WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 19, 2025 – 05:10 pm GMT

PDB ID	:	9QFU
Title	:	Human Tryptase beta-2 (hTPSB2) complexed with covalent inhibitor Compound #1
Authors	:	Porta, A.; Manelfi, C.; Talarico, C.; Beccari, A.R.; Brindisi, M.; Summa, V.; Iaconis, D.; Gobbi, M.; Beeg, M.
Deposited on	:	2025-03-12
Resolution	:	1.98 Å(reported)

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

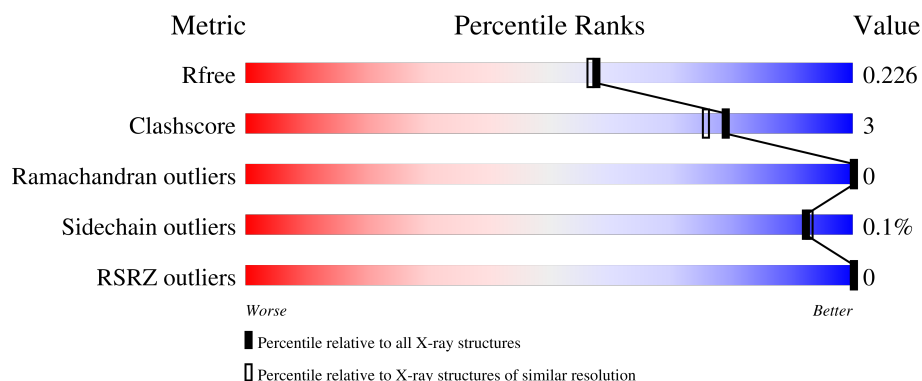|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance ⓘ

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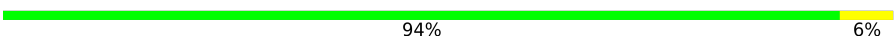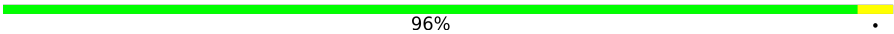*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.1%
RSRZ outliers		0

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	243	94% 6%
1	B	243	94% 6%
1	C	243	95% 5%
1	D	243	96% •

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
6	ACT	A	310	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 8818 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 Tryptase beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	10	9	0
			1994	1277	347	355	15			
1	B	243	Total	C	N	O	S	15	7	0
			1972	1262	343	352	15			
1	C	243	Total	C	N	O	S	13	8	0
			1974	1262	345	352	15			
1	D	243	Total	C	N	O	S	14	12	0
			2013	1291	348	358	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	HIS	ARG	variant	UNP P20231
A	37	GLY	ASP	variant	UNP P20231
A	38	PRO	ARG	variant	UNP P20231
A	117	LYS	ASN	conflict	UNP P20231
B	36	HIS	ARG	variant	UNP P20231
B	37	GLY	ASP	variant	UNP P20231
B	38	PRO	ARG	variant	UNP P20231
B	117	LYS	ASN	conflict	UNP P20231
C	36	HIS	ARG	variant	UNP P20231
C	37	GLY	ASP	variant	UNP P20231
C	38	PRO	ARG	variant	UNP P20231
C	117	LYS	ASN	conflict	UNP P20231
D	36	HIS	ARG	variant	UNP P20231
D	37	GLY	ASP	variant	UNP P20231
D	38	PRO	ARG	variant	UNP P20231
D	117	LYS	ASN	conflict	UNP P20231

- Molecule 2 is {N}-[(1 {S},2 {S})-6-azanyl-1-[5-[[4-[2-(3,4-dichlorophenyl)ethoxy]phenyl]methyl]-1,2,4-oxadiazol-3-yl]-1-oxidanyl-hexan-2-yl]-4-fluoranyl-benzamide (three-letter code: A1I52) (formula: $C_{30}H_{31}Cl_2FN_4O_4$) (labeled as "Ligand of Interest" by depositor).

A1I52
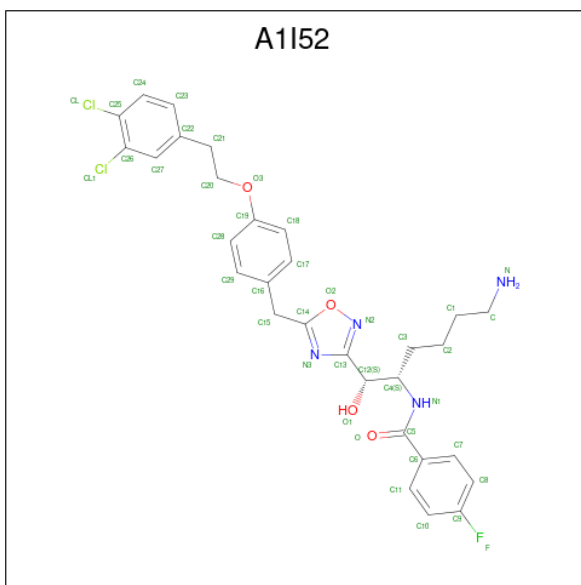
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			41	30	2	1	4	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			41	30	2	1	4	4		
2	C	1	Total	C	Cl	F	N	O	0	0
			41	30	2	1	4	4		
2	D	1	Total	C	Cl	F	N	O	0	1
			46	34	3	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).

SO4
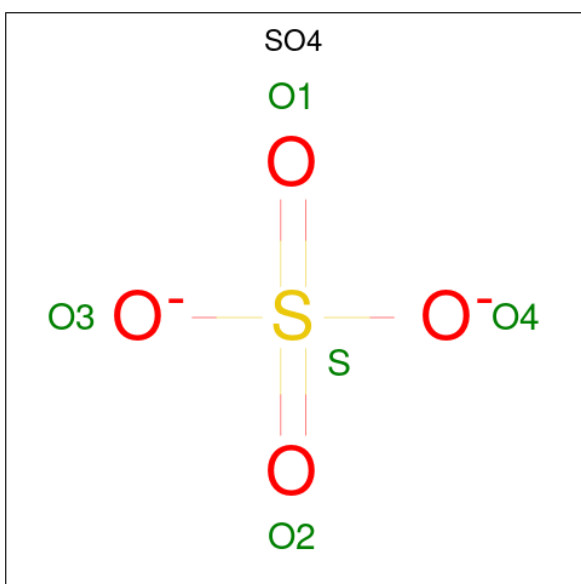
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).

