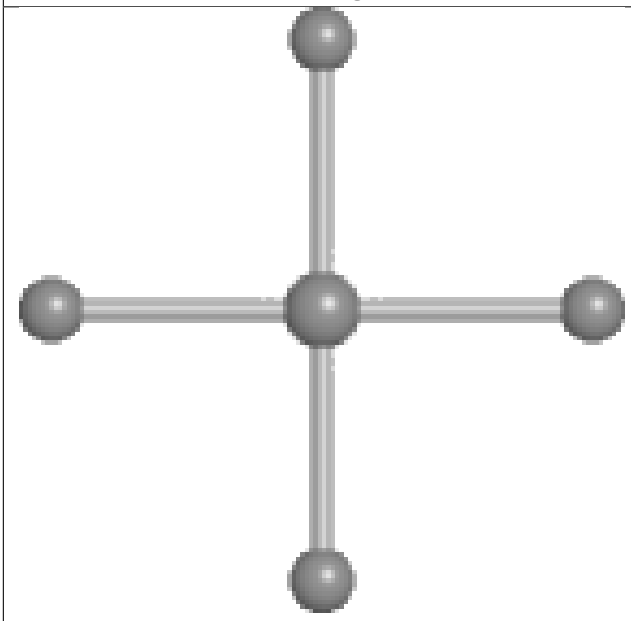

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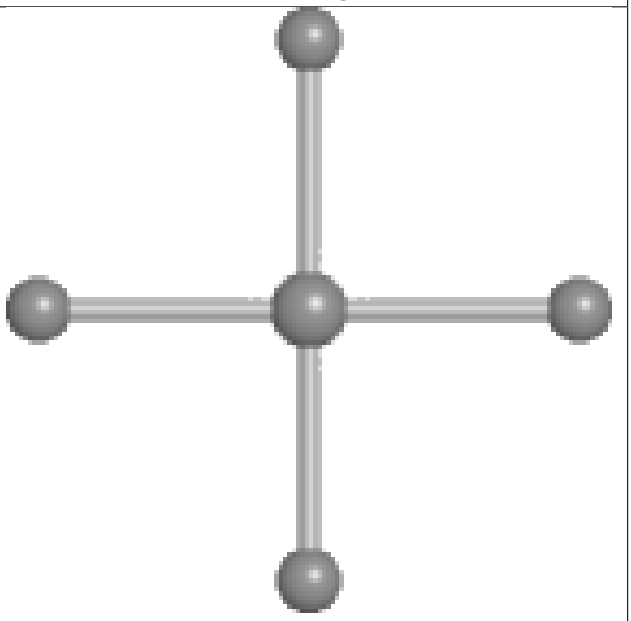
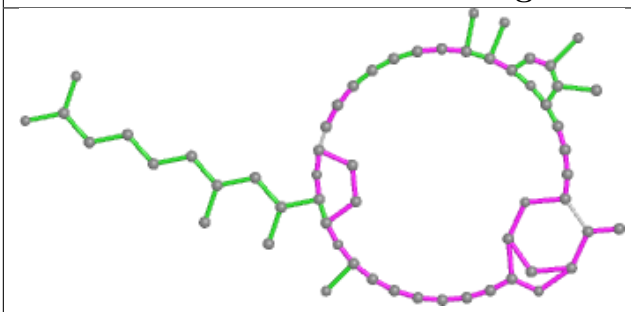


Rings

Ligand SRN C 1205



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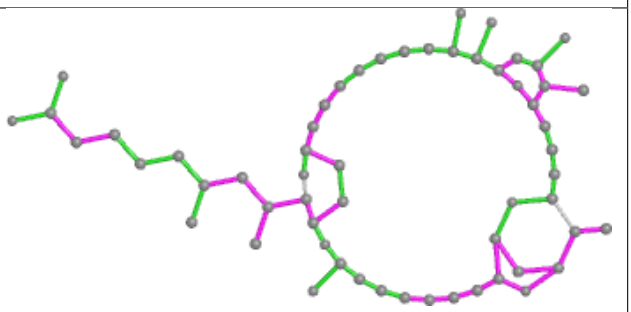
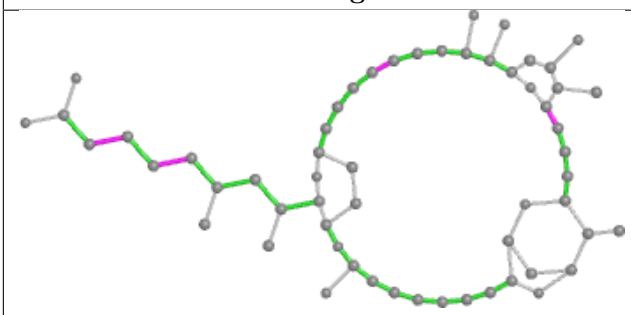


Bond angles



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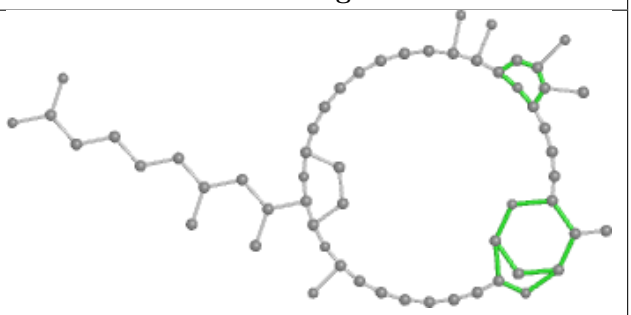
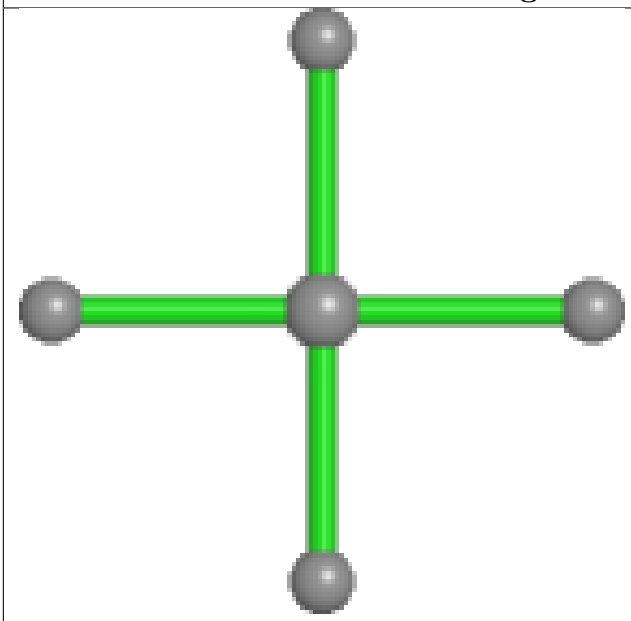


Rings

Ligand SO4 C 1206



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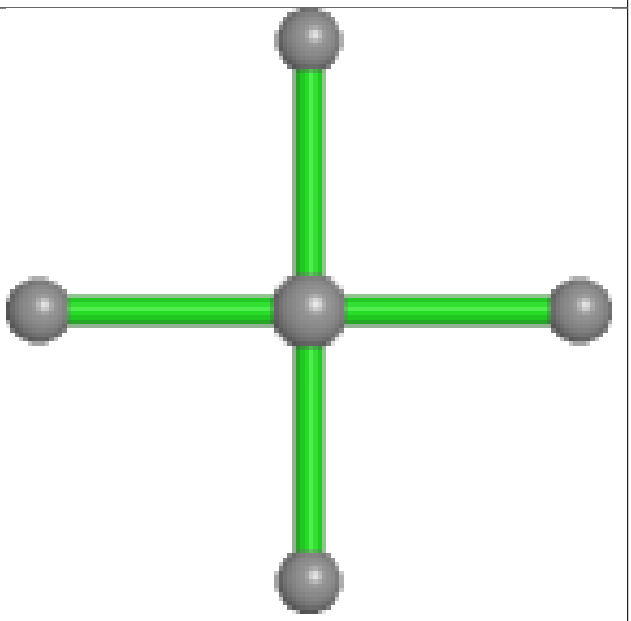

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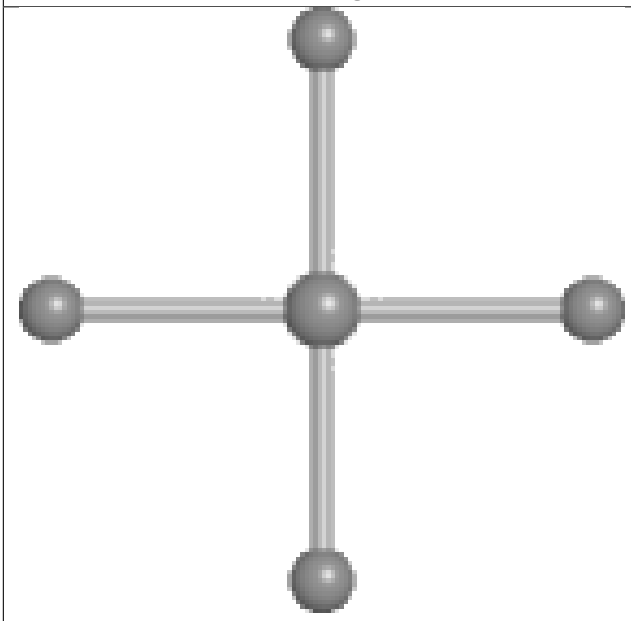

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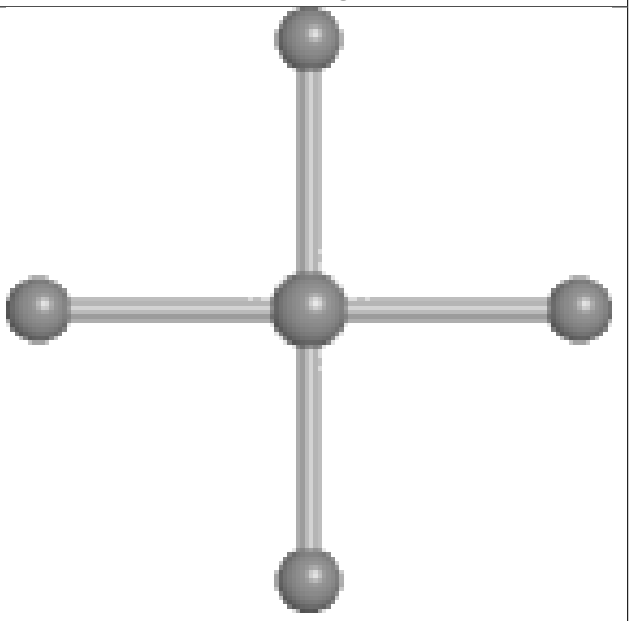
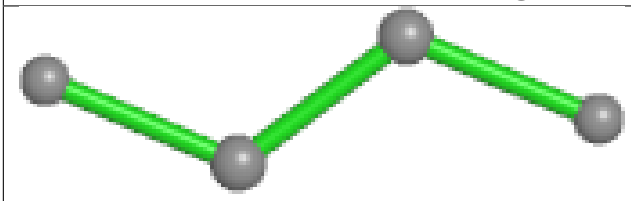


Rings

Ligand EDO D 2009



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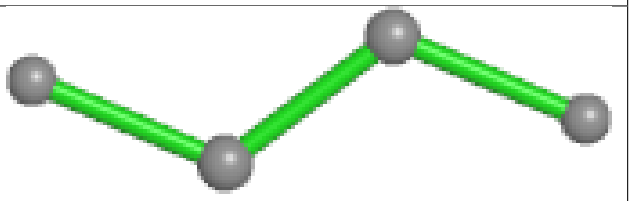

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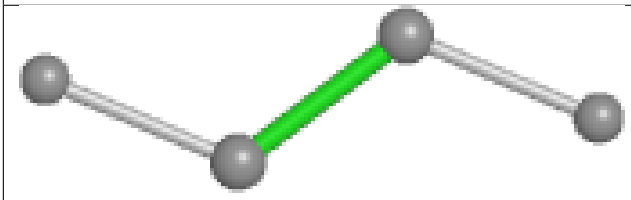

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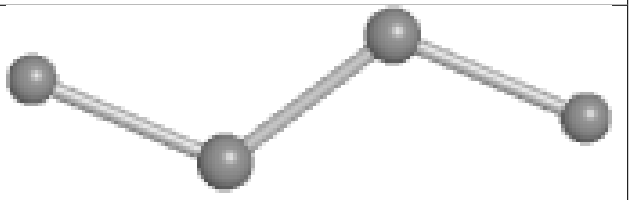
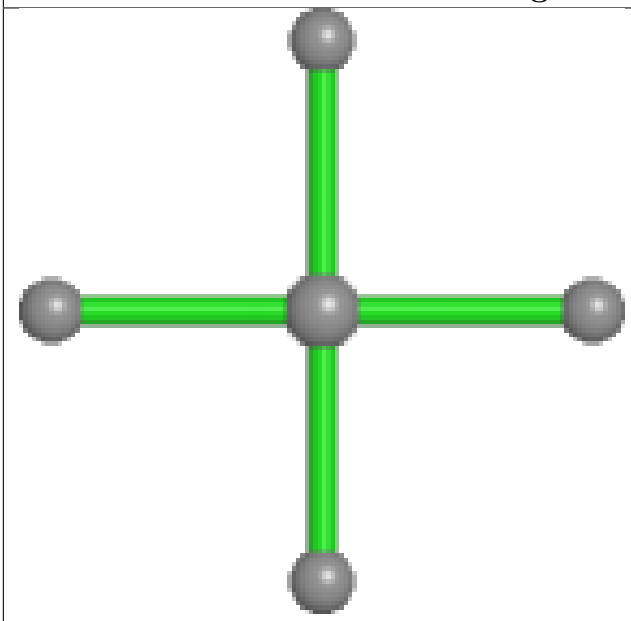


Rings

Ligand SO4 F 502



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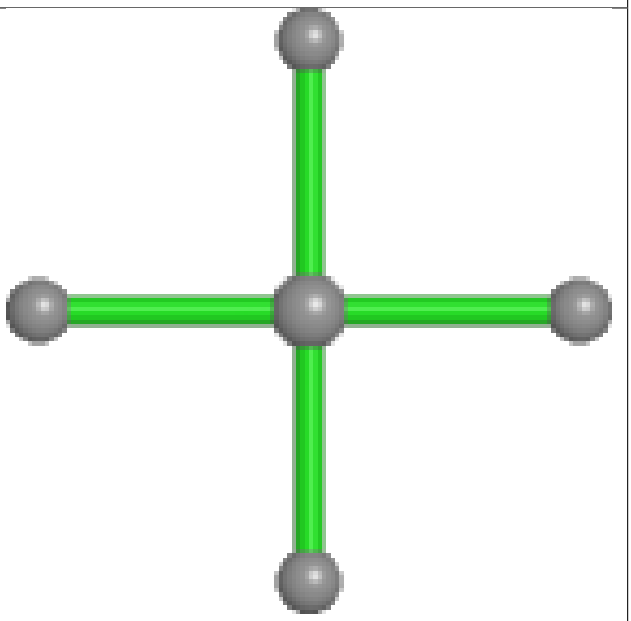

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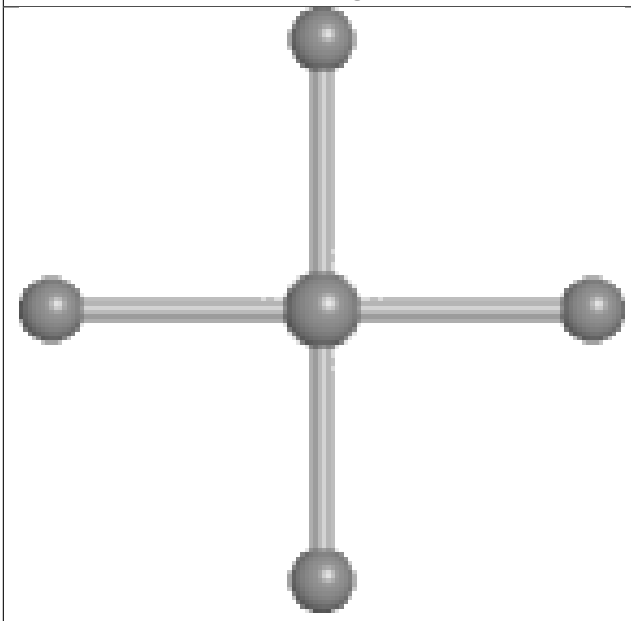

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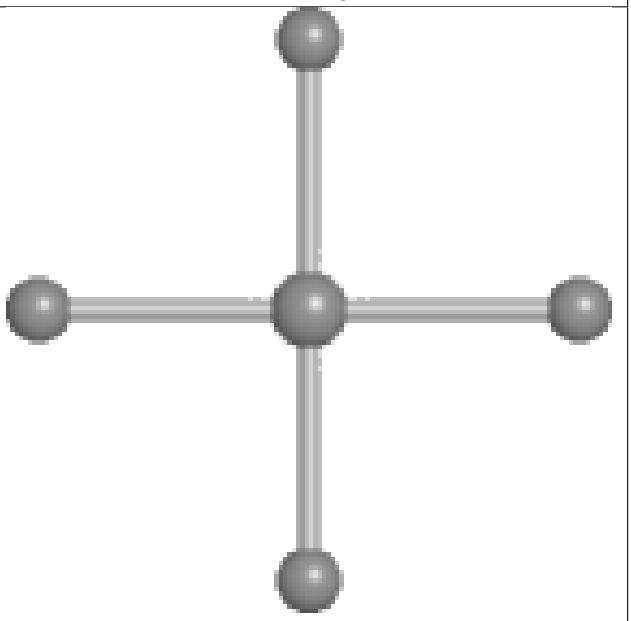
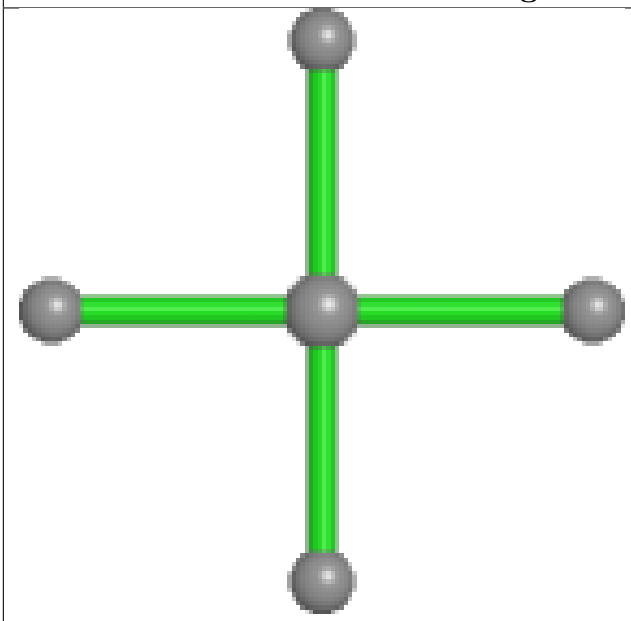
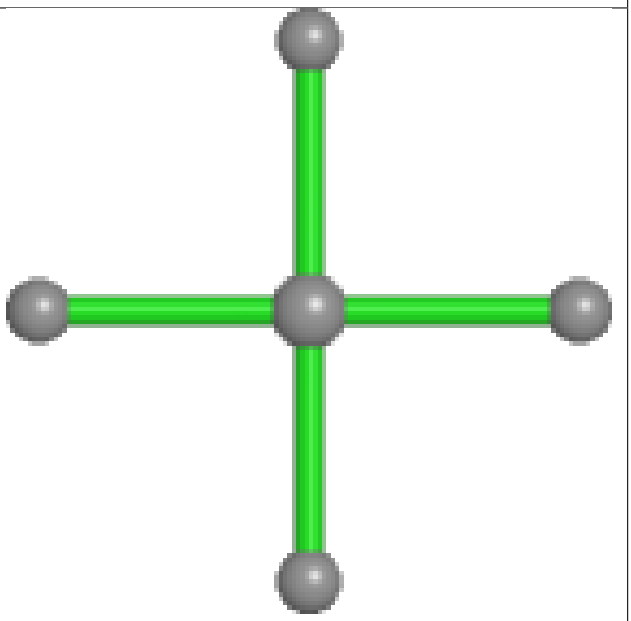