PEG
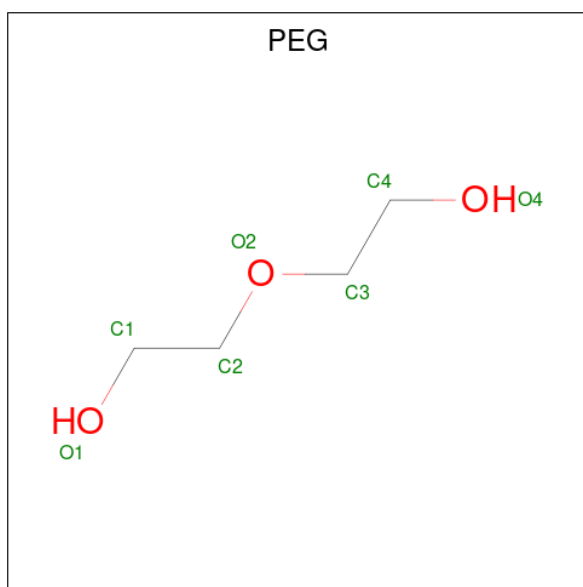
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0
4	D	1	Total 7	C 4	O 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).
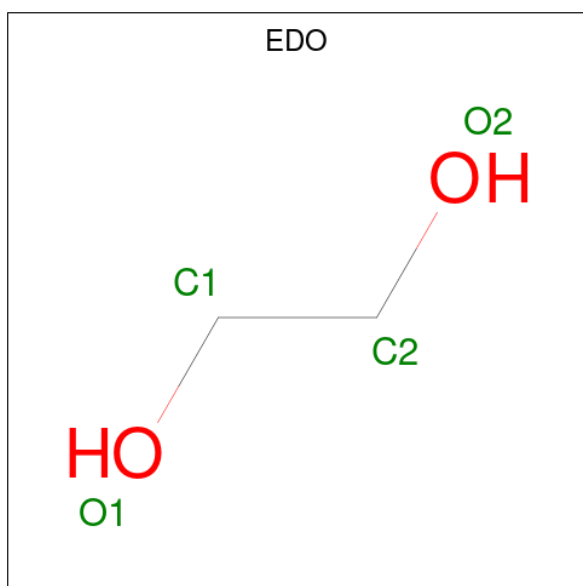
EDO

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

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).

ACT

OXT

O⁻

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

GOL

C3

OH O3

C1 C2

HO

OH

O1

O2
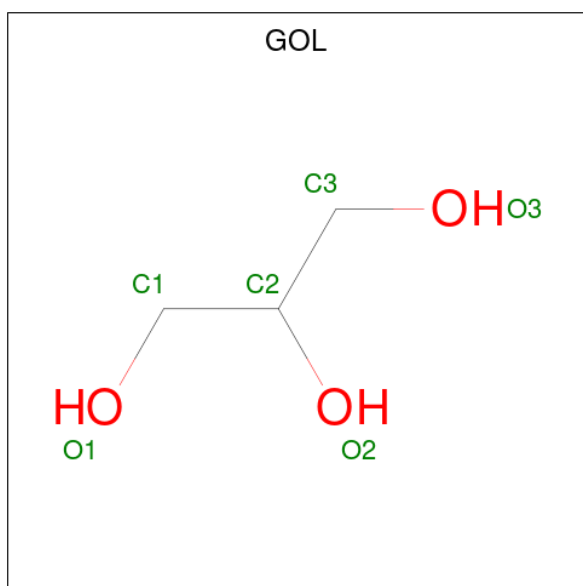
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	149	Total 149	O 149	0	1
8	B	120	Total 120	O 120	0	1
8	C	115	Total 115	O 115	0	0
8	D	140	Total 140	O 140	0	1

3 Residue-property plots ⓘ

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

• Molecule 1: Tryptase beta-2

Chain A:

• Molecule 1: Tryptase beta-2

Chain B:

• Molecule 1: Tryptase beta-2

Chain C:
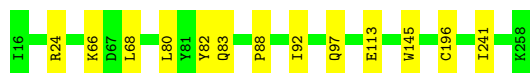
• Molecule 1: Tryptase beta-2

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	78.55Å 78.55Å 165.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.93 – 1.98 62.93 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.93-1.98) 99.7 (62.93-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.98Å)	Xtriage
Refinement program	REFMAC v.5.8.0267	Depositor
R, R_{free}	0.177 , 0.221 0.184 , 0.226	Depositor DCC
R_{free} test set	4239 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.486 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8818	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: A1I52, GOL, SO4, EDO, PEG, ACT

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	0.73	0/2068	0.89	2/2833 (0.1%)
1	B	0.73	0/2044	0.86	0/2799
1	C	0.73	0/2043	0.86	0/2798
1	D	0.73	0/2093	0.88	0/2866
All	All	0.73	0/8248	0.87	2/11296 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	238	ARG	NE-CZ-NH2	-5.28	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1994	0	1905	10	0
1	B	1972	0	1891	12	0
1	C	1974	0	1892	8	0
1	D	2013	0	1930	7	0
2	A	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	41	0	0	2	0
2	C	41	0	0	0	0
2	D	46	0	0	1	0
3	A	20	0	0	2	0
3	B	15	0	0	1	0
3	C	25	0	0	1	0
3	D	20	0	0	0	0
4	A	7	0	10	0	0
4	D	7	0	10	0	0
5	A	12	0	18	0	0
5	B	12	0	18	0	0
5	C	20	0	30	0	0
5	D	16	0	24	0	0
6	A	4	0	3	3	0
6	B	4	0	3	0	0
6	C	4	0	3	0	0
7	B	6	0	8	2	0
8	A	149	0	0	3	0
8	B	120	0	0	3	0
8	C	115	0	0	4	0
8	D	140	0	0	2	0
All	All	8818	0	7745	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 41 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)
3:B:307:SO4:O1	8:B:401:HOH:O	1.87	0.91
1:B:66:LYS:NZ	8:B:402:HOH:O	2.20	0.75
1:B:254:HIS:ND1	8:B:403:HOH:O	2.27	0.66
1:A:66:LYS:NZ	8:A:403:HOH:O	2.23	0.62
1:A:141[A]:TRP:CH2	6:A:310:ACT:H3	2.34	0.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	250/243 (103%)	242 (97%)	8 (3%)	0	100	100
1	B	248/243 (102%)	241 (97%)	7 (3%)	0	100	100
1	C	249/243 (102%)	242 (97%)	7 (3%)	0	100	100
1	D	253/243 (104%)	245 (97%)	8 (3%)	0	100	100
All	All	1000/972 (103%)	970 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	217/208 (104%)	217 (100%)	0	100	100
1	B	215/208 (103%)	215 (100%)	0	100	100
1	C	214/208 (103%)	214 (100%)	0	100	100
1	D	220/208 (106%)	219 (100%)	1 (0%)	86	86
All	All	866/832 (104%)	865 (100%)	1 (0%)	92	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	117	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	GLN
1	B	235	GLN
1	C	97	GLN
1	C	235	GLN
1	D	237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

42 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	$\#|Z| > 2$
5	EDO	B	308	-	3,3,3	0.19	0	2,2,2	0.25	0
5	EDO	B	309	-	3,3,3	0.10	0	2,2,2	0.23	0
3	SO4	C	305	-	4,4,4	0.38	0	6,6,6	0.07	0
5	EDO	C	309	-	3,3,3	0.24	0	2,2,2	0.26	0
5	EDO	C	310	-	3,3,3	0.05	0	2,2,2	0.23	0
3	SO4	D	306	-	4,4,4	0.32	0	6,6,6	0.16	0
6	ACT	A	310	-	3,3,3	0.61	0	3,3,3	1.15	0
3	SO4	B	302	-	4,4,4	0.38	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	EDO	A	309	-	3,3,3	0.13	0	2,2,2	0.40	0
5	EDO	B	306	-	3,3,3	0.11	0	2,2,2	0.23	0
3	SO4	B	307	-	4,4,4	0.35	0	6,6,6	0.19	0
5	EDO	D	310	-	3,3,3	0.16	0	2,2,2	0.40	0
5	EDO	A	307	-	3,3,3	0.17	0	2,2,2	0.18	0
5	EDO	C	312	-	3,3,3	0.16	0	2,2,2	0.35	0
4	PEG	A	306	-	6,6,6	0.23	0	5,5,5	0.29	0
3	SO4	A	302	-	4,4,4	0.41	0	6,6,6	0.18	0
5	EDO	D	307	-	3,3,3	0.11	0	2,2,2	0.61	0
2	A1I52	D	301[A]	-	40,44,44	0.70	1 (2%)	50,59,59	1.19	4 (8%)
3	SO4	C	308	-	4,4,4	0.23	0	6,6,6	0.33	0
3	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.22	0
4	PEG	D	308	-	6,6,6	0.22	0	5,5,5	0.22	0
3	SO4	C	303	-	4,4,4	0.38	0	6,6,6	0.20	0
3	SO4	A	304	-	4,4,4	0.32	0	6,6,6	0.09	0
5	EDO	A	308	-	3,3,3	0.09	0	2,2,2	0.15	0
3	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.17	0
2	A1I52	C	301	1	40,44,44	0.85	1 (2%)	50,59,59	0.92	3 (6%)
5	EDO	D	309	-	3,3,3	0.26	0	2,2,2	0.17	0
3	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.30	0
6	ACT	B	304	-	3,3,3	1.23	0	3,3,3	0.54	0
3	SO4	C	304	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	A	305	-	4,4,4	0.30	0	6,6,6	0.26	0
5	EDO	C	311	-	3,3,3	0.06	0	2,2,2	0.37	0
6	ACT	C	307	-	3,3,3	1.25	0	3,3,3	0.86	0
2	A1I52	A	301	1	40,44,44	0.80	1 (2%)	50,59,59	1.02	2 (4%)
7	GOL	B	305	-	5,5,5	0.12	0	5,5,5	0.65	0
3	SO4	B	303	-	4,4,4	0.32	0	6,6,6	0.19	0
2	A1I52	B	301	1	40,44,44	0.80	1 (2%)	50,59,59	0.86	3 (6%)
5	EDO	D	304	-	3,3,3	0.16	0	2,2,2	0.21	0
5	EDO	C	306	-	3,3,3	0.14	0	2,2,2	0.47	0
3	SO4	C	302	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	D	305	-	4,4,4	0.34	0	6,6,6	0.12	0
2	A1I52	D	301[B]	-	40,44,44	0.69	1 (2%)	50,59,59	1.17	4 (8%)

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
5	EDO	B	308	-	-	1/1/1/1	-

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	309	-	-	0/1/1/1	-
5	EDO	C	309	-	-	0/1/1/1	-
5	EDO	C	310	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	B	306	-	-	1/1/1/1	-
5	EDO	D	310	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	C	312	-	-	1/1/1/1	-
4	PEG	A	306	-	-	1/4/4/4	-
5	EDO	D	307	-	-	0/1/1/1	-
2	A1I52	D	301[A]	-	-	8/26/31/31	0/4/4/4
4	PEG	D	308	-	-	1/4/4/4	-
5	EDO	A	308	-	-	1/1/1/1	-
2	A1I52	C	301	1	-	8/26/31/31	0/4/4/4
5	EDO	D	309	-	-	1/1/1/1	-
5	EDO	C	311	-	-	1/1/1/1	-
2	A1I52	A	301	1	-	6/26/31/31	0/4/4/4
7	GOL	B	305	-	-	2/4/4/4	-
2	A1I52	B	301	1	-	7/26/31/31	0/4/4/4
5	EDO	D	304	-	-	1/1/1/1	-
5	EDO	C	306	-	-	0/1/1/1	-
2	A1I52	D	301[B]	-	-	8/26/31/31	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1I52	C12-C4	4.51	1.59	1.53
2	B	301	A1I52	C12-C4	3.84	1.58	1.53
2	A	301	A1I52	C12-C4	3.50	1.57	1.53
2	D	301[A]	A1I52	C12-C4	2.68	1.56	1.53
2	D	301[B]	A1I52	C12-C4	2.68	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1I52	C13-C12-C4	-4.22	106.58	111.31
2	D	301[A]	A1I52	C13-C12-C4	-4.12	106.69	111.31
2	D	301[B]	A1I52	C13-C12-C4	-4.12	106.69	111.31
2	D	301[A]	A1I52	C3-C4-N1	-4.03	105.03	110.33
2	D	301[B]	A1I52	C3-C4-N1	-4.03	105.03	110.33