Rings

Ligand SO4 C 1201



Bond lengths



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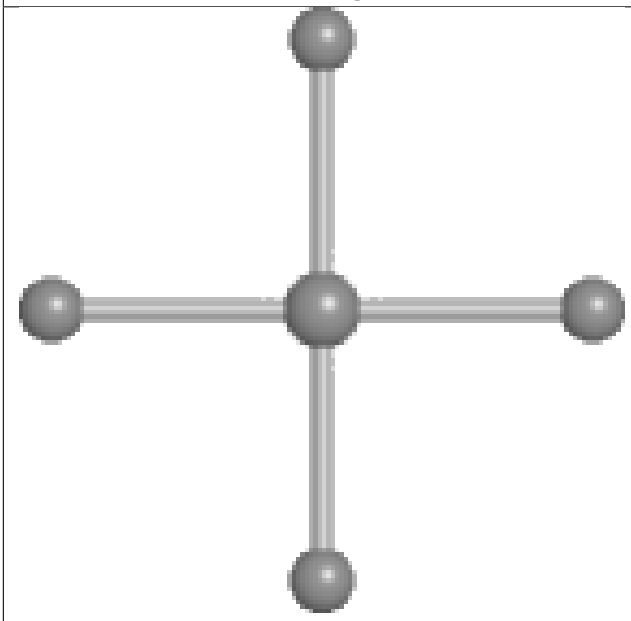
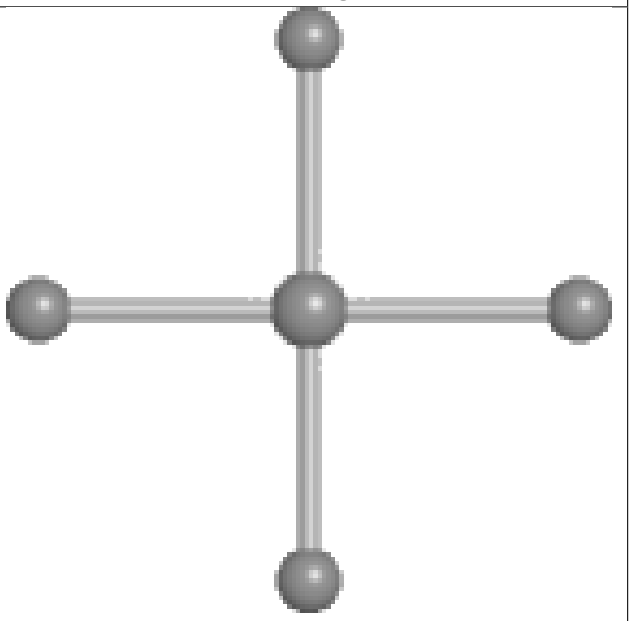
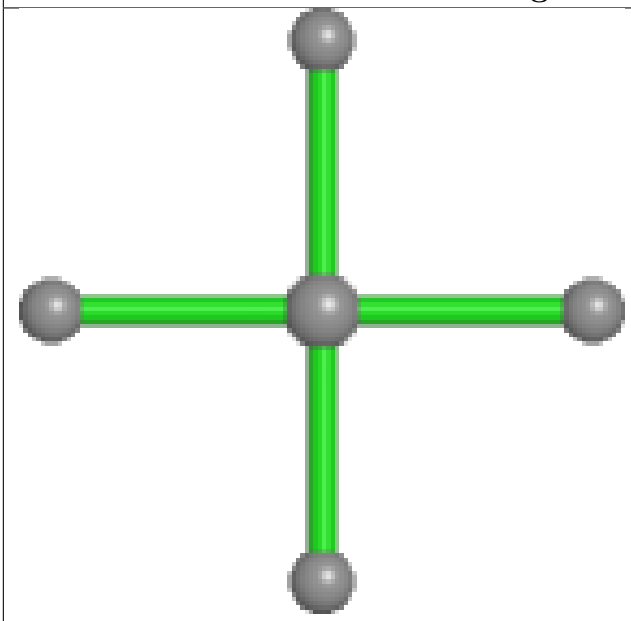


Torsions

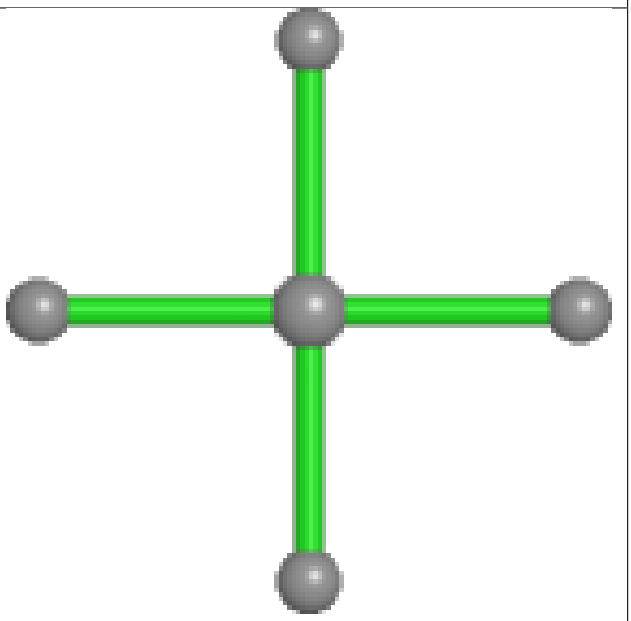


Rings

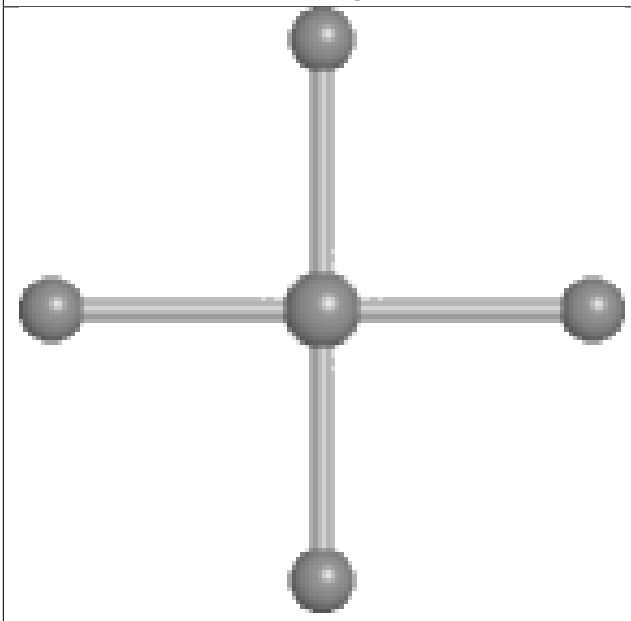
Ligand SO4 F 501



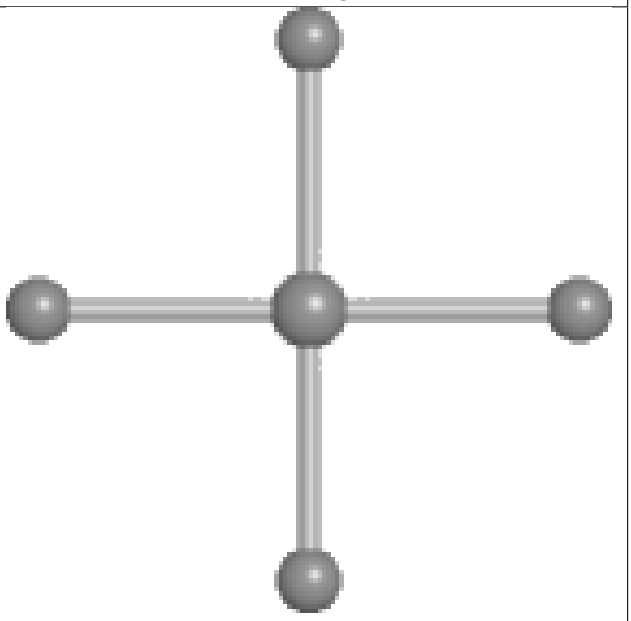
Bond lengths



Bond angles

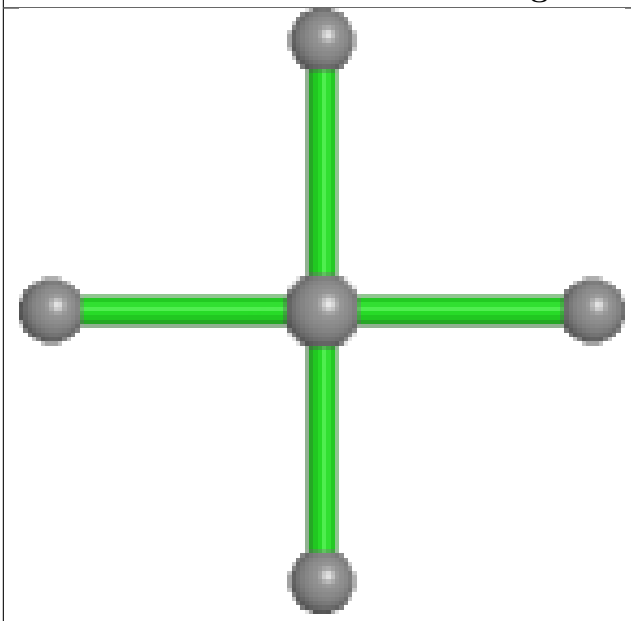


Torsions



Rings

Ligand SO4 F 505



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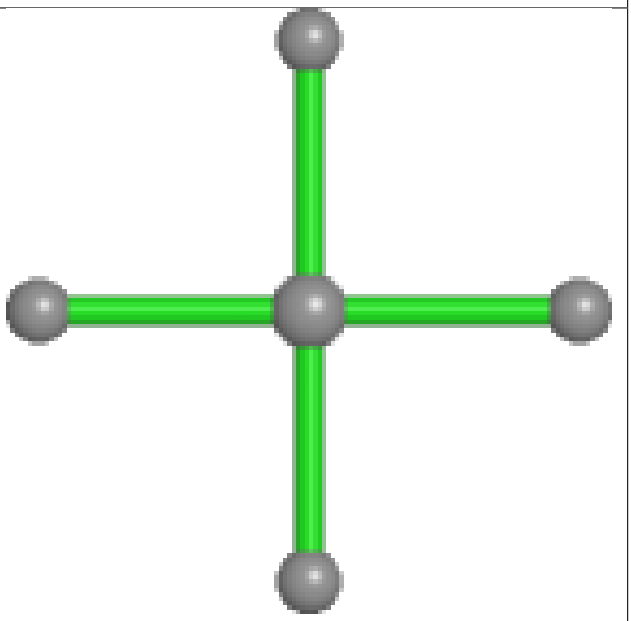

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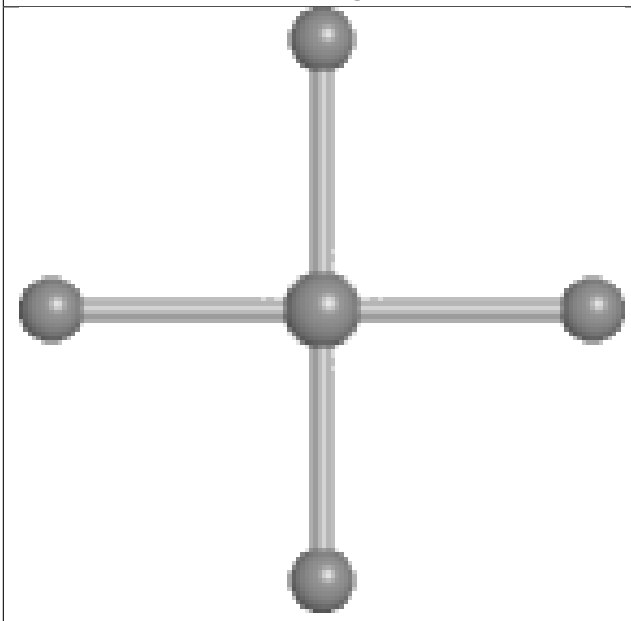
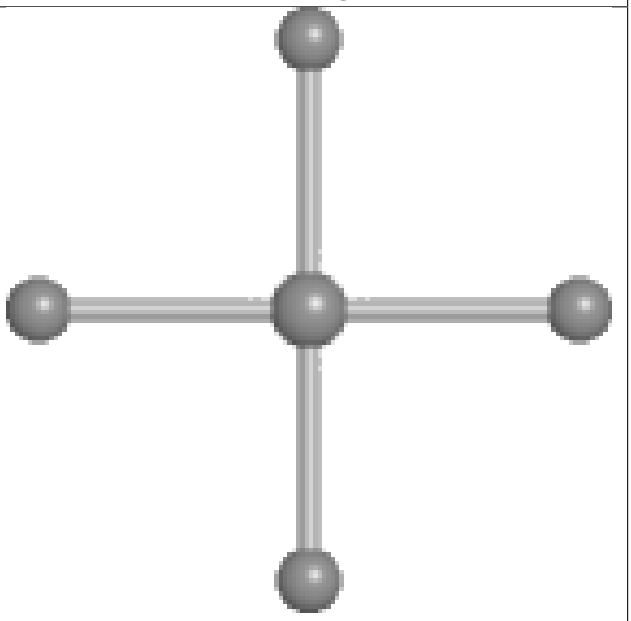
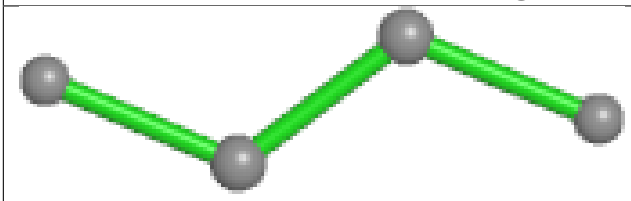


Torsions



Rings

Ligand EDO D 2011



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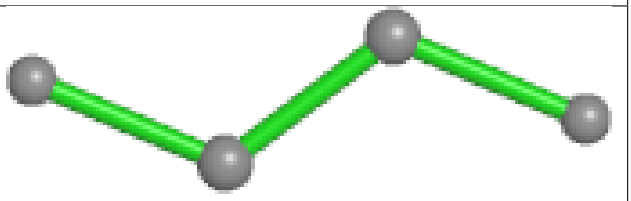
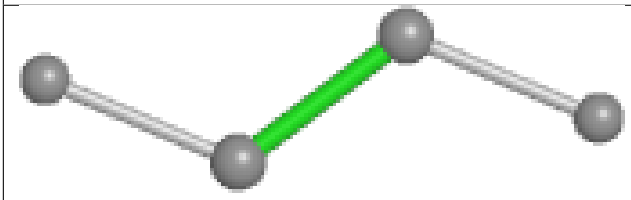


Bond angles



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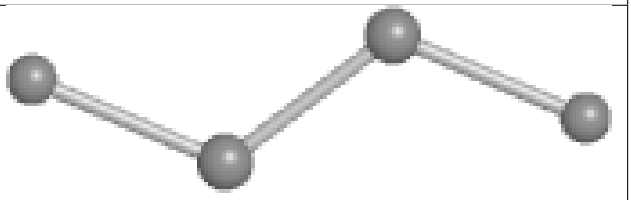
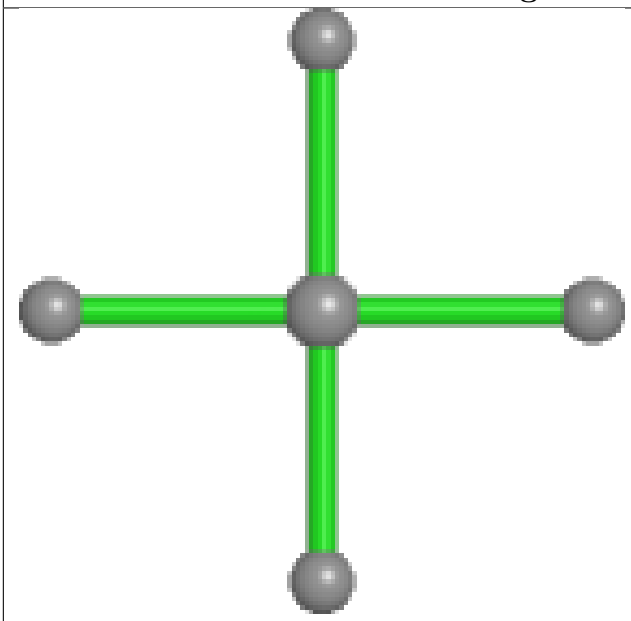


Rings

Ligand SO4 C 1202



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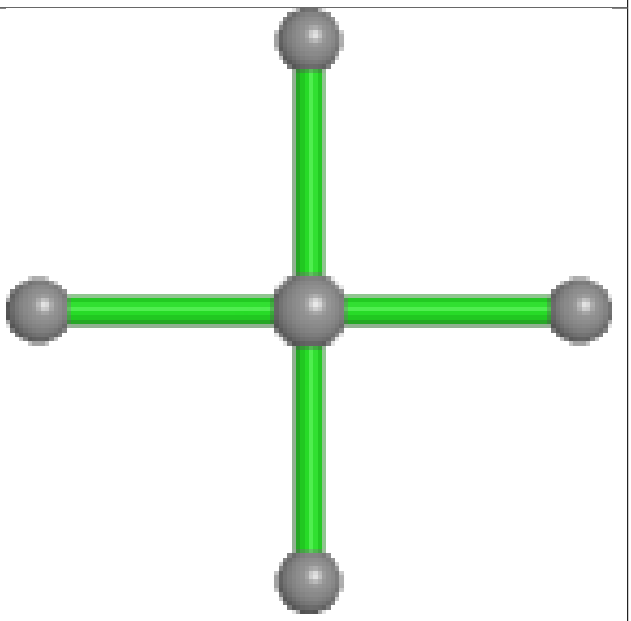
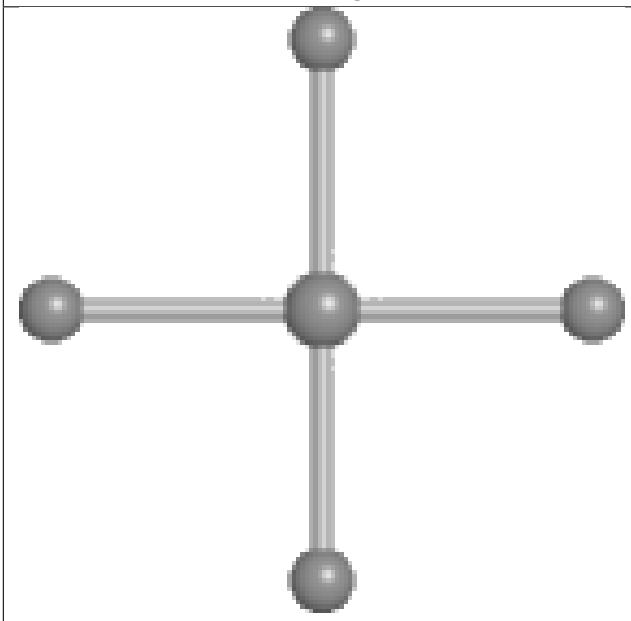
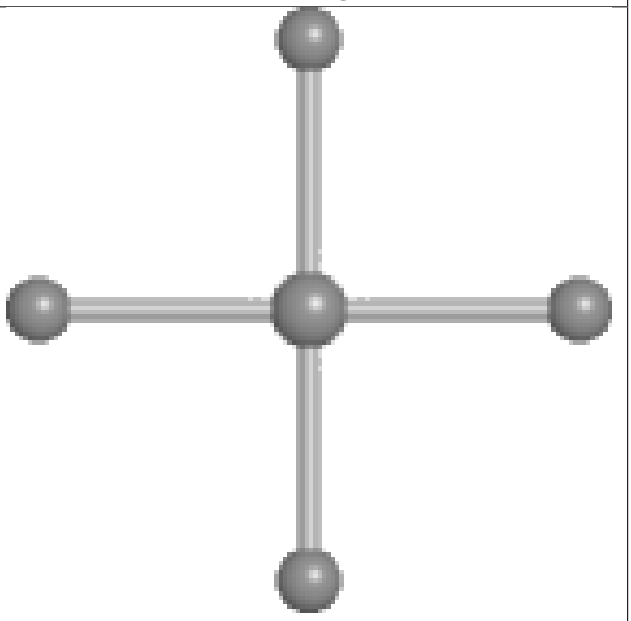


Bond angles

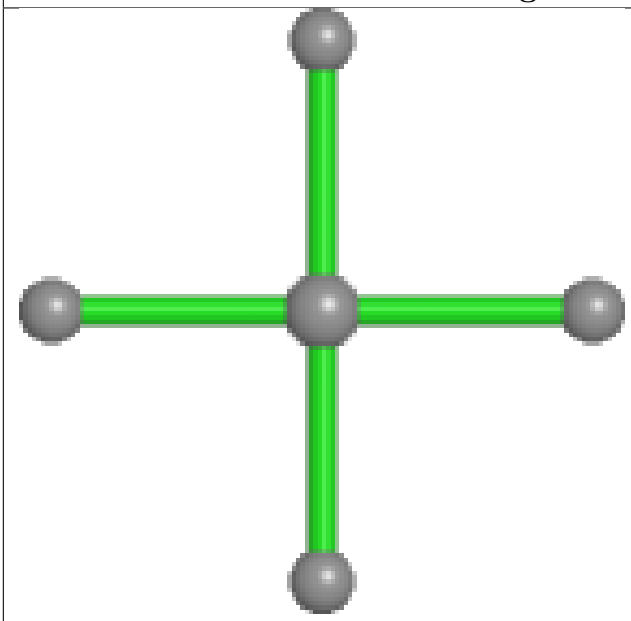


Torsions

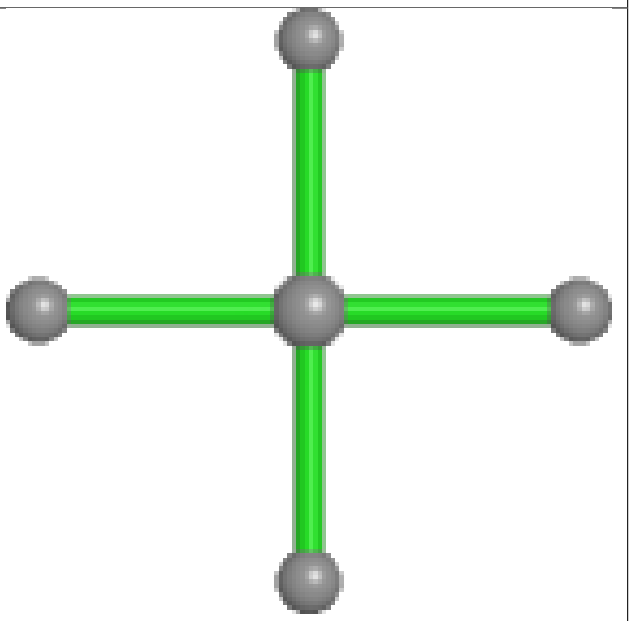


Rings

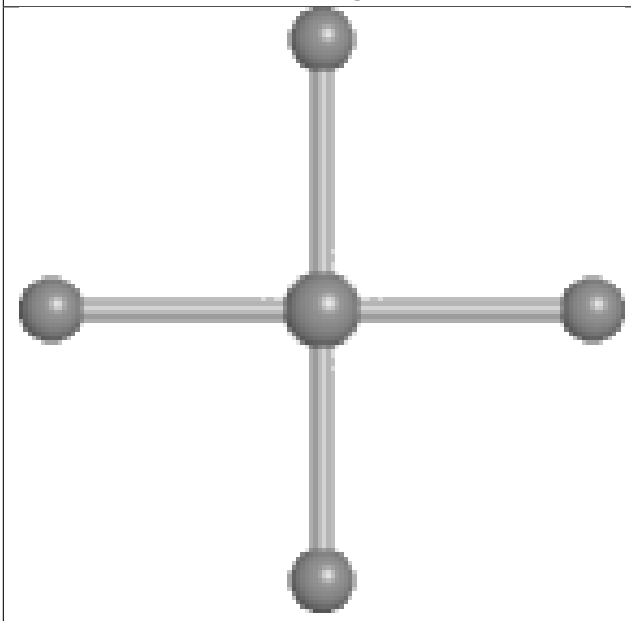
Ligand SO4 D 2003



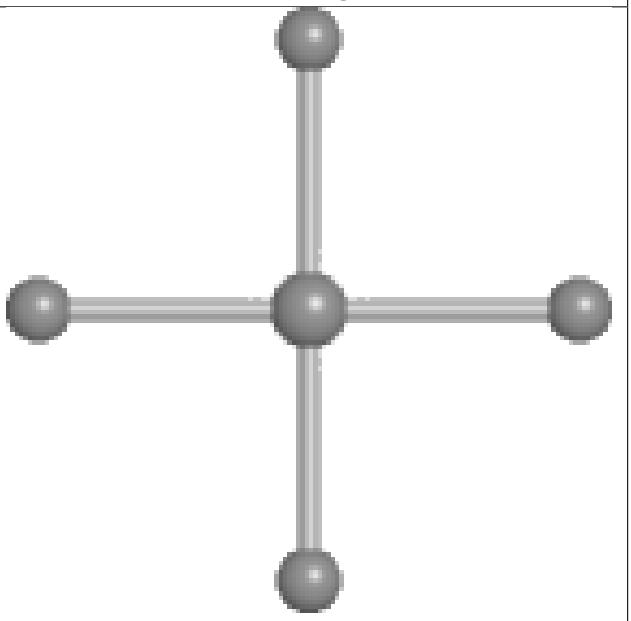
Bond lengths



Bond angles

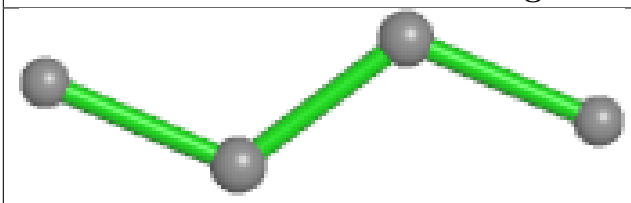


Torsions



Rings

Ligand EDO F 506



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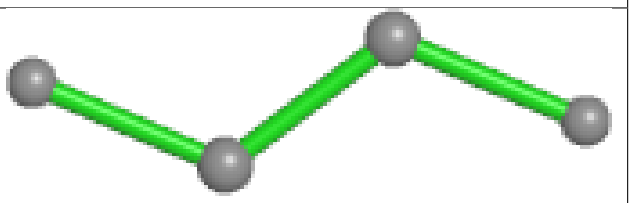
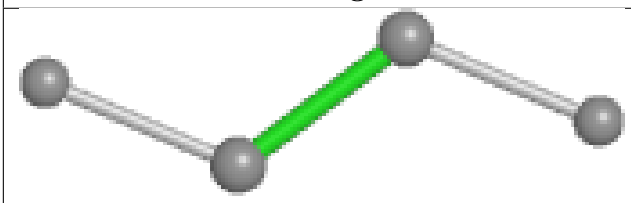


Bond angles



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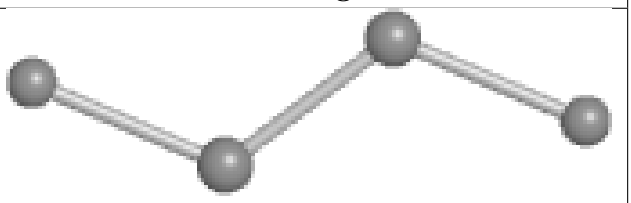
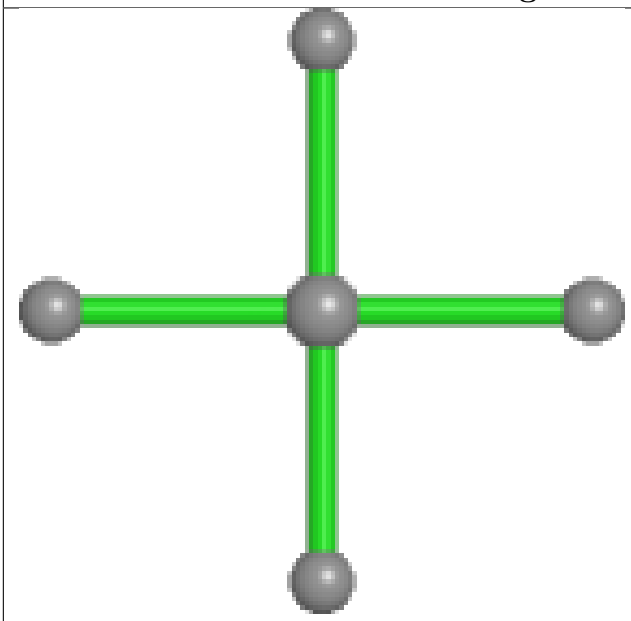


Rings

Ligand SO4 D 2004



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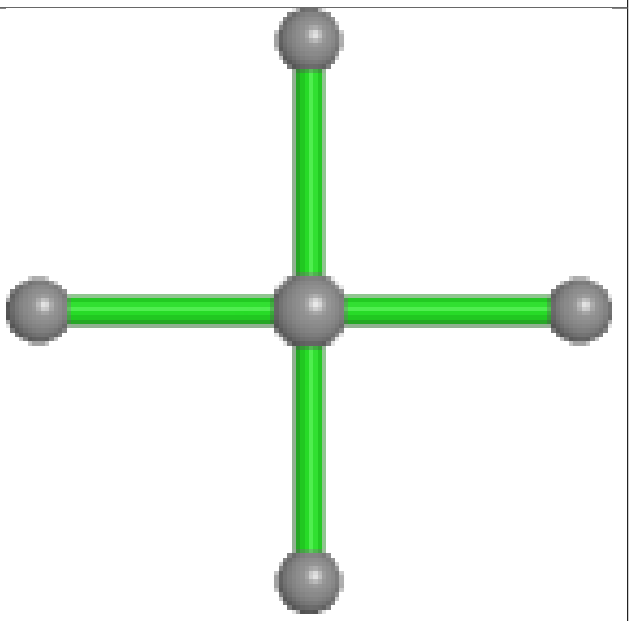
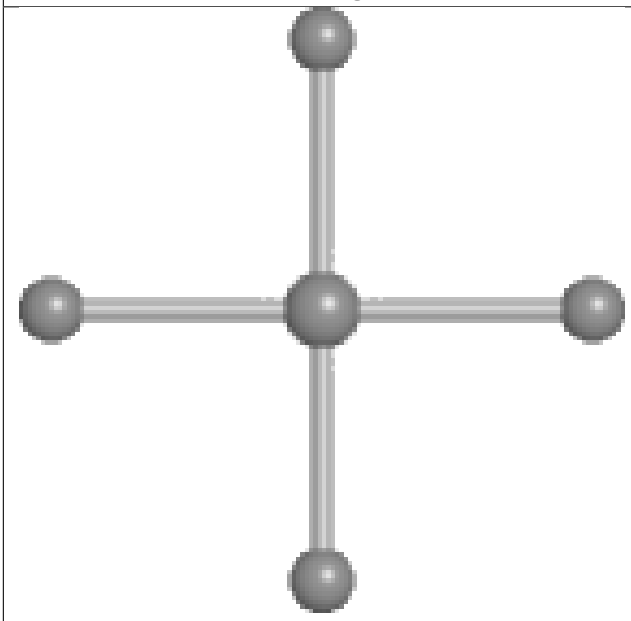


Bond angles



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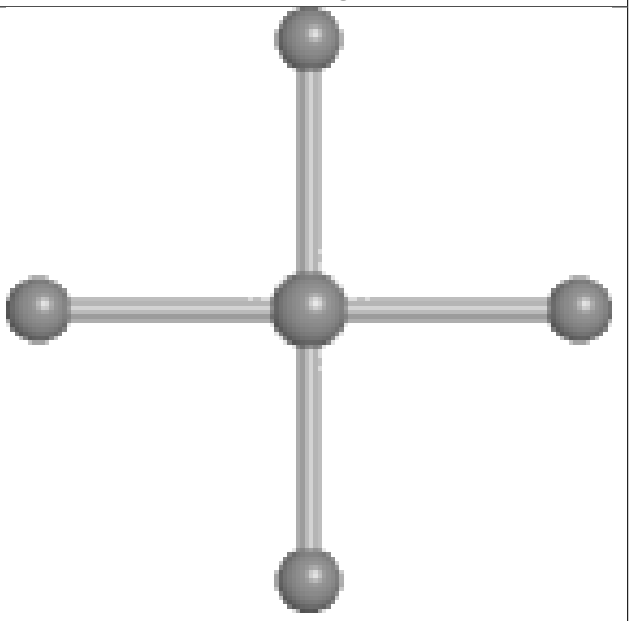
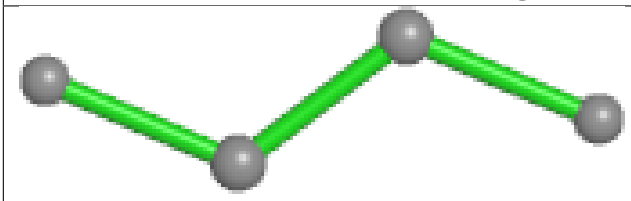


Rings

Ligand EDO C 1207



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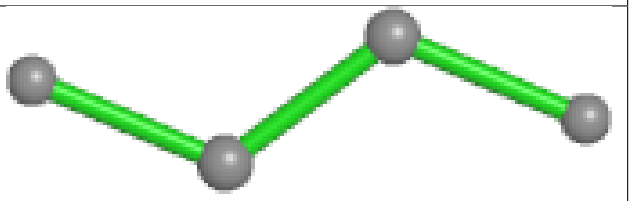
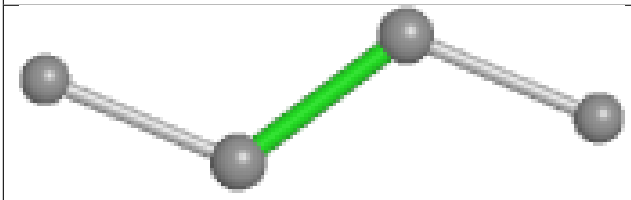


Bond angles



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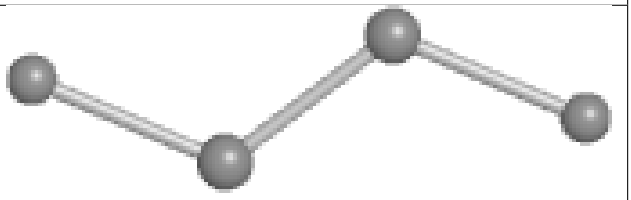
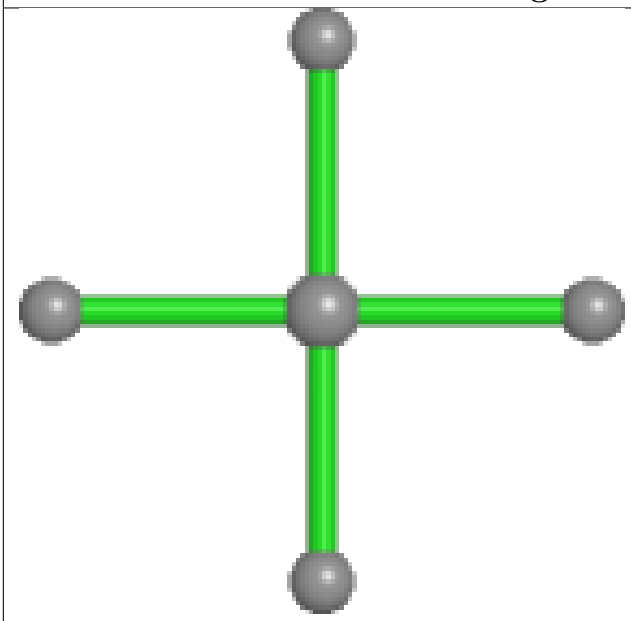
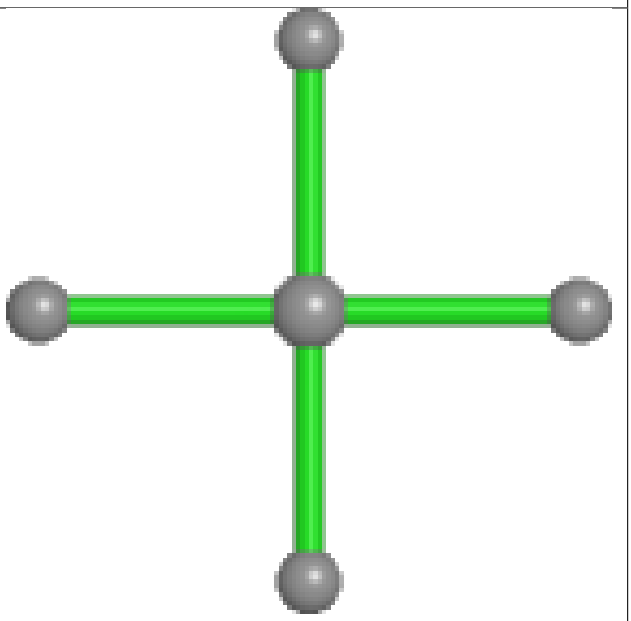