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	A1I52	N3-C14-C15-C16
2	C	301	A1I52	N3-C14-C15-C16
7	B	305	GOL	C1-C2-C3-O3
2	C	301	A1I52	O-C5-C6-C7
2	C	301	A1I52	O-C5-C6-C11

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	310	ACT	3	0
3	B	307	SO4	1	0
3	A	302	SO4	1	0
2	D	301[A]	A1I52	1	0
3	C	308	SO4	1	0
3	A	305	SO4	1	0
2	A	301	A1I52	1	0
7	B	305	GOL	2	0
2	B	301	A1I52	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 B 308

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 309

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 C 305

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 309

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 310

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 306

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT A 310

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 309

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 306

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 307

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 310

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 307

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 312

Bond lengths

Bond angles

Torsions

Rings

Ligand PEG A 306

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 307

Bond lengths

Bond angles

Torsions

Rings

Ligand A1I52 D 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 C 308
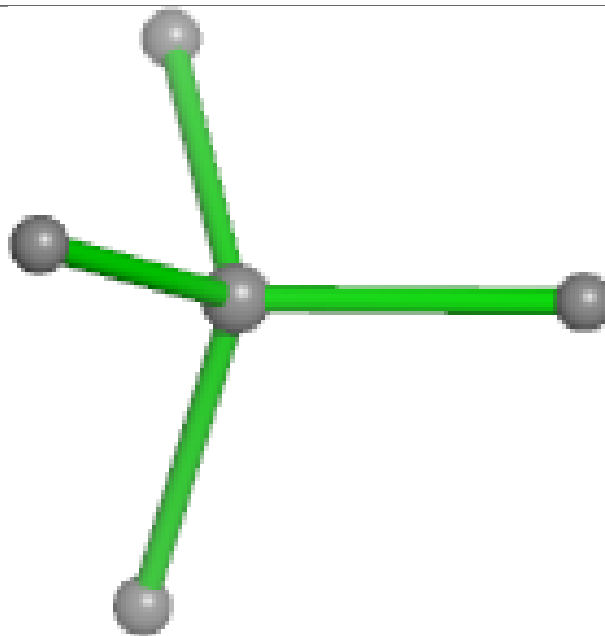
Bond lengths
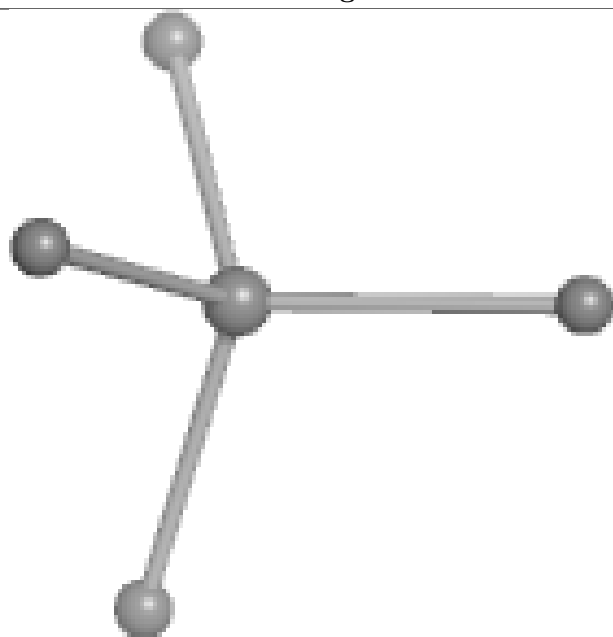
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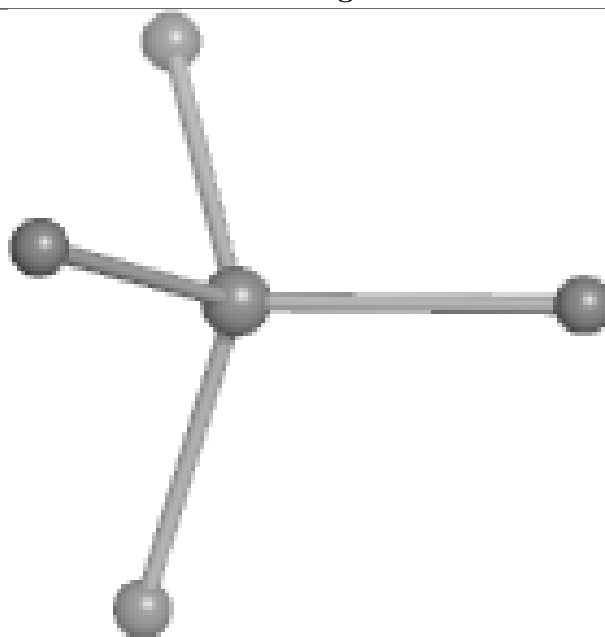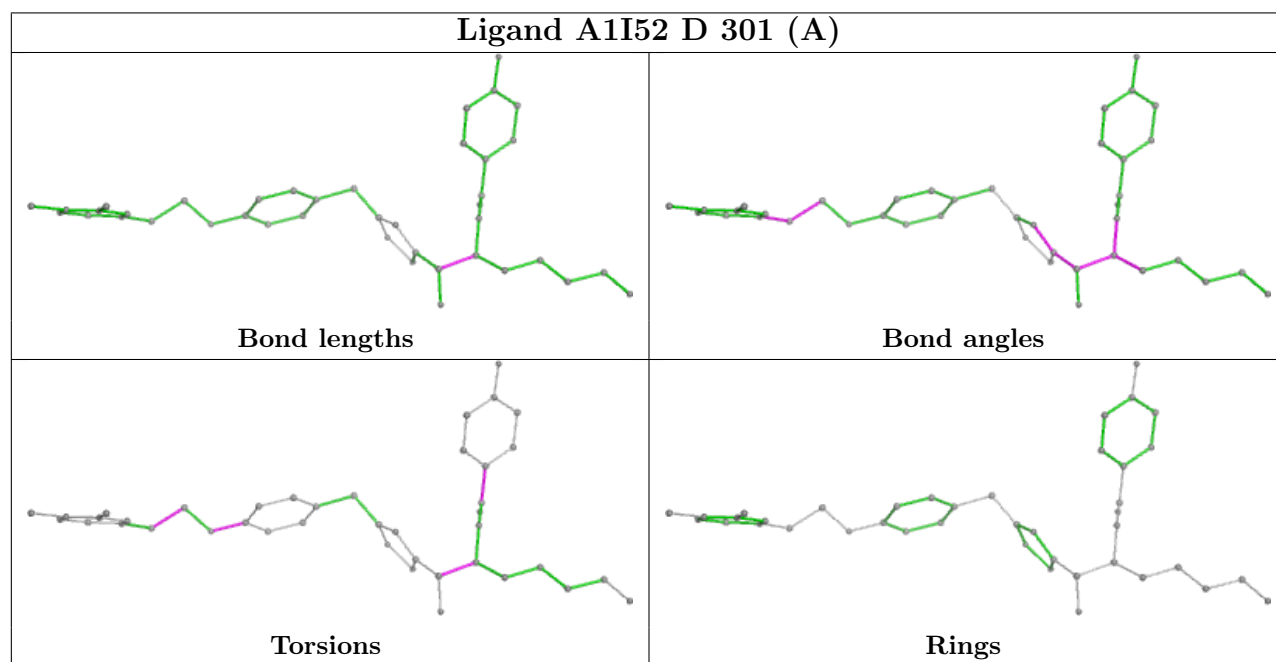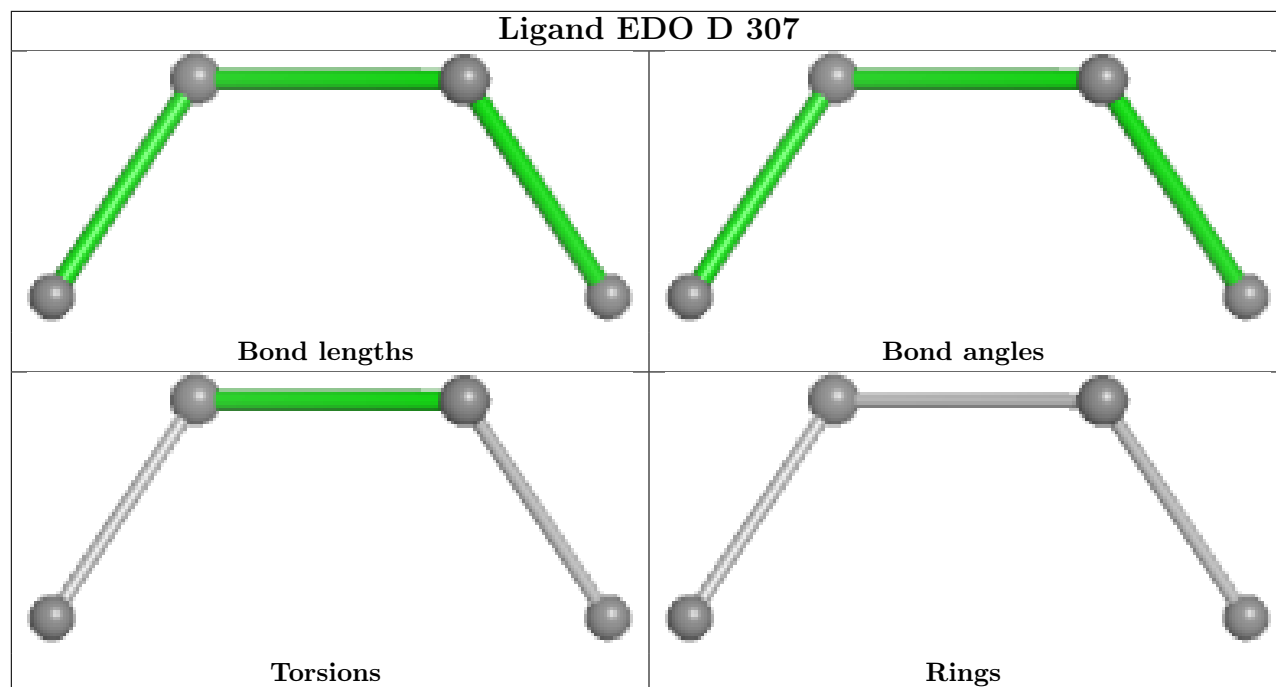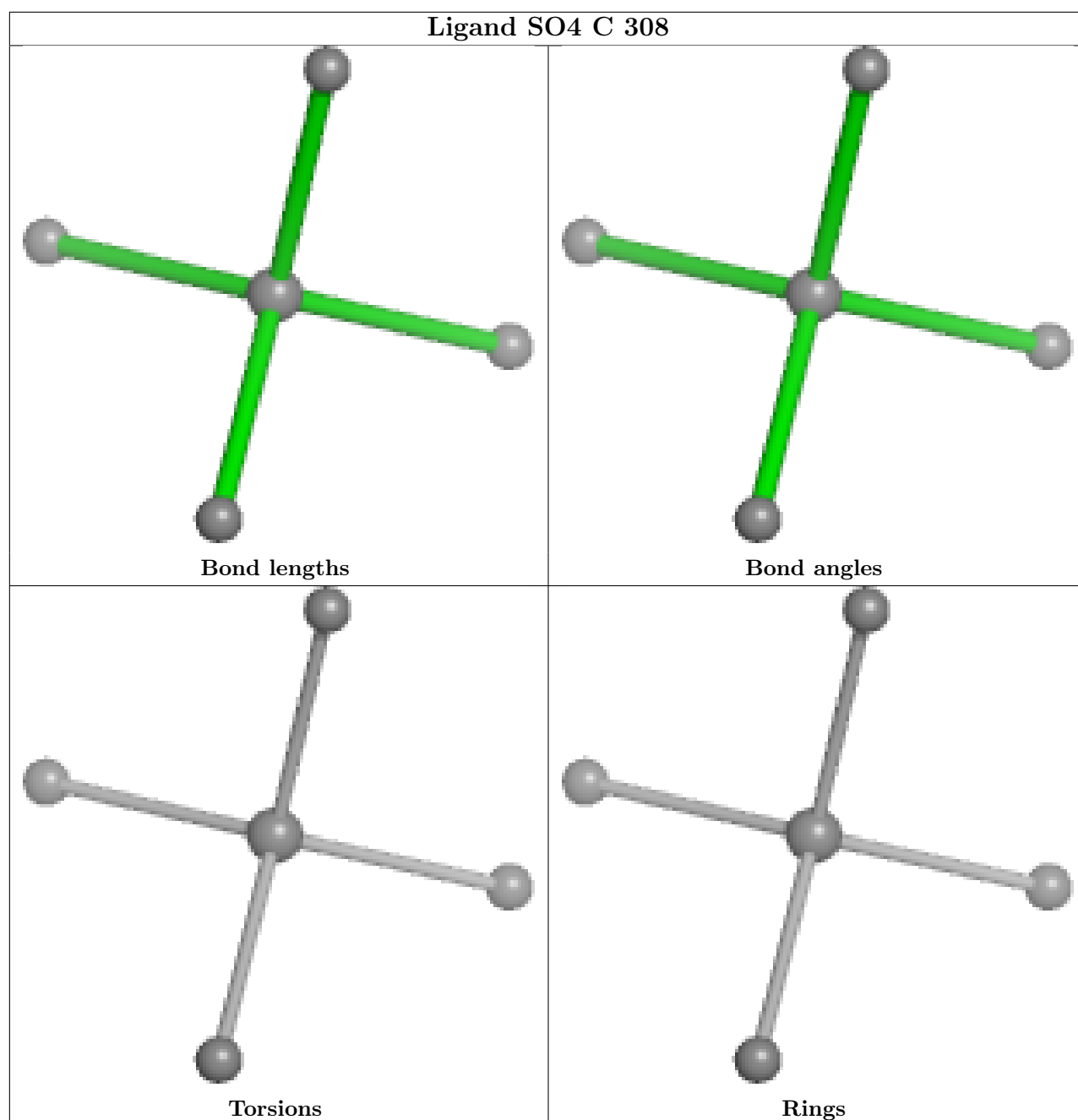
Torsions

Rings

Ligand SO4 A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand PEG D 308

Bond lengths

Bond angles

Torsions

Rings
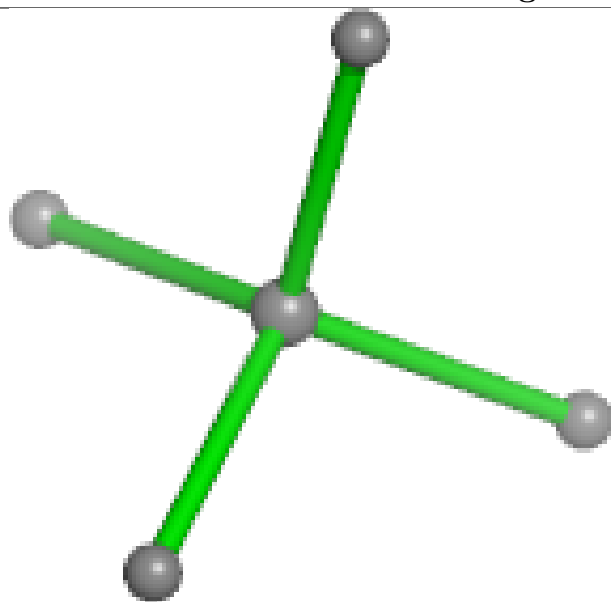
Ligand SO4 C 303
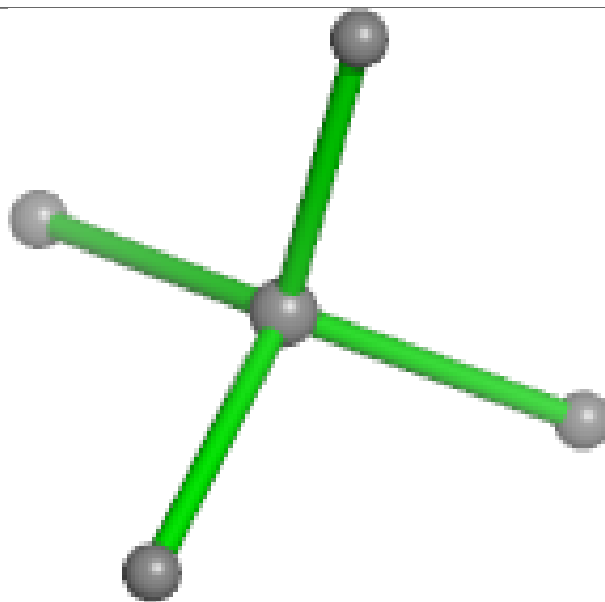
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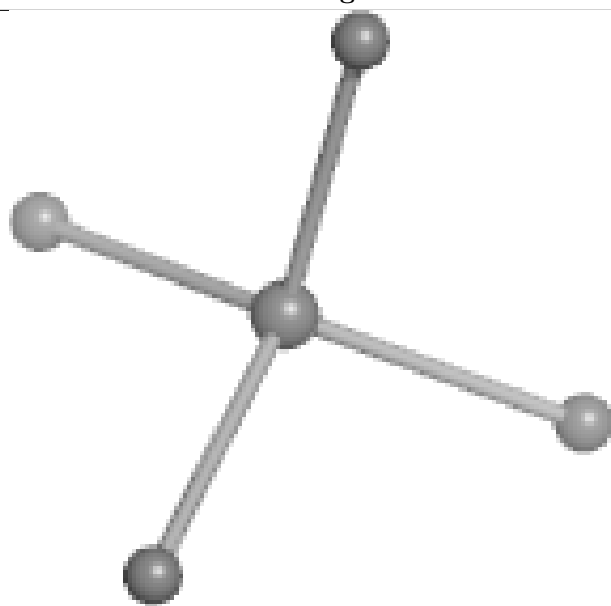
Bond angles
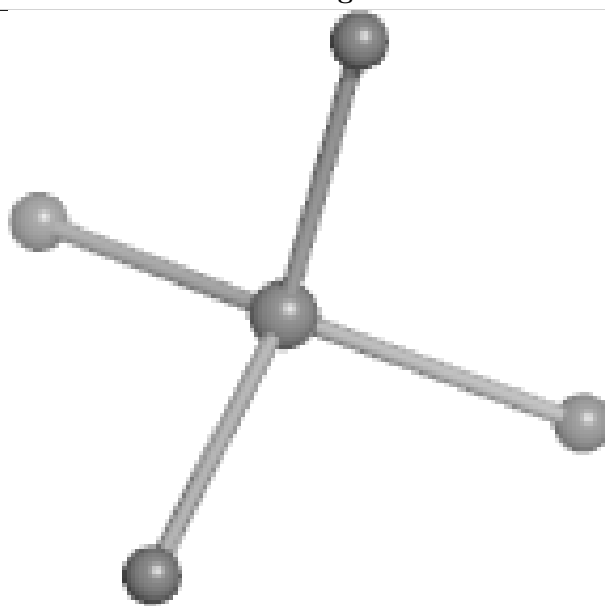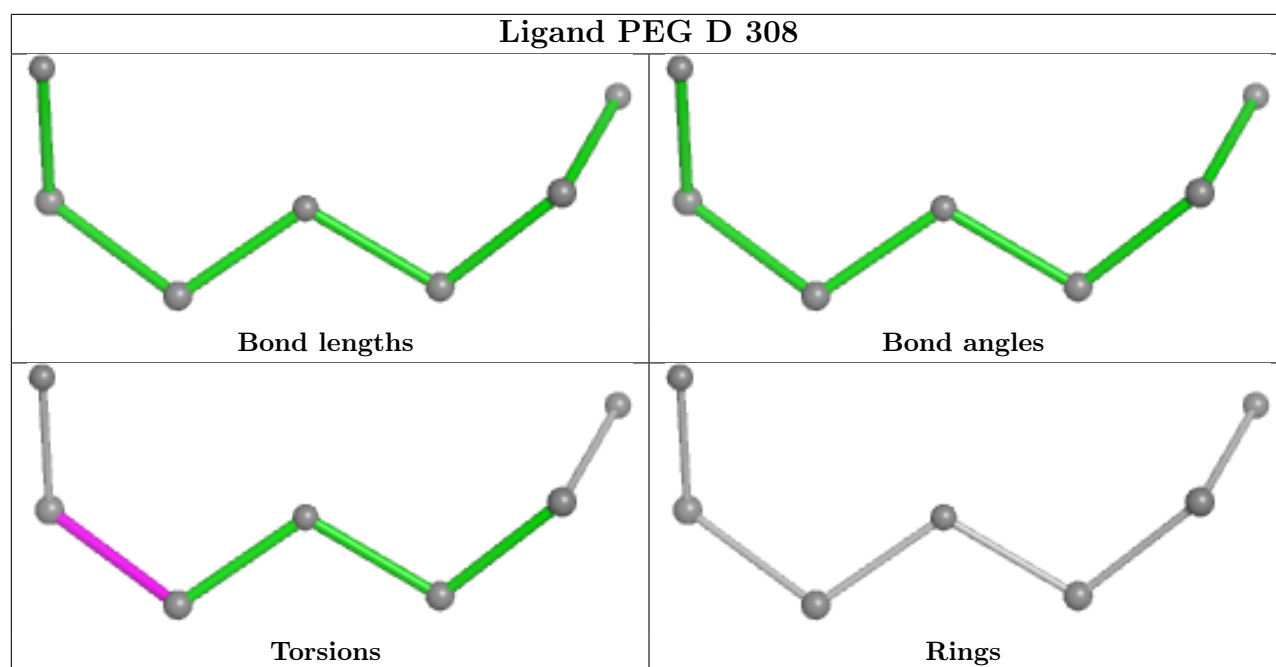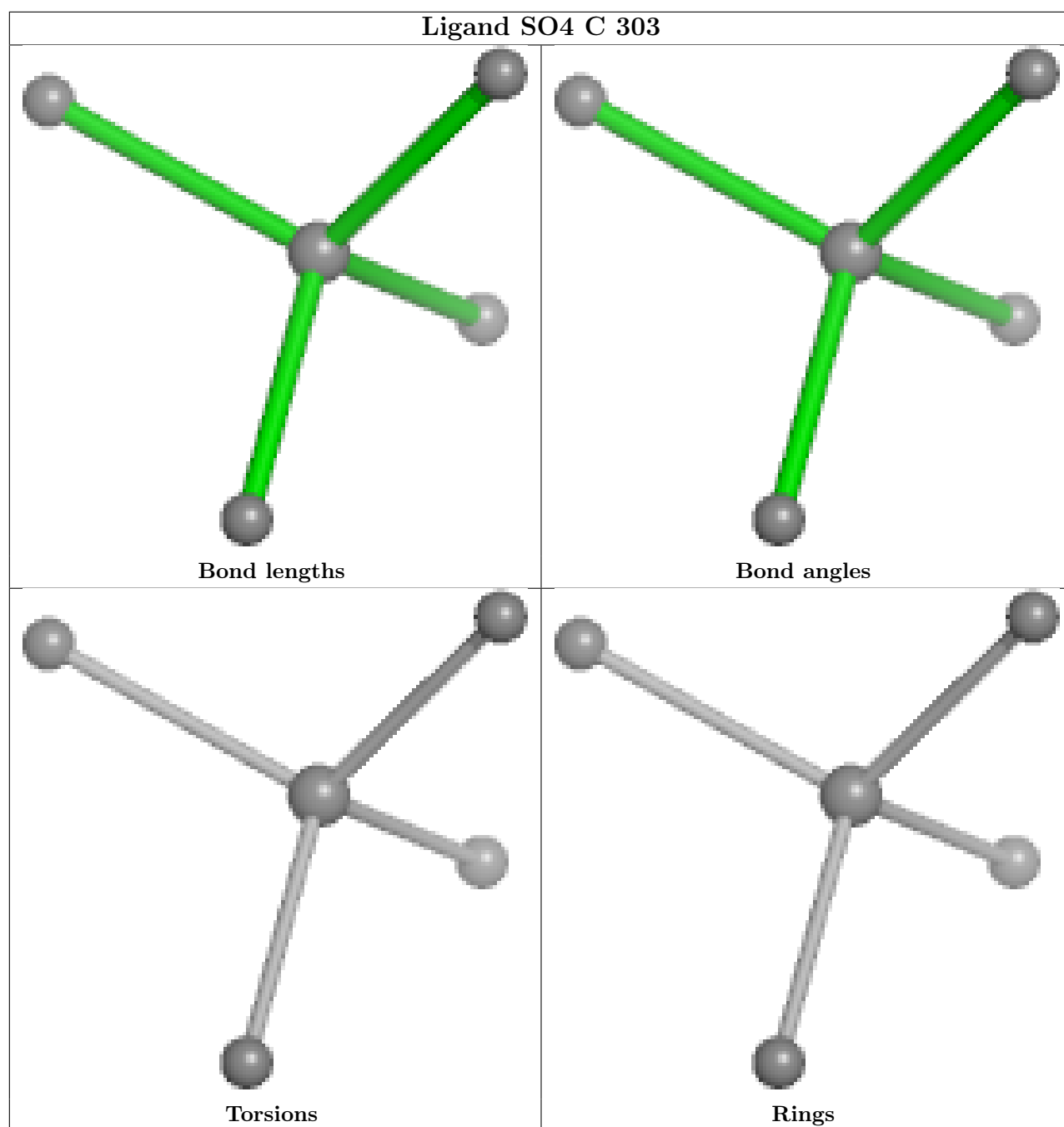
Torsions

Rings

Ligand SO4 A 304

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 308
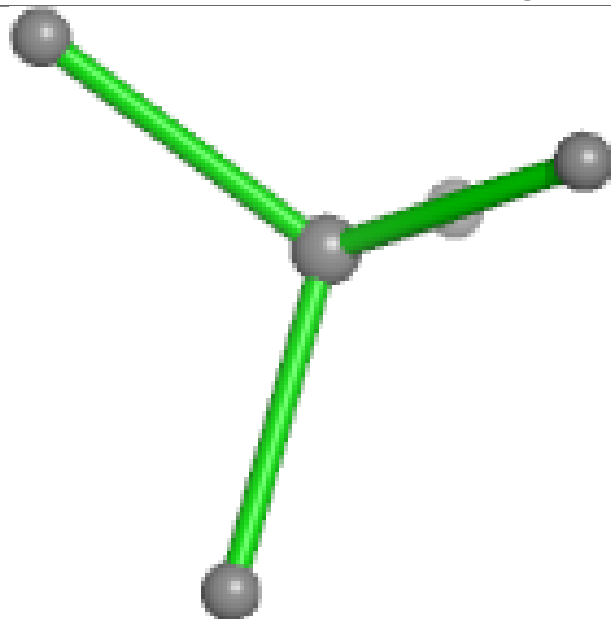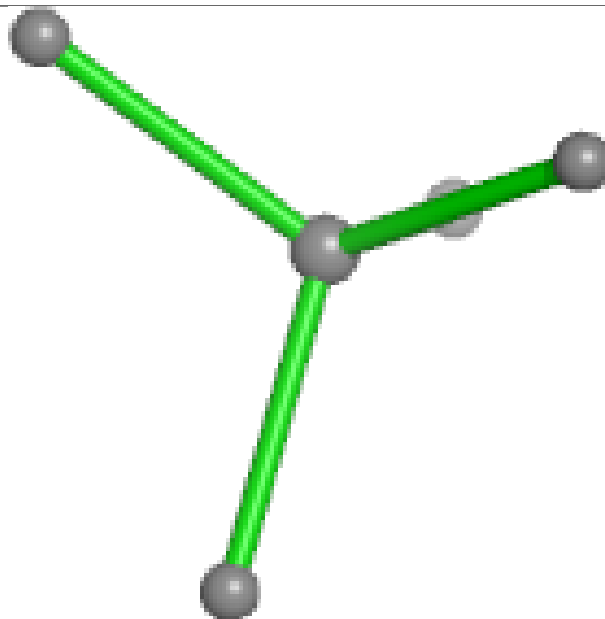
Bond lengths
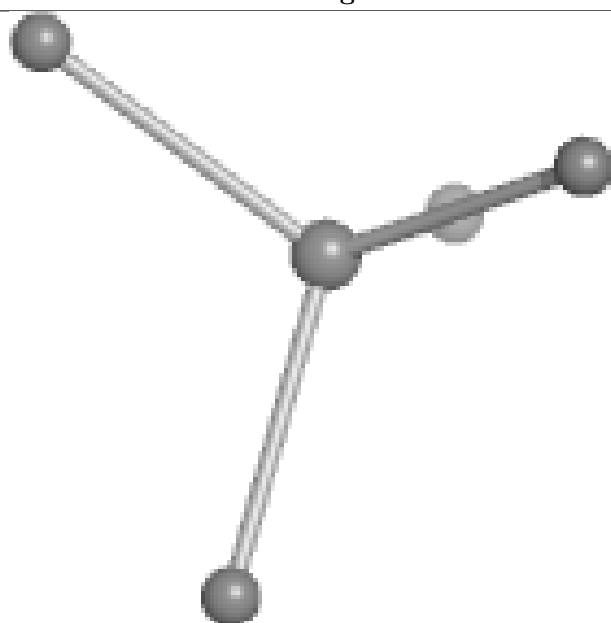
Bond angles
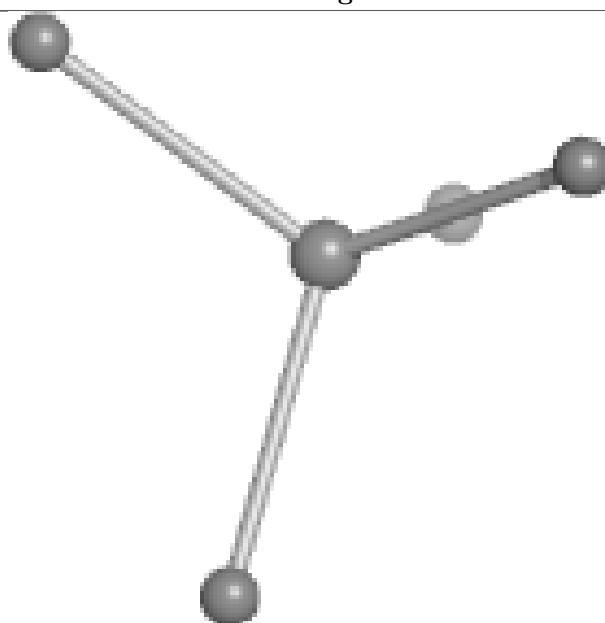