Rings

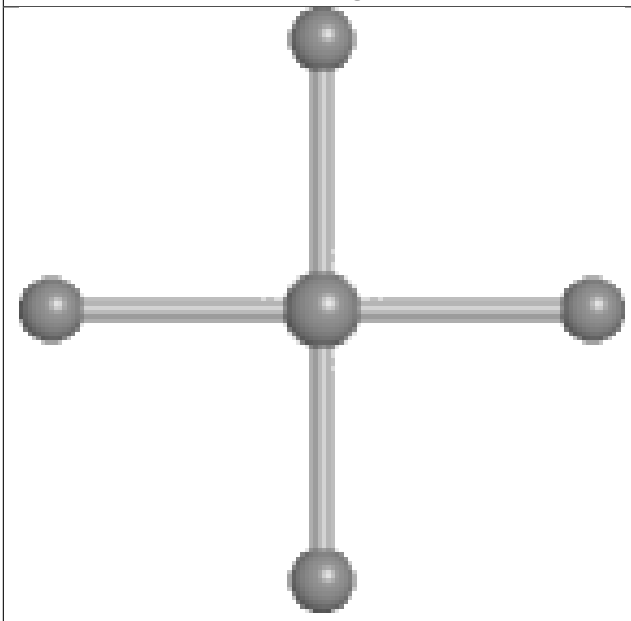
Ligand SO4 F 503



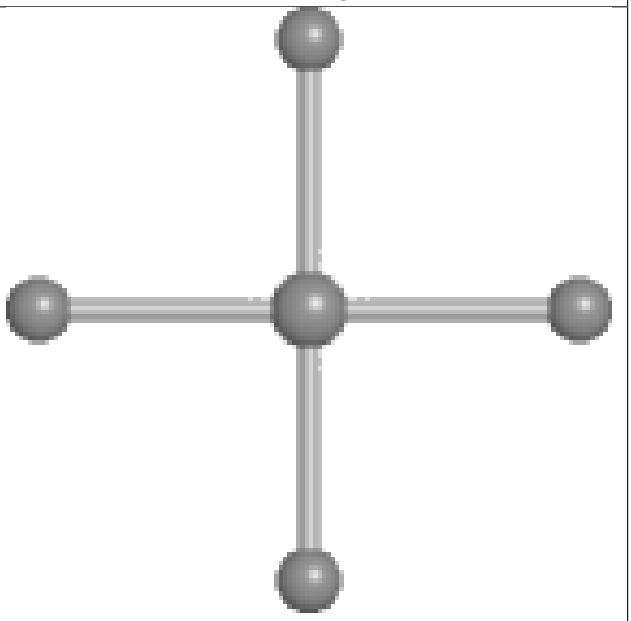
Bond lengths



Bond angles

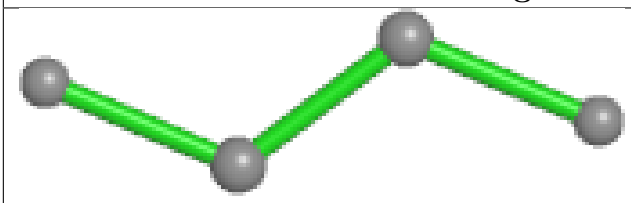


Torsions



Rings

Ligand EDO C 1204



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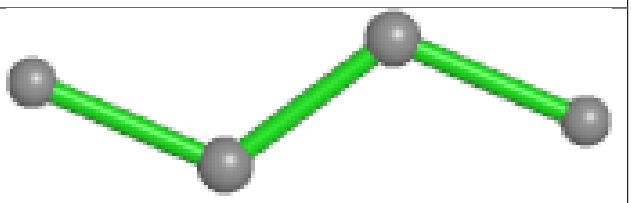

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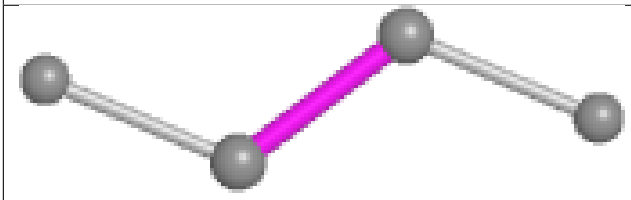
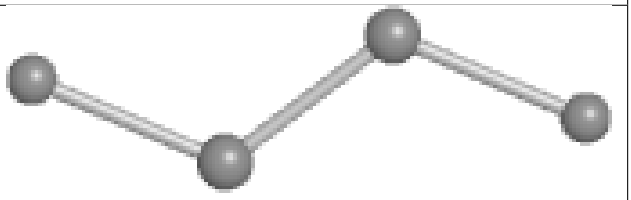
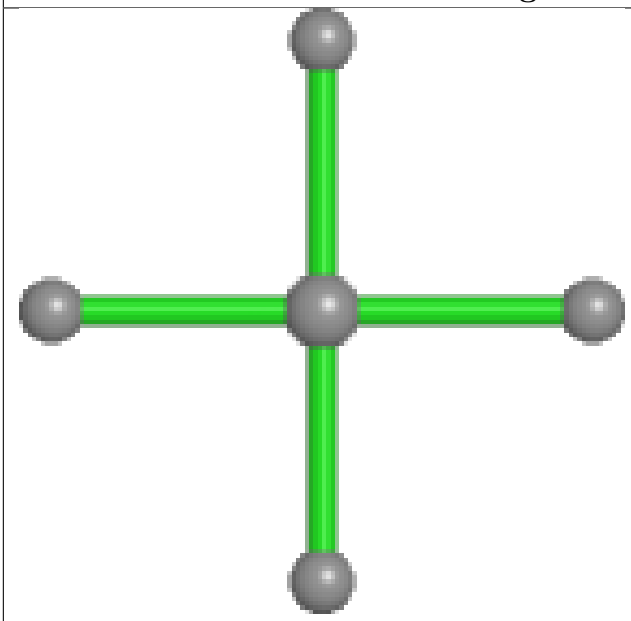


Torsions



Rings

Ligand SO4 D 2010



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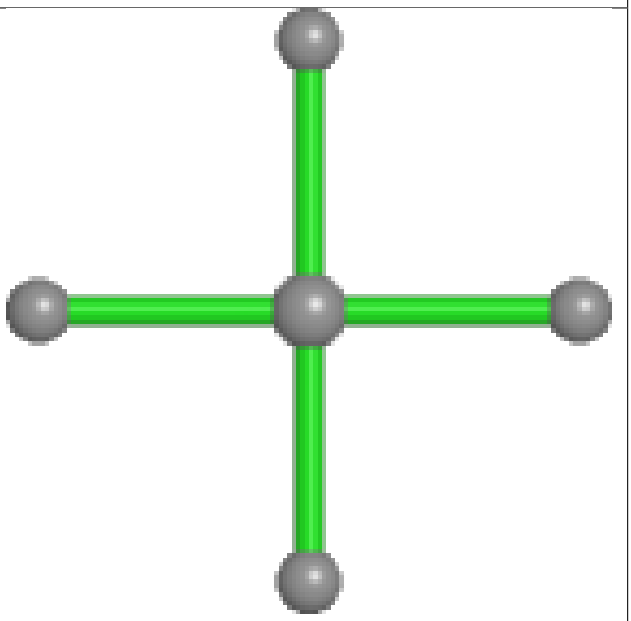

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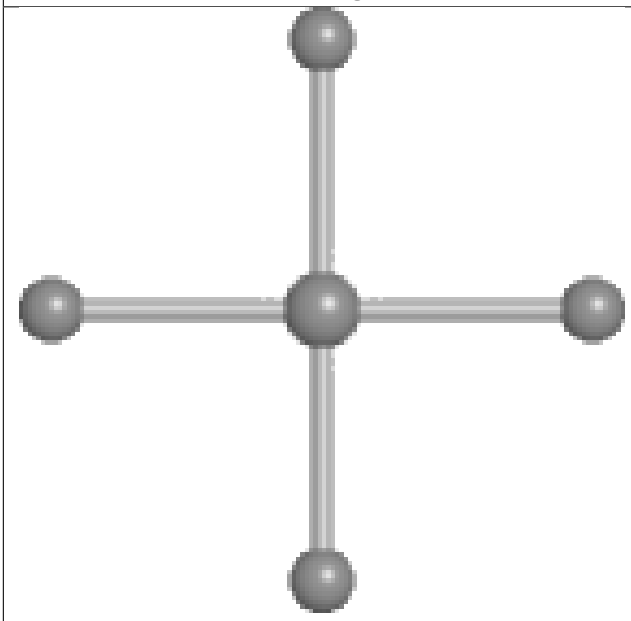

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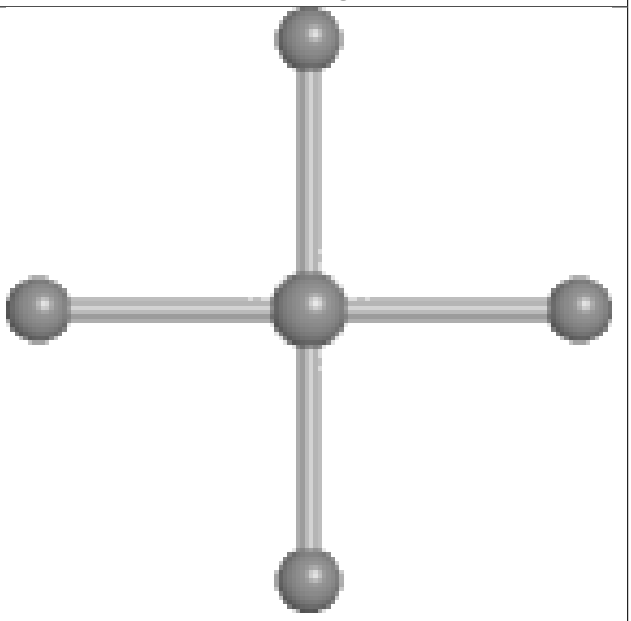
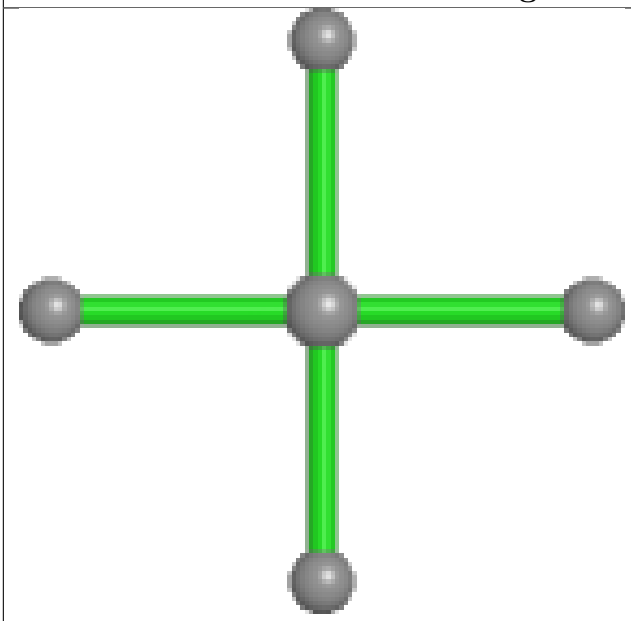
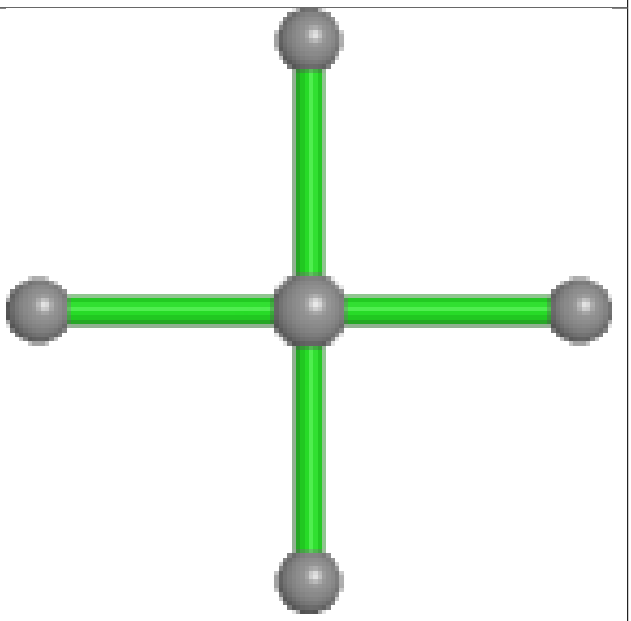


Rings

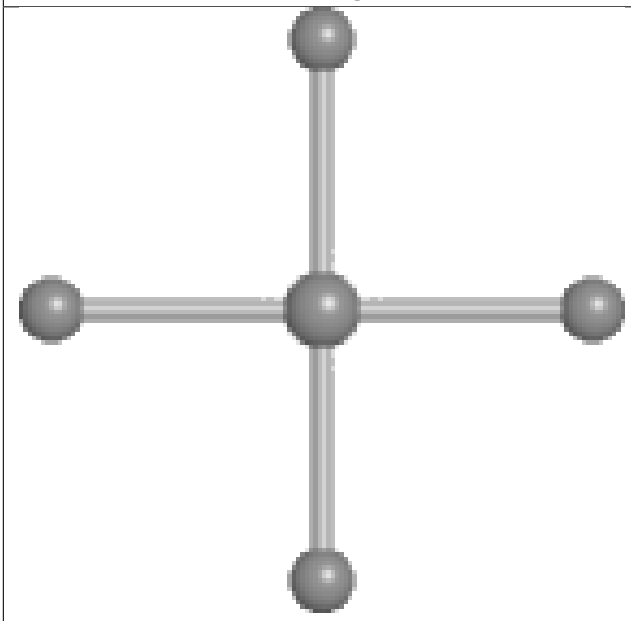
Ligand SO4 D 2005



Bond lengths



Bond angles



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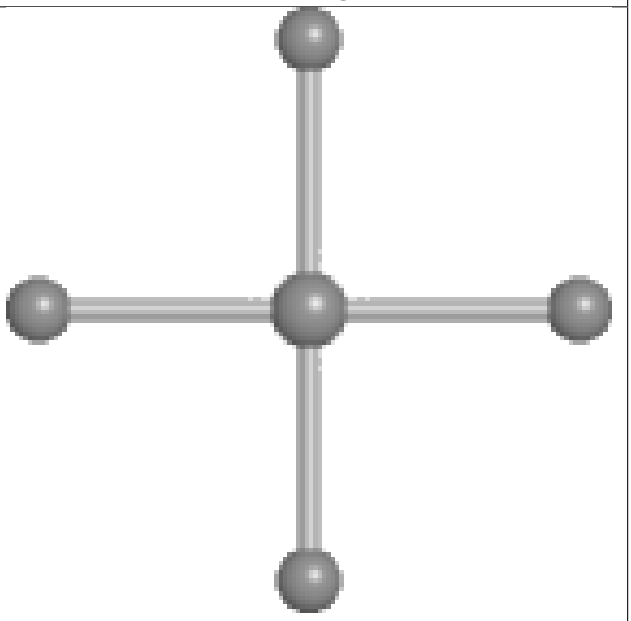
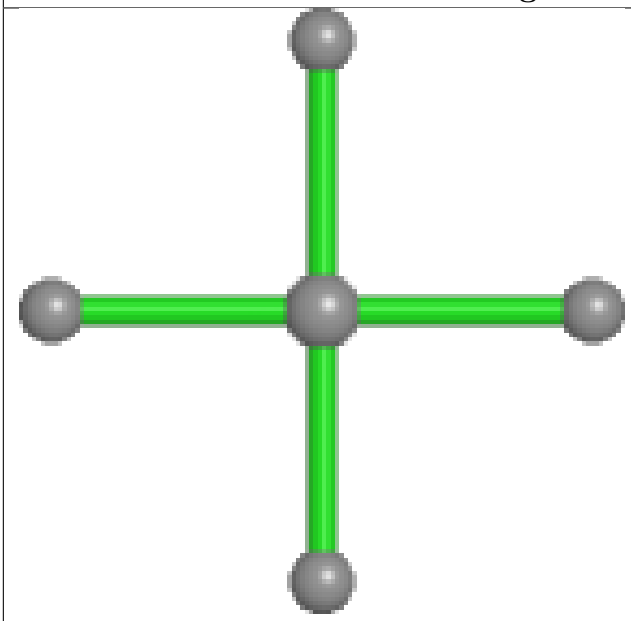
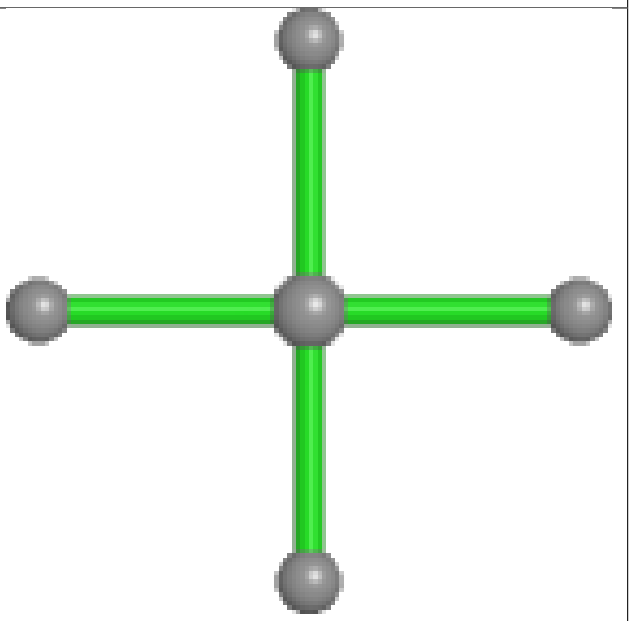


Rings

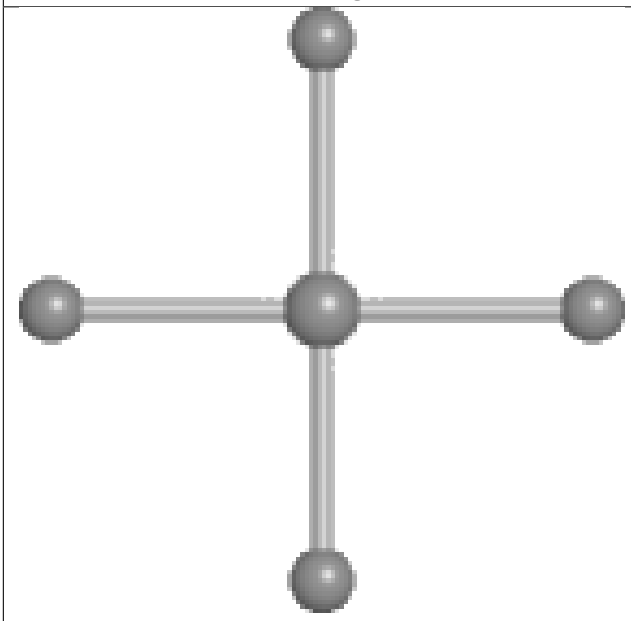
Ligand SO4 D 2006



Bond lengths



Bond angles



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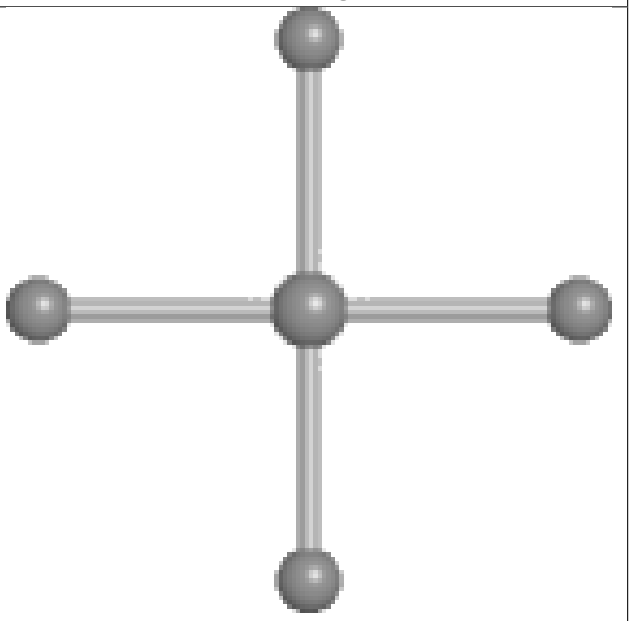
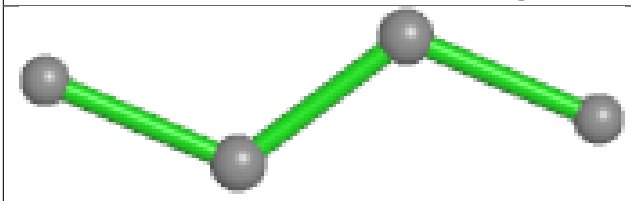
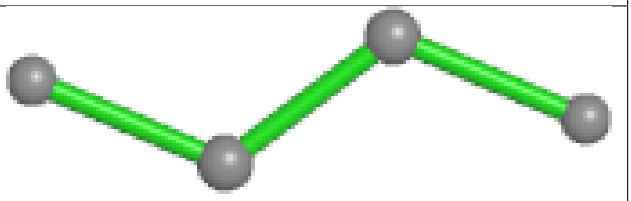
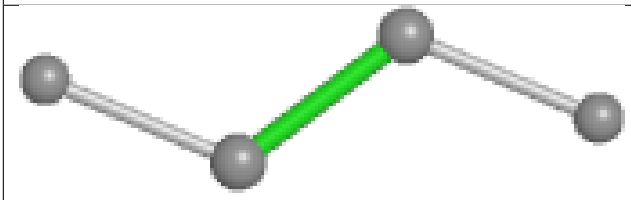
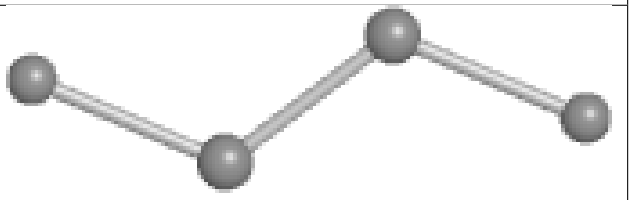


Rings

Ligand EDO D 2007	
	
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, 95^{th} 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	218/350 (62%)	-0.17	5 (2%) 60 39	76, 105, 138, 165	0
1	B	233/350 (66%)	0.18	7 (3%) 50 27	98, 133, 157, 174	0
1	T	53/350 (15%)	1.32	10 (18%) 1 0	128, 168, 199, 204	0
2	C	1099/1169 (94%)	0.05	37 (3%) 45 24	54, 104, 178, 205	0
3	D	1246/1317 (94%)	-0.12	10 (0%) 86 74	46, 91, 152, 196	0
4	E	76/107 (71%)	-0.07	0 100 100	67, 98, 140, 151	0
5	F	305/466 (65%)	-0.30	0 100 100	50, 90, 142, 186	0
6	G	0/17	-	-	-	-
7	J	83/114 (72%)	-0.26	0 100 100	80, 117, 166, 183	0
8	O	31/31 (100%)	-0.82	0 100 100	64, 81, 105, 111	0
9	P	26/26 (100%)	-0.85	0 100 100	76, 87, 113, 119	0
All	All	3370/4297 (78%)	-0.06	69 (2%) 65 45	46, 101, 169, 205	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	350	GLY	4.6
1	T	263	CYS	4.5
2	C	190	LEU	4.5
2	C	228	LEU	4.3
1	B	1	MET	4.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

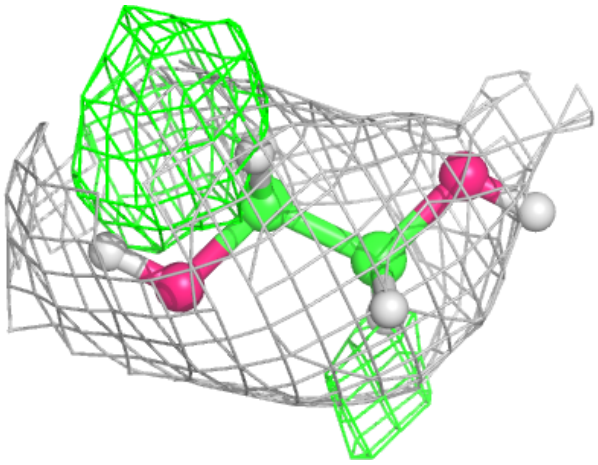
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

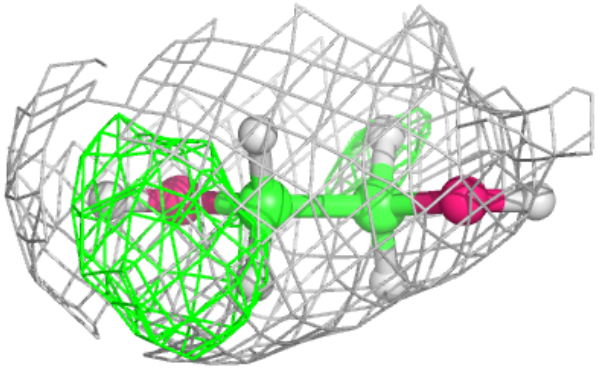
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	C	1207	4/4	0.62	0.30	107,129,144,144	0
11	EDO	D	2008	4/4	0.65	0.29	93,111,125,126	0
11	EDO	D	2007	4/4	0.68	0.40	102,123,135,156	0
10	SO4	F	504	5/5	0.78	0.22	133,134,157,163	0
10	SO4	C	1203	5/5	0.80	0.33	114,140,180,183	0
11	EDO	F	506	4/4	0.83	0.32	101,121,130,156	0
11	EDO	D	2009	4/4	0.86	0.36	90,108,124,137	0
11	EDO	D	2011	4/4	0.87	0.25	76,107,133,133	0
10	SO4	F	505	5/5	0.87	0.56	116,128,134,152	0
10	SO4	C	1202	5/5	0.89	0.10	116,120,146,158	0
10	SO4	D	2006	5/5	0.89	0.14	113,121,139,140	0
10	SO4	C	1206	5/5	0.90	0.26	127,131,156,410	0
10	SO4	F	503	5/5	0.91	0.13	105,109,129,136	0
10	SO4	D	2005	5/5	0.91	0.44	104,115,141,154	0
10	SO4	D	2010	5/5	0.91	0.14	94,120,151,152	0
12	SRN	C	1205	58/58	0.92	0.29	79,97,136,149	0
11	EDO	C	1204	4/4	0.93	0.35	61,88,105,113	0
10	SO4	C	1201	5/5	0.94	0.29	133,138,162,170	0
10	SO4	D	2004	5/5	0.94	0.18	98,103,114,125	0
10	SO4	F	501	5/5	0.95	0.08	122,128,139,153	0
10	SO4	D	2003	5/5	0.96	0.22	74,87,102,109	0
13	ZN	D	2002	1/1	0.96	0.23	134,134,134,134	0
13	ZN	D	2001	1/1	0.98	0.21	77,77,77,77	0
10	SO4	F	502	5/5	0.98	0.15	90,91,130,137	0

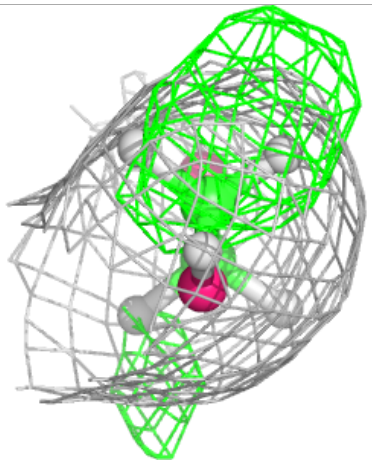
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EDO C 1207:

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

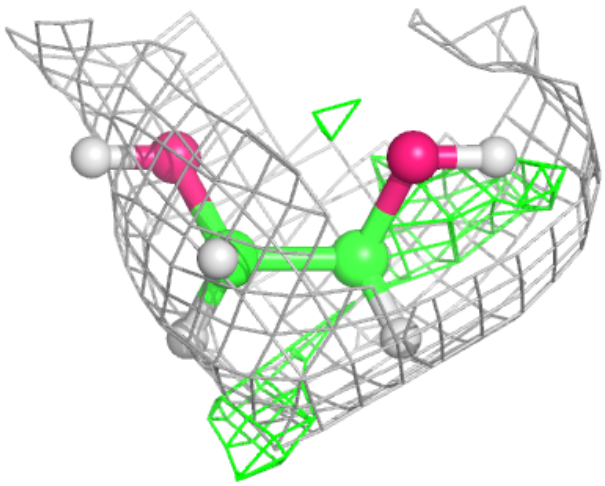


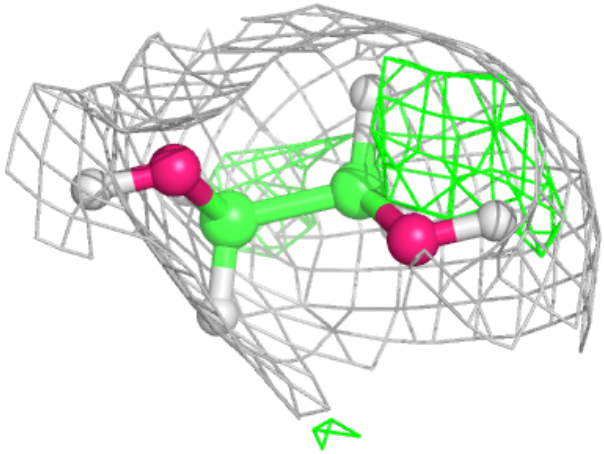


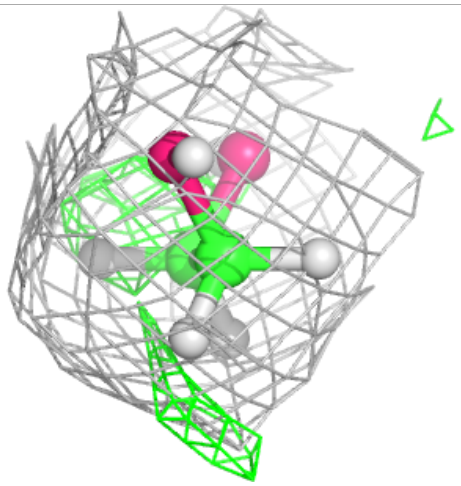


Electron density around EDO D 2008:

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

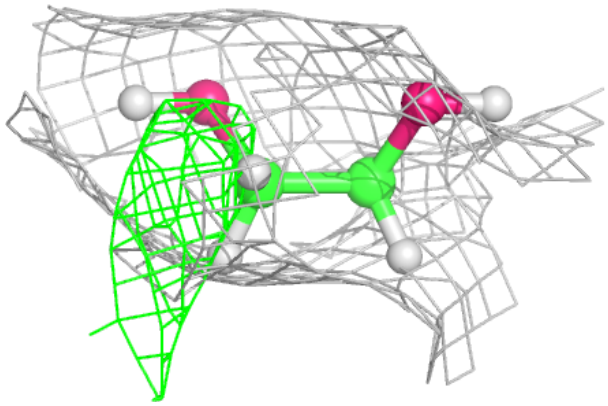


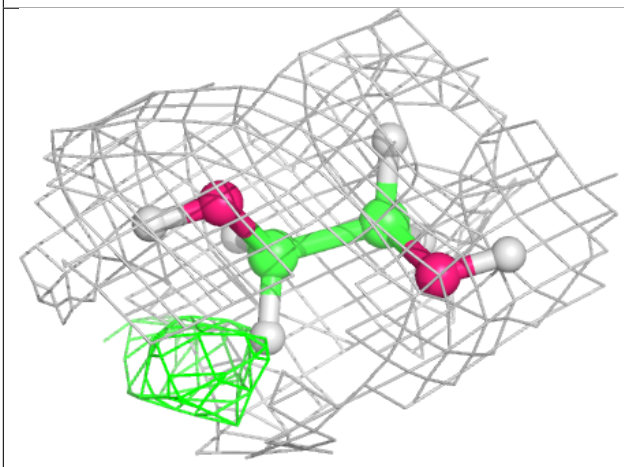


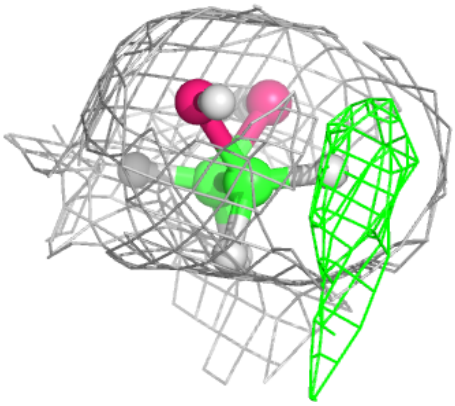


Electron density around EDO D 2007:

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

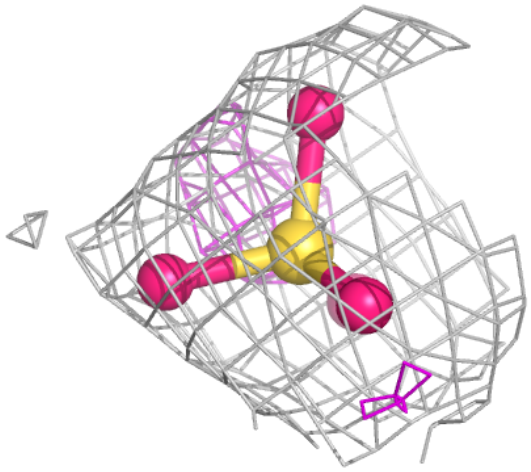


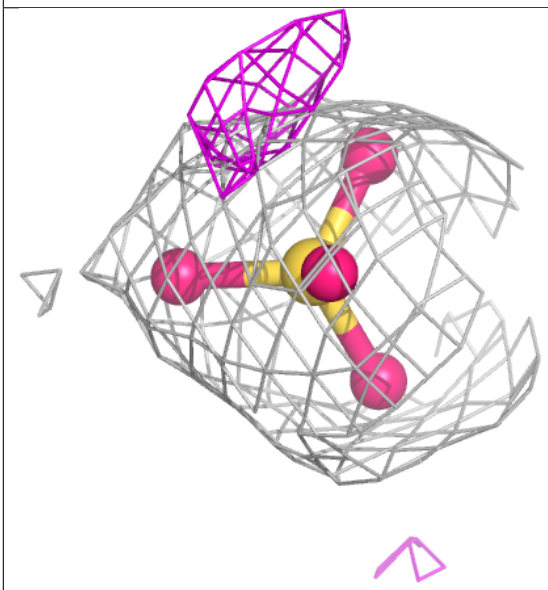


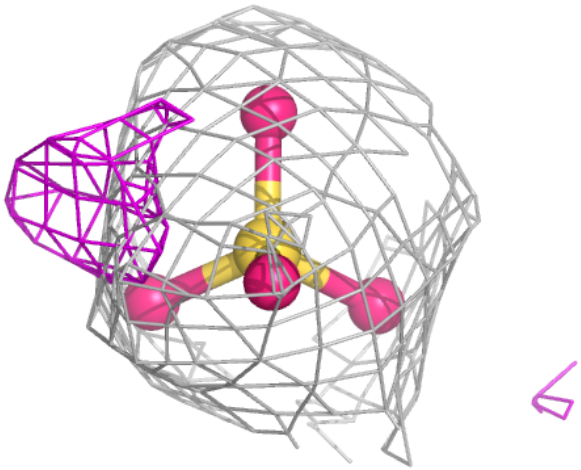


Electron density around SO4 F 504:

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

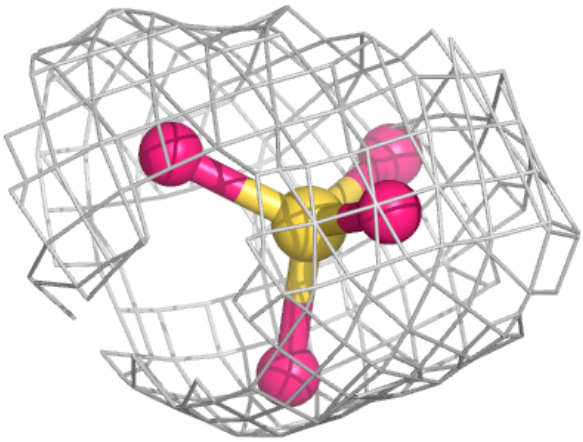


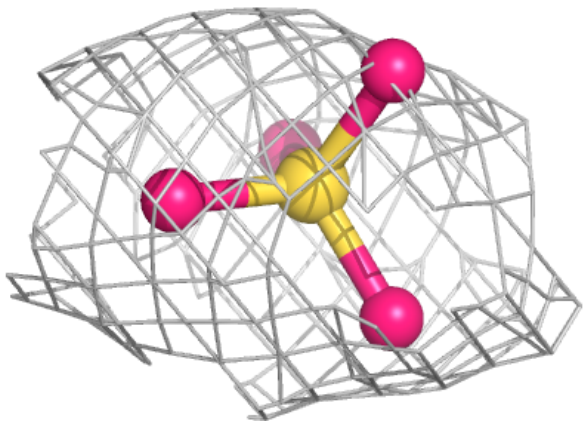


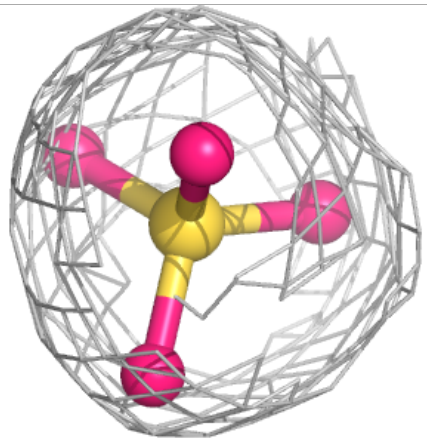


Electron density around SO4 C 1203:

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

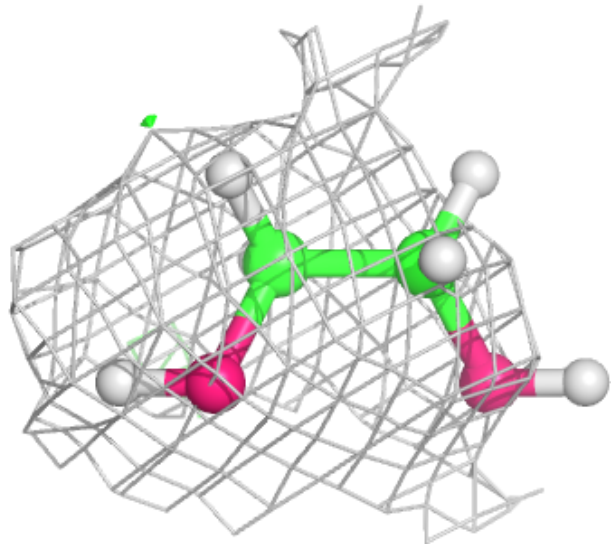


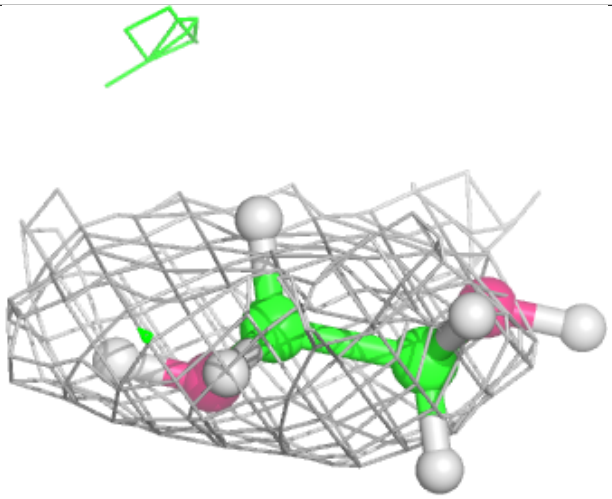


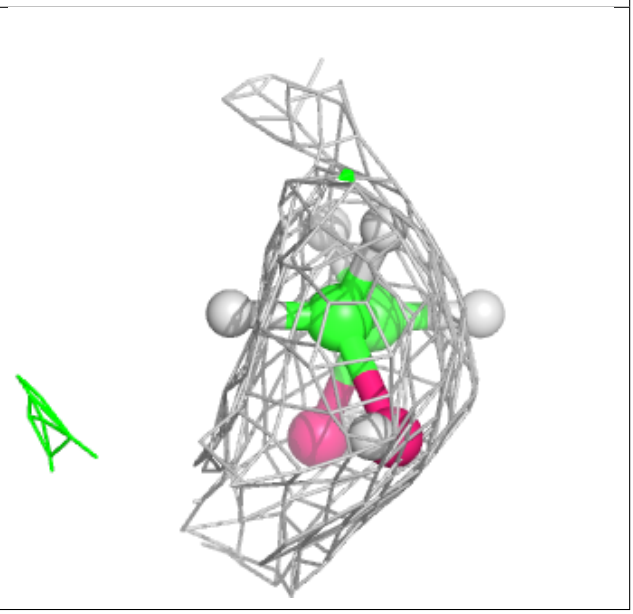


Electron density around EDO F 506:

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

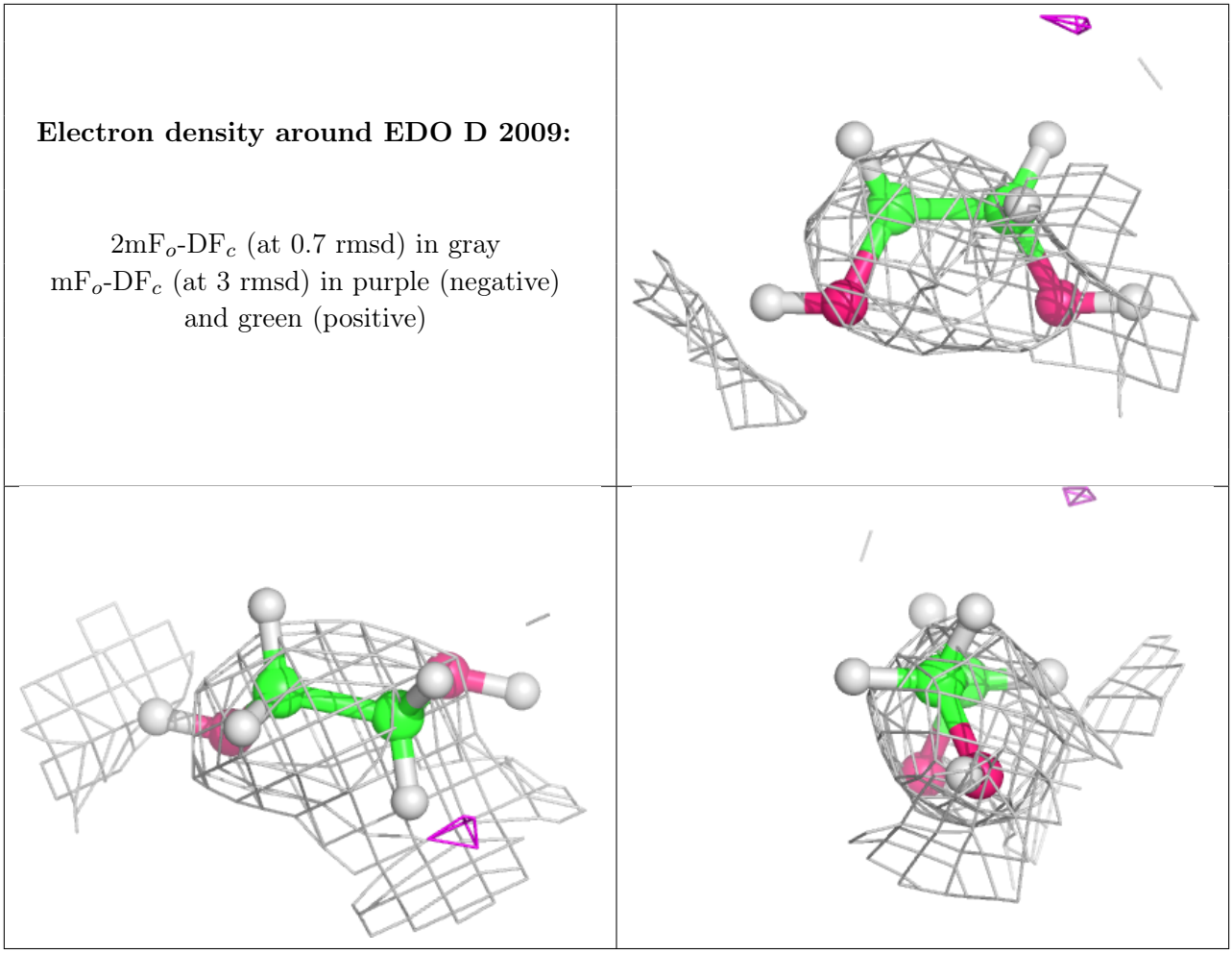






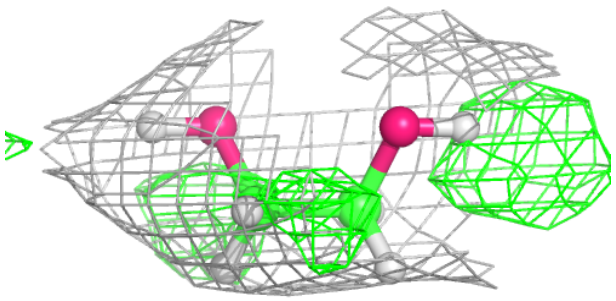
Electron density around EDO D 2009:

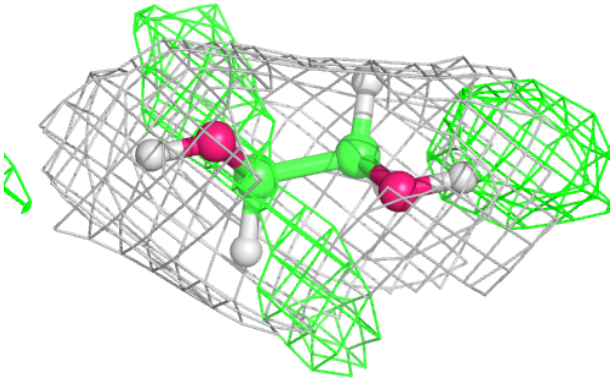
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

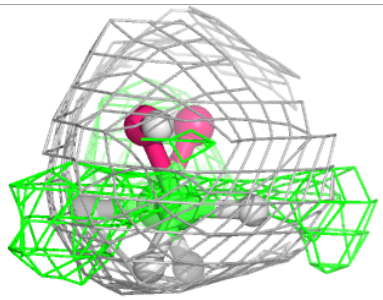


Electron density around EDO D 2011:

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

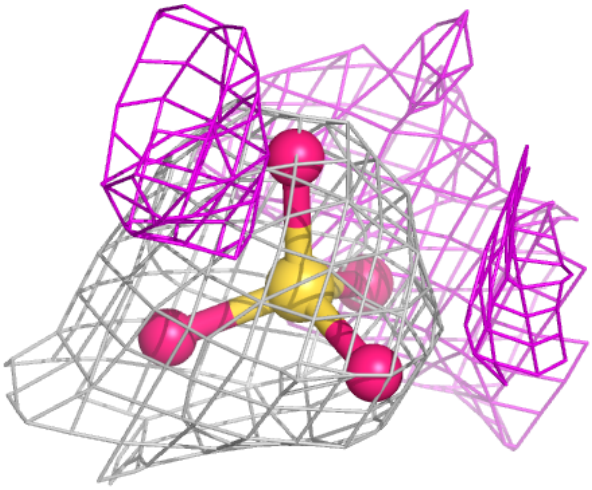


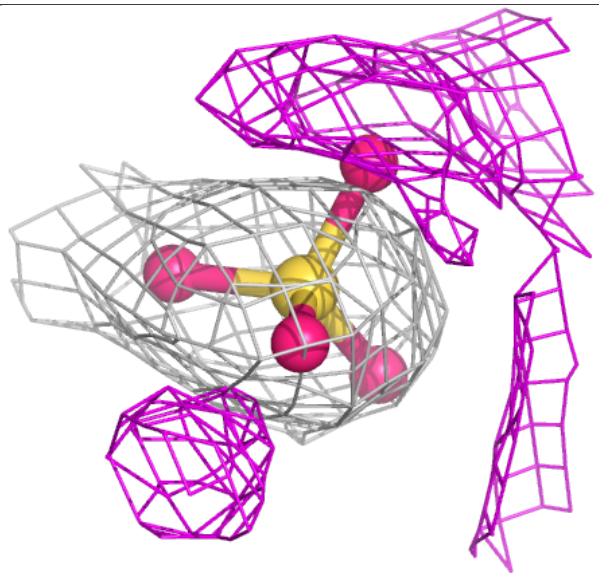


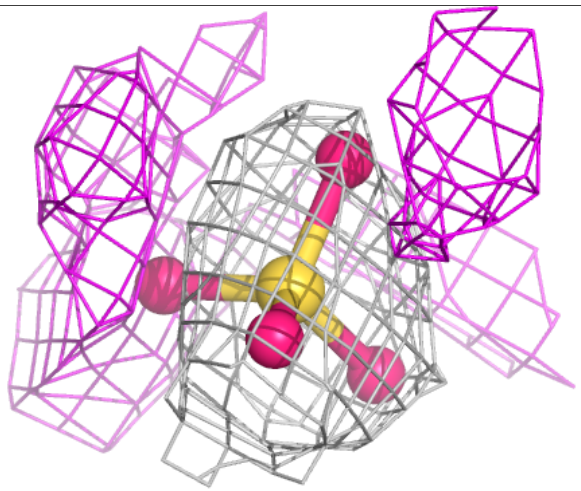


Electron density around SO4 F 505:

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

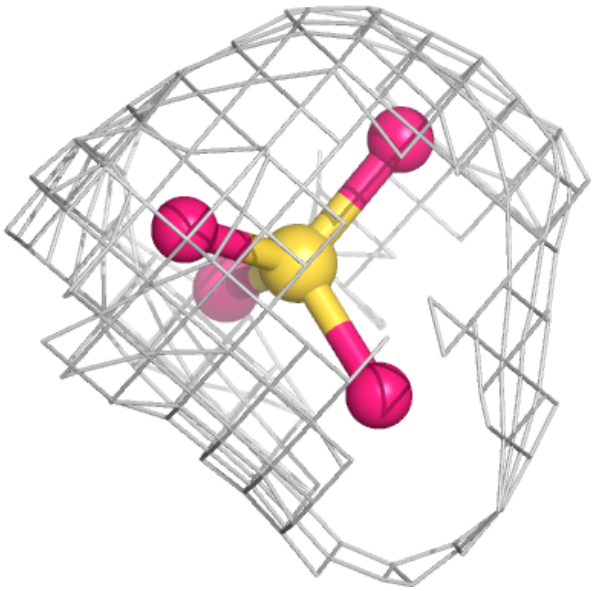


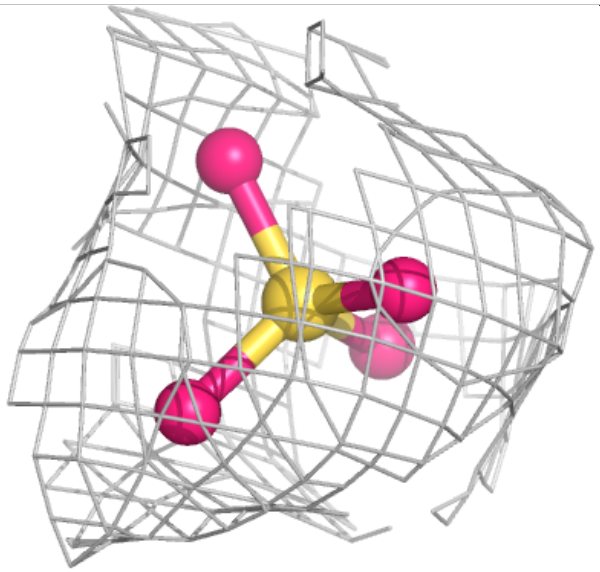


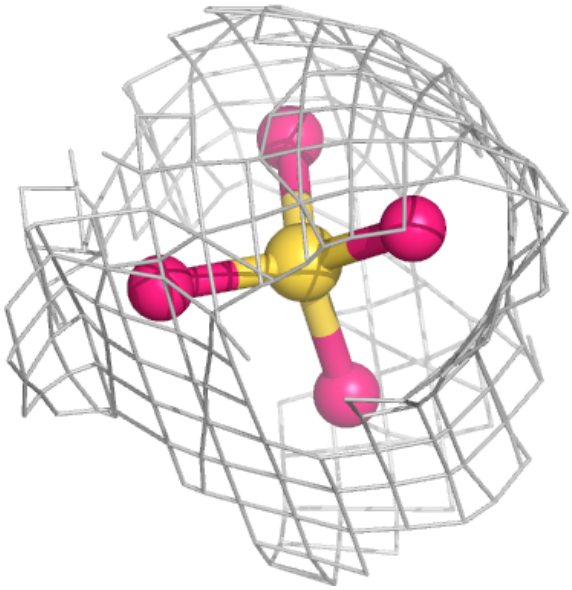


Electron density around SO4 C 1202:

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

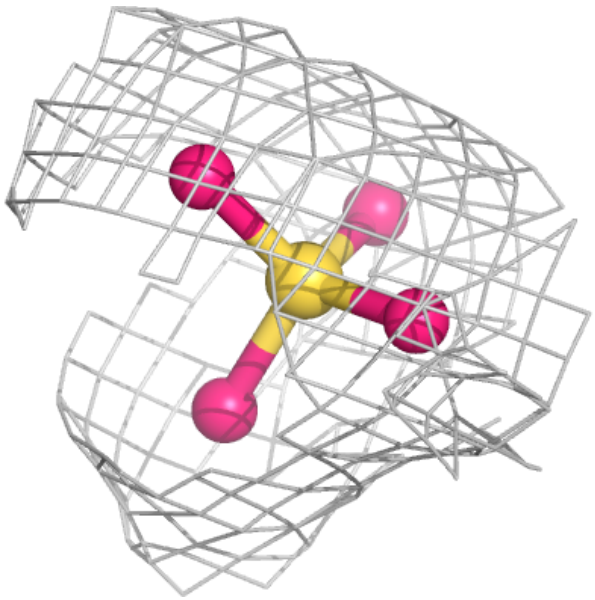


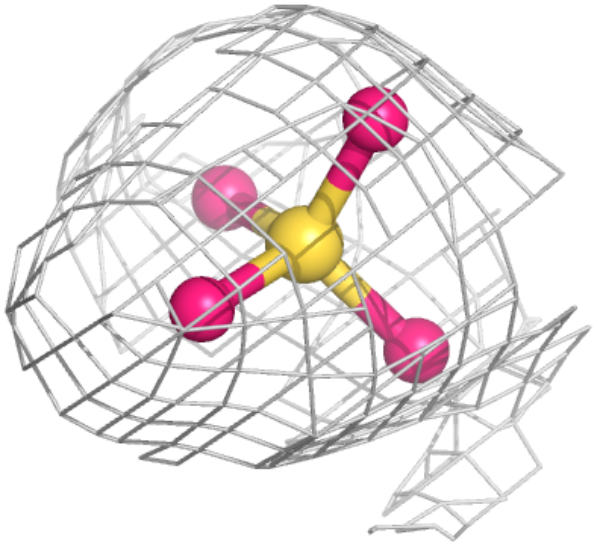


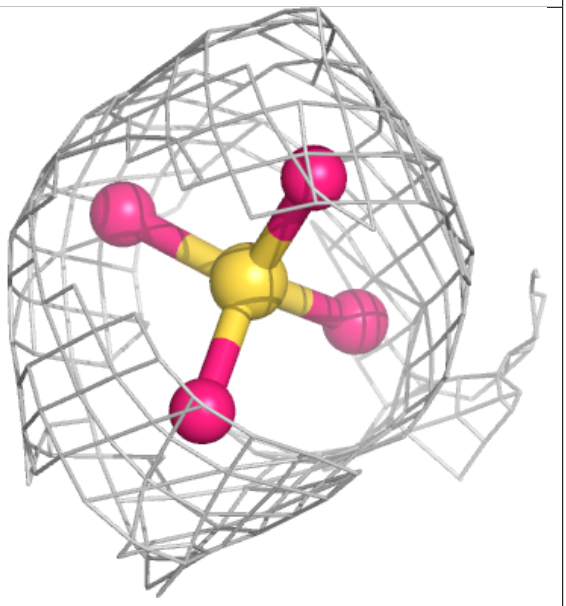


Electron density around SO4 D 2006:

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

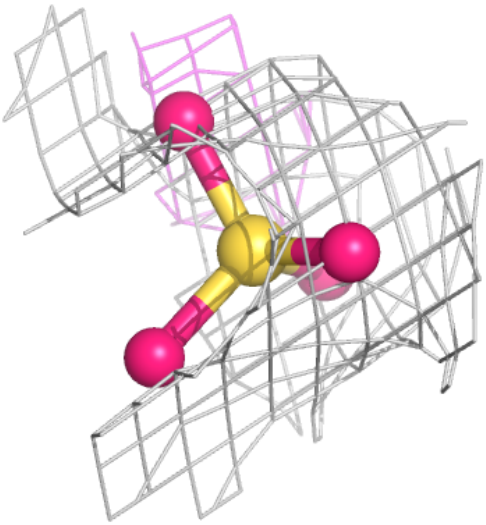


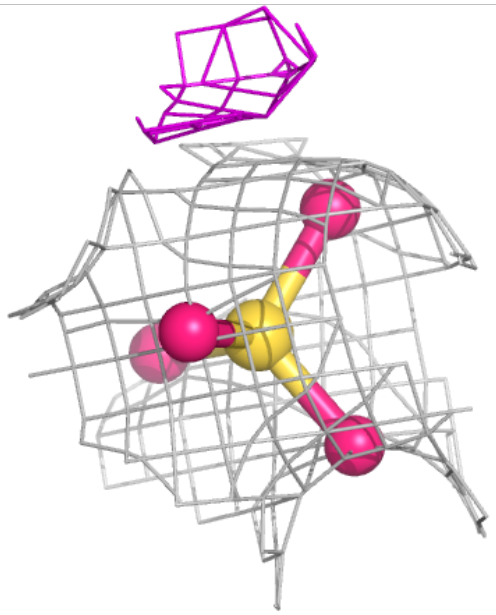


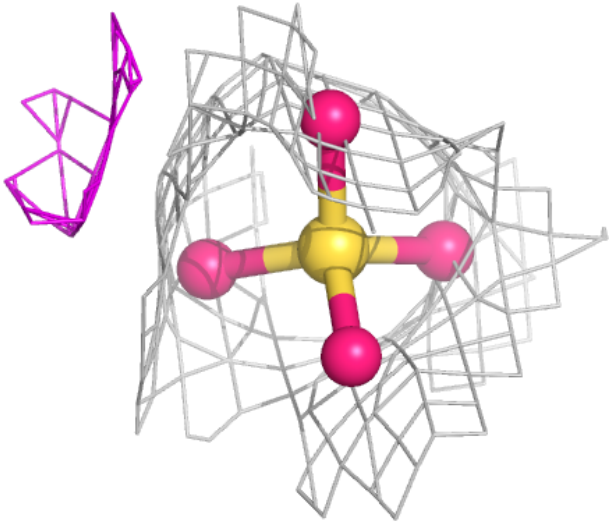


Electron density around SO4 C 1206:

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

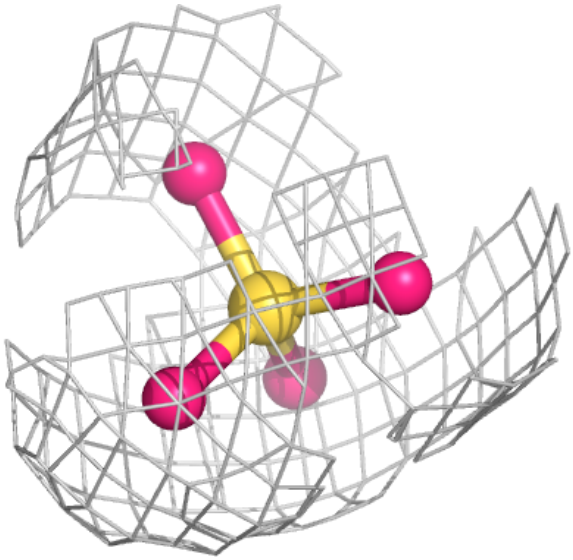


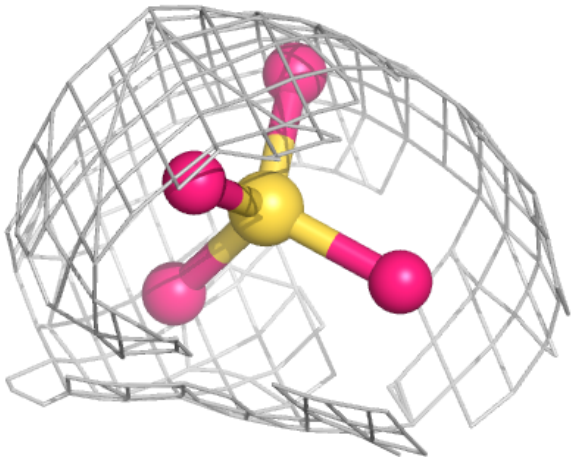


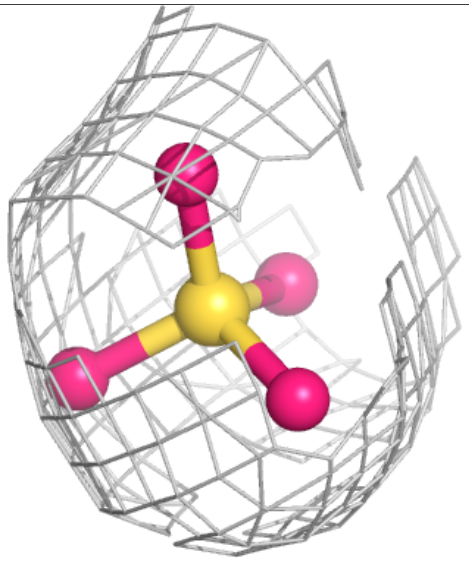


Electron density around SO4 F 503:

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

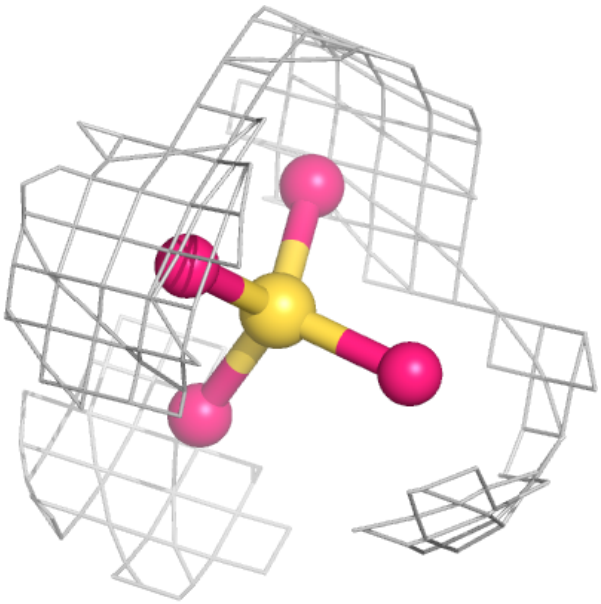


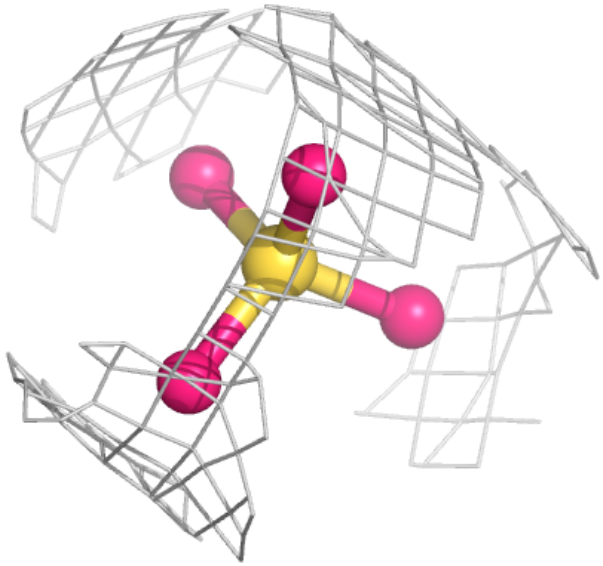


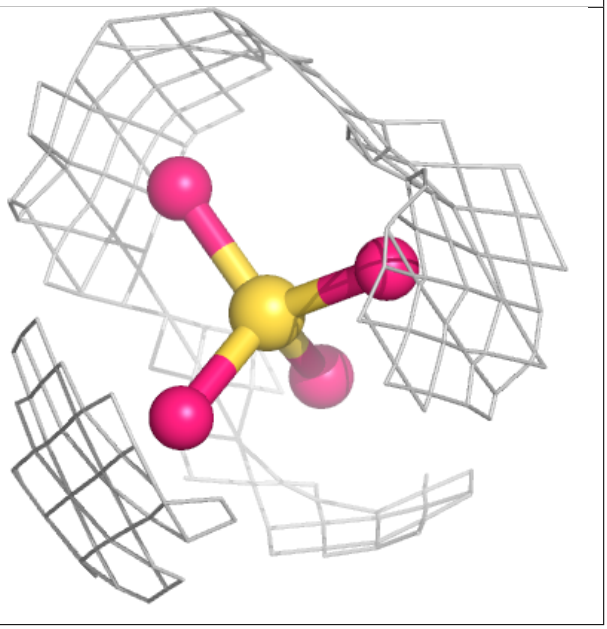


Electron density around SO4 D 2005:

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

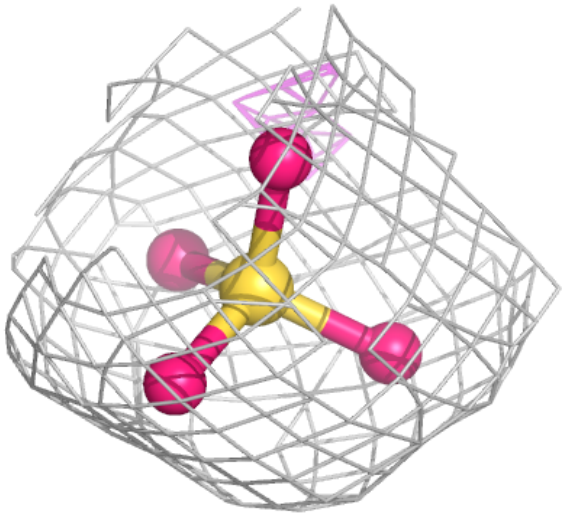


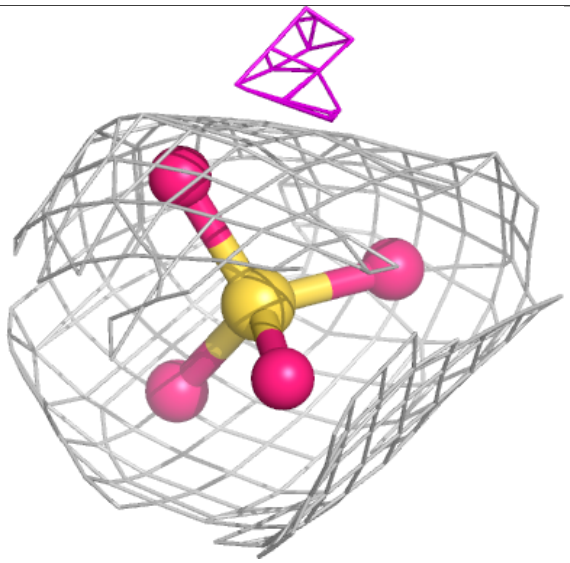


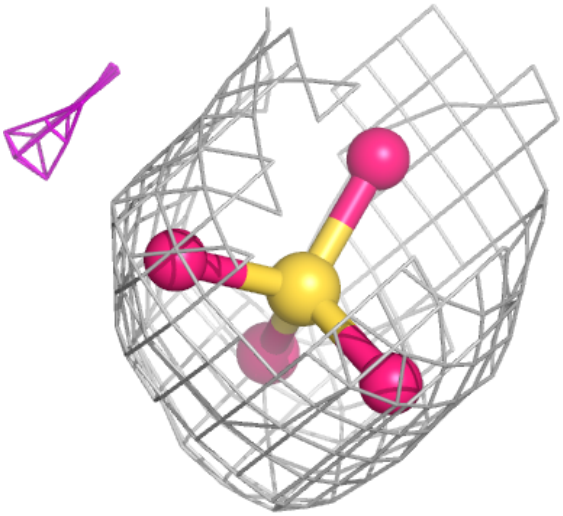


Electron density around SO4 D 2010:

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

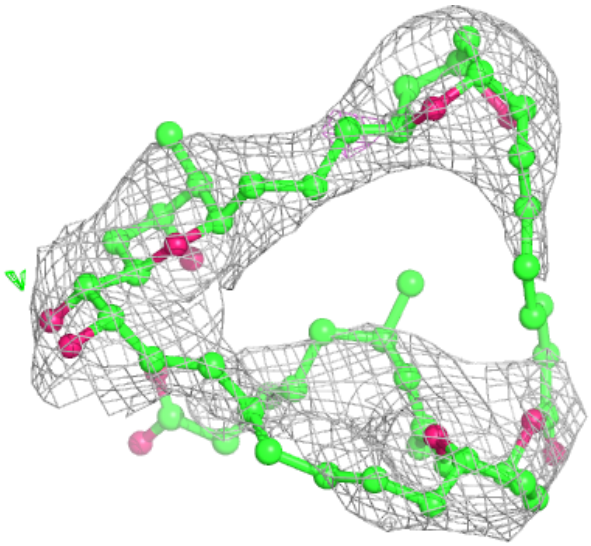


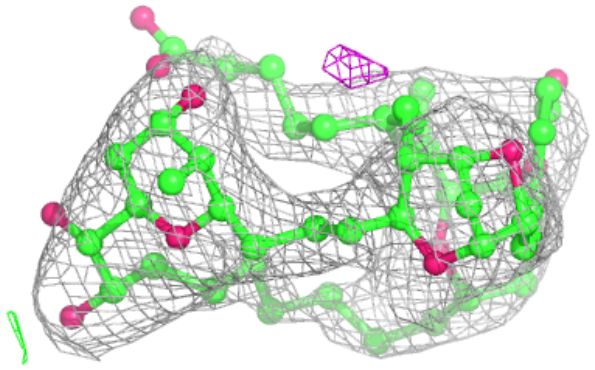


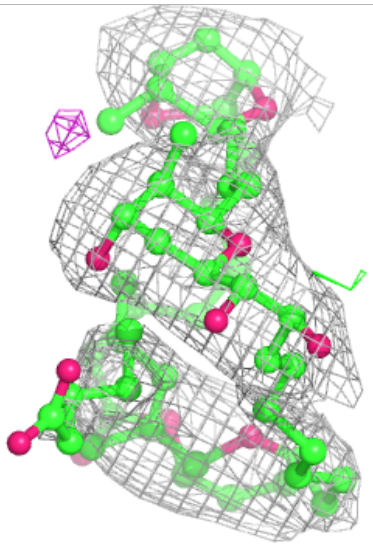


Electron density around SRN C 1205:

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

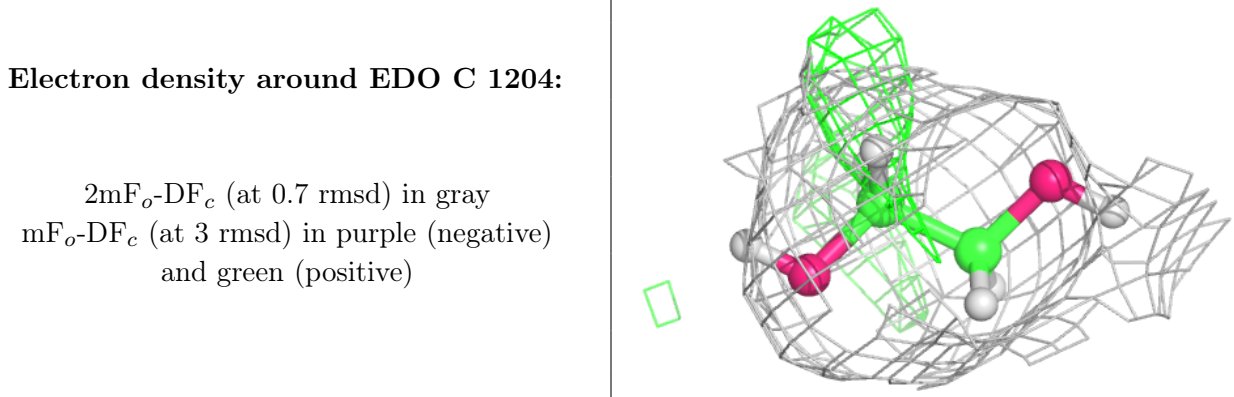


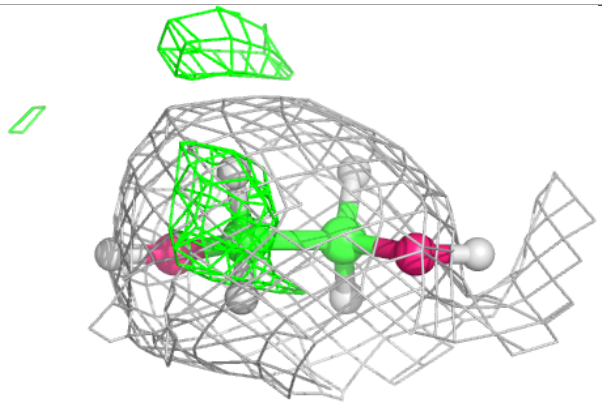


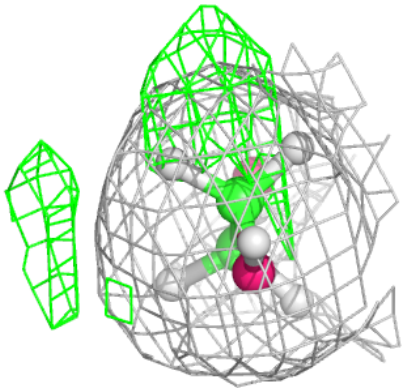


Electron density around EDO C 1204:

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

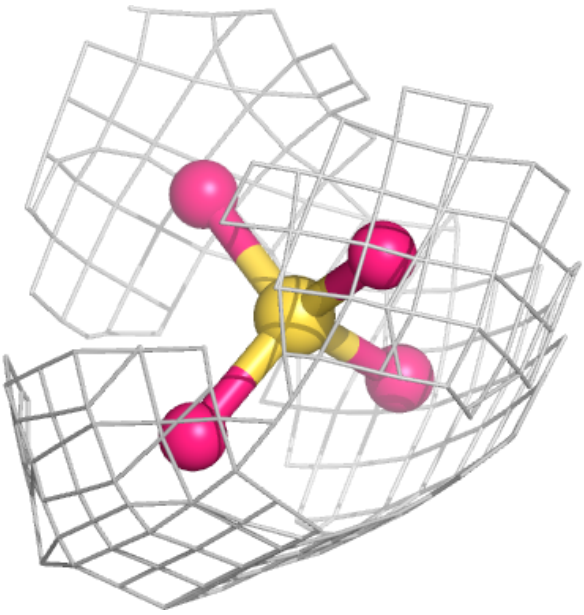


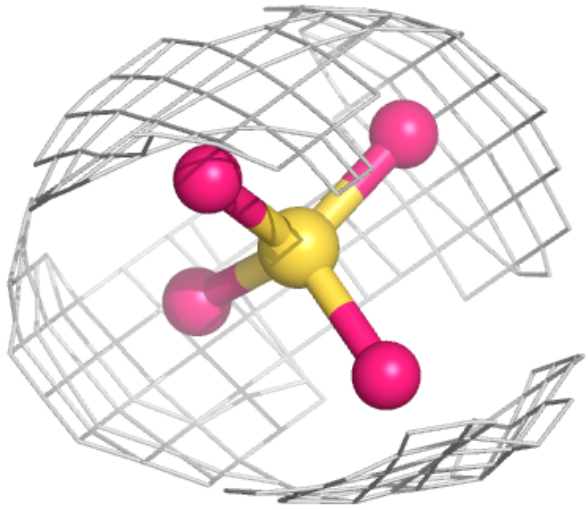


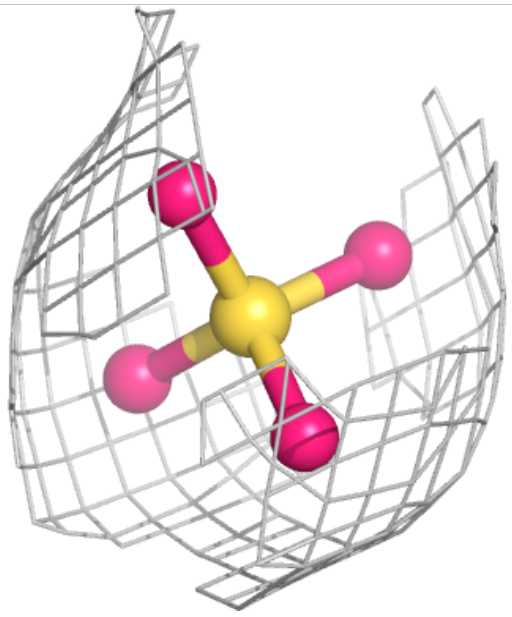


Electron density around SO4 C 1201:

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

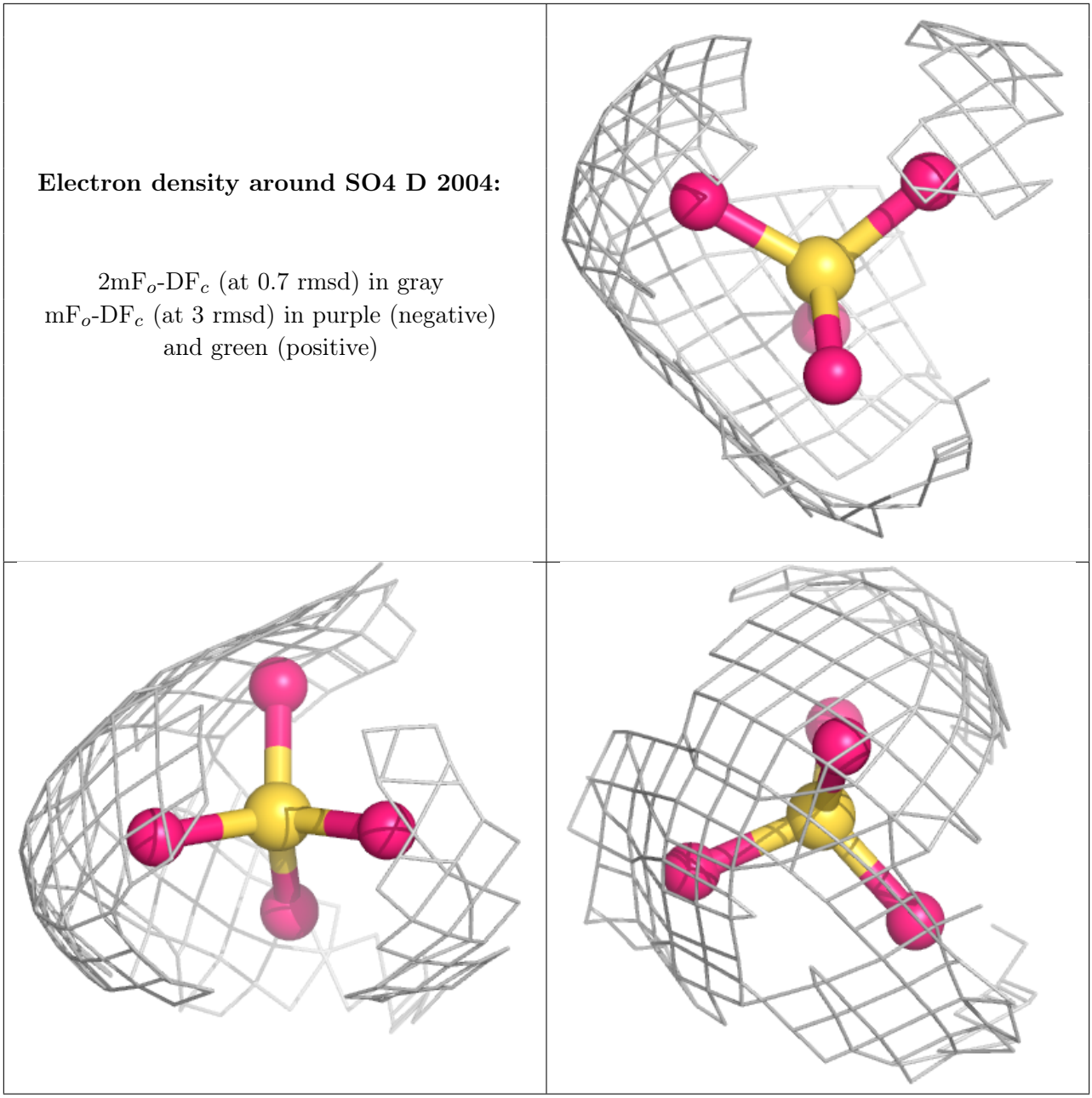






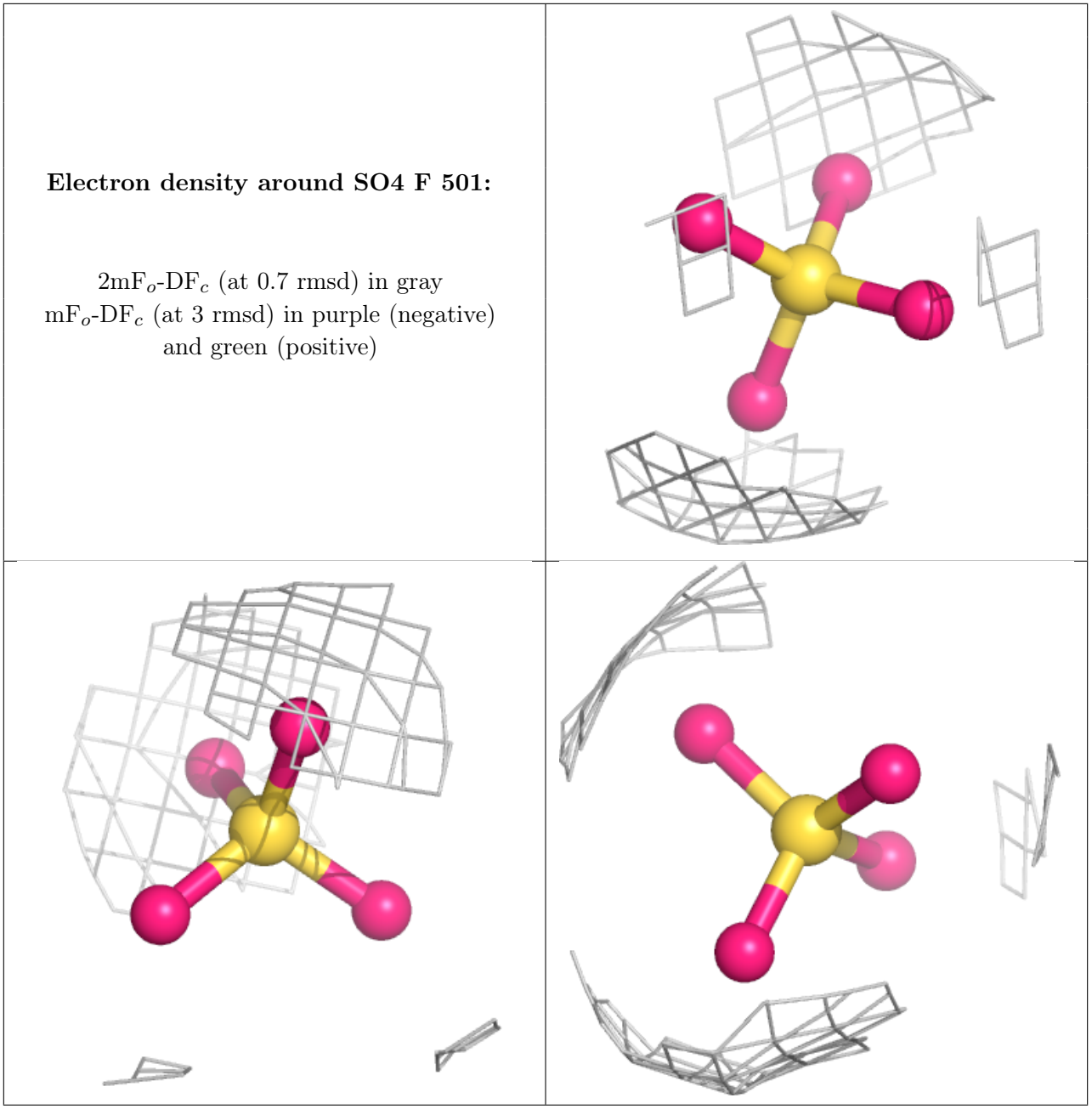
Electron density around SO4 D 2004:

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



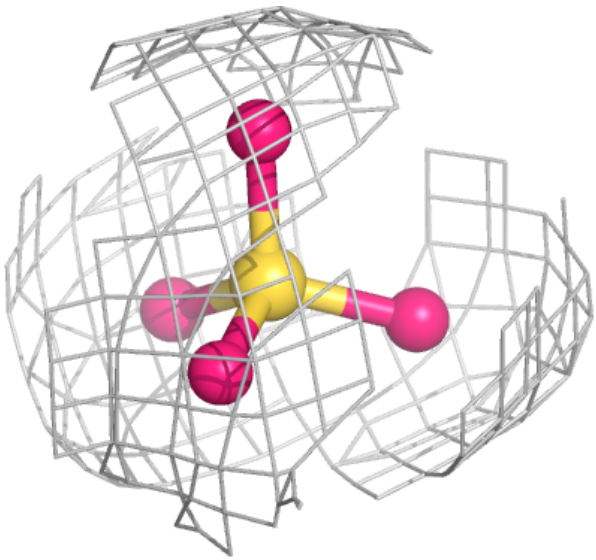
Electron density around SO4 F 501:

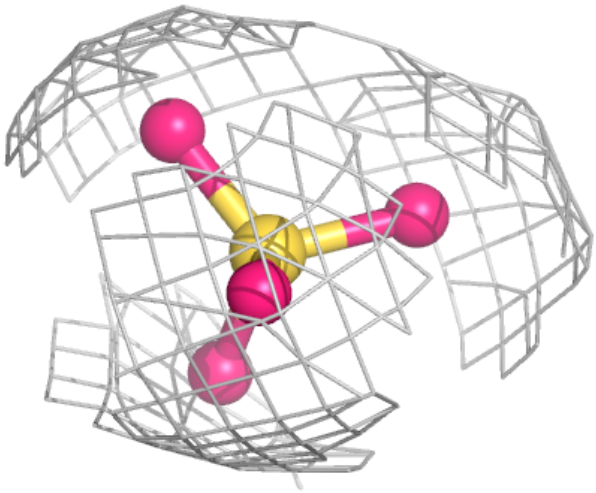
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

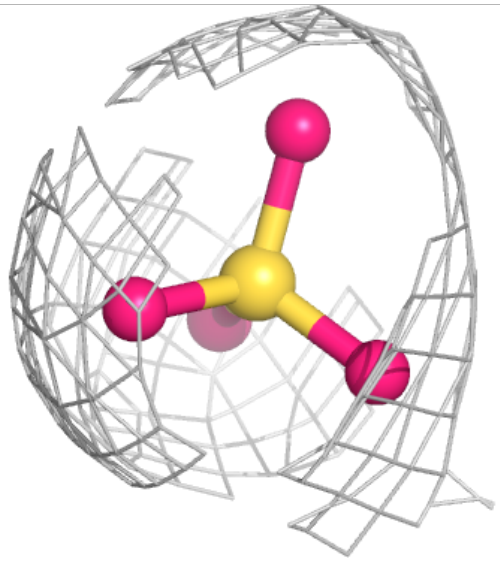


Electron density around SO4 D 2003:

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

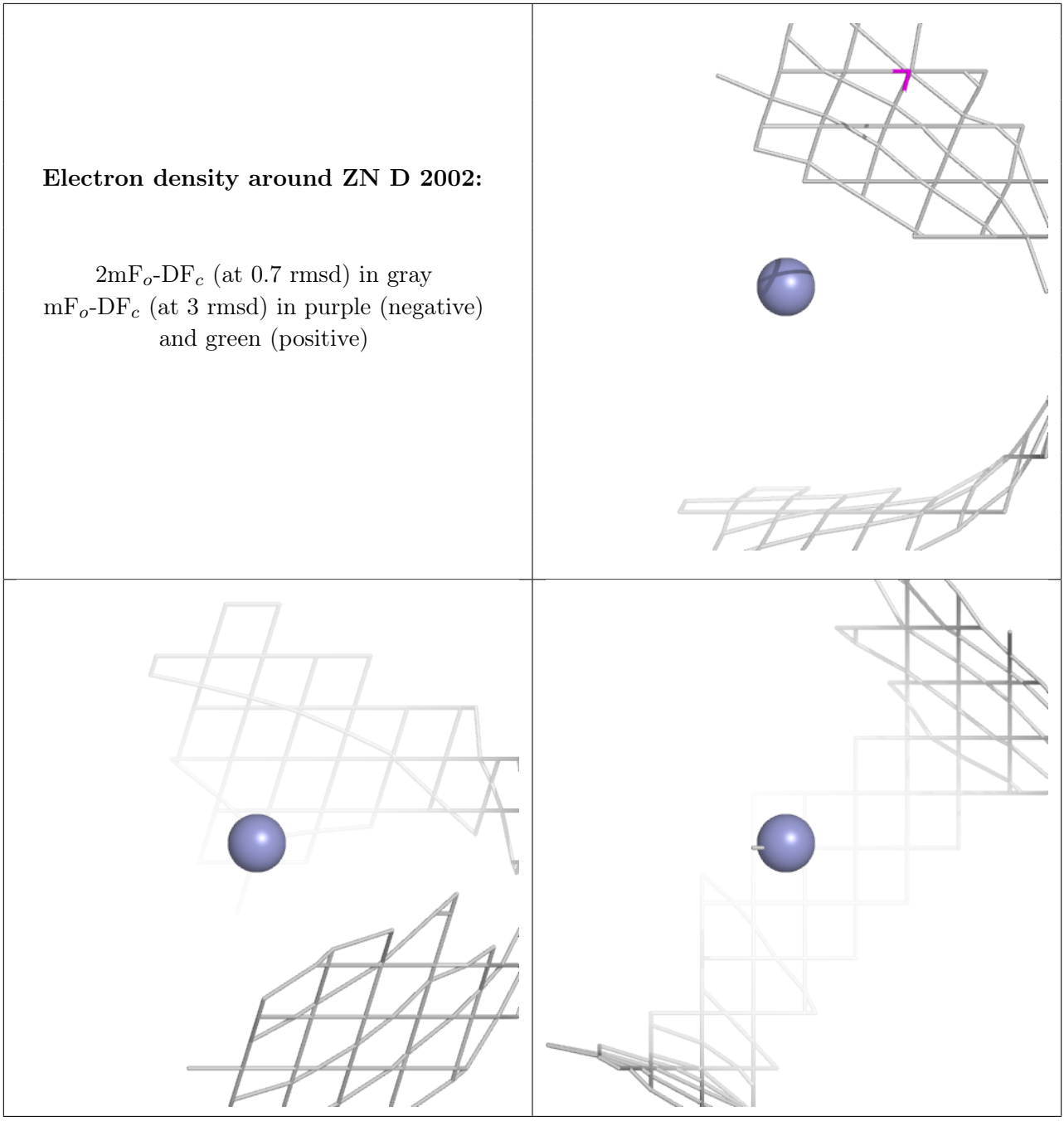






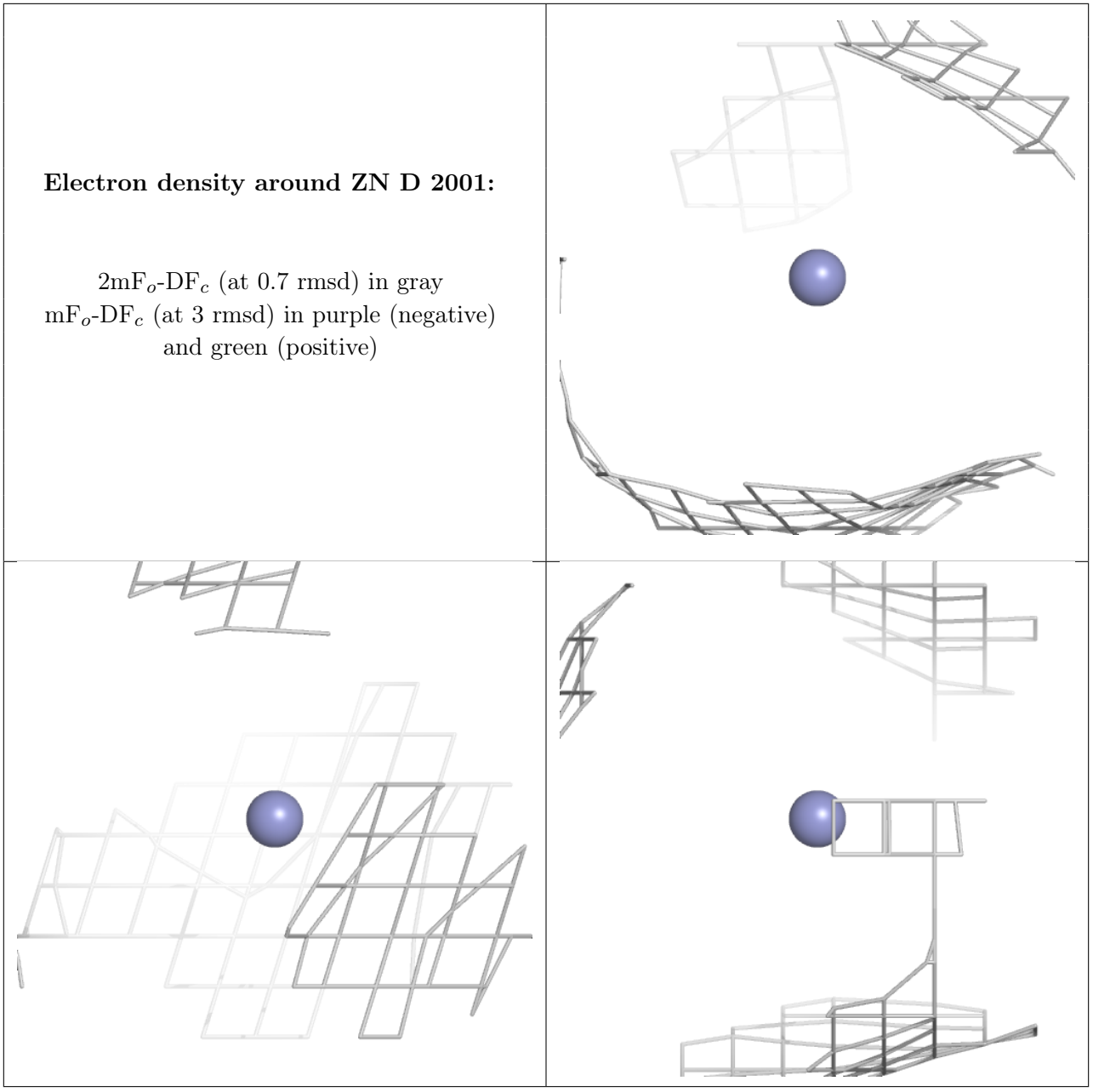
Electron density around ZN D 2002:

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



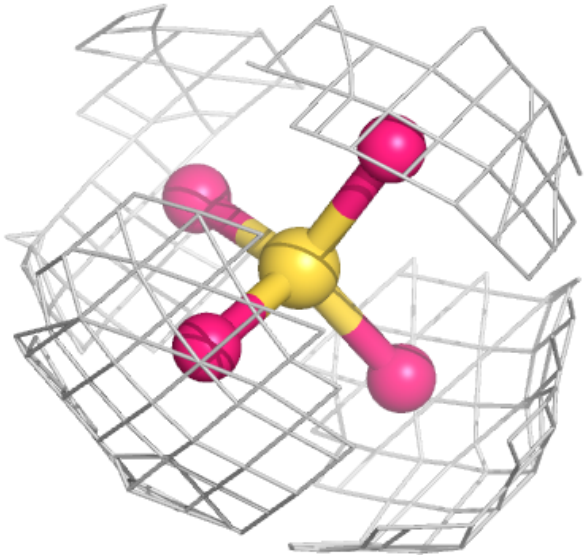
Electron density around ZN D 2001:

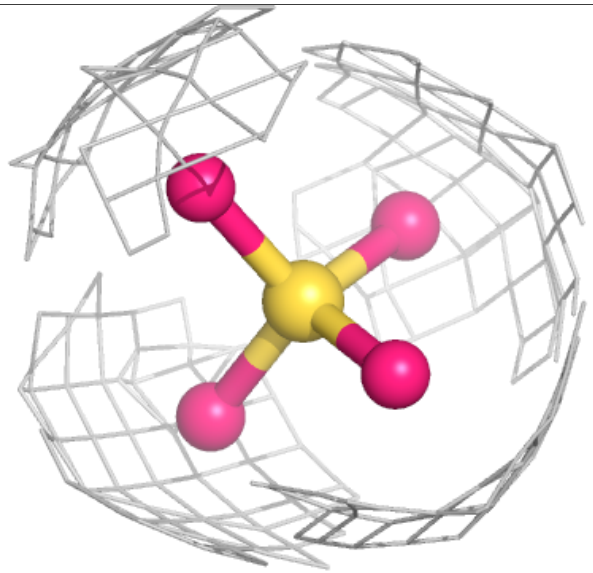
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

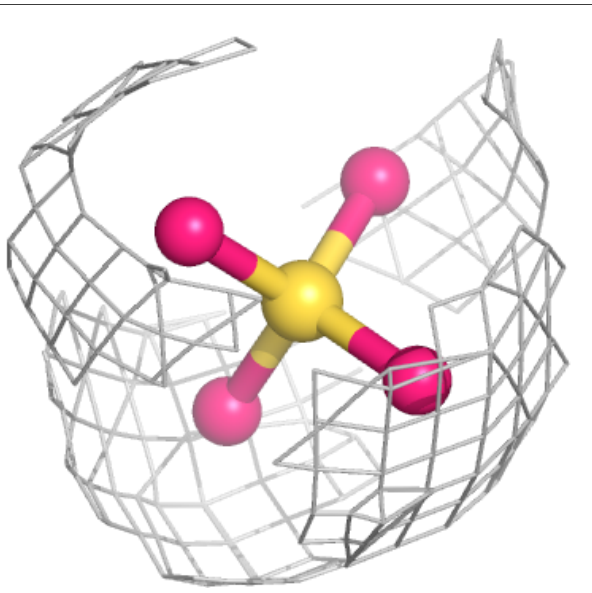


Electron density around SO4 F 502:

$2mF_o$-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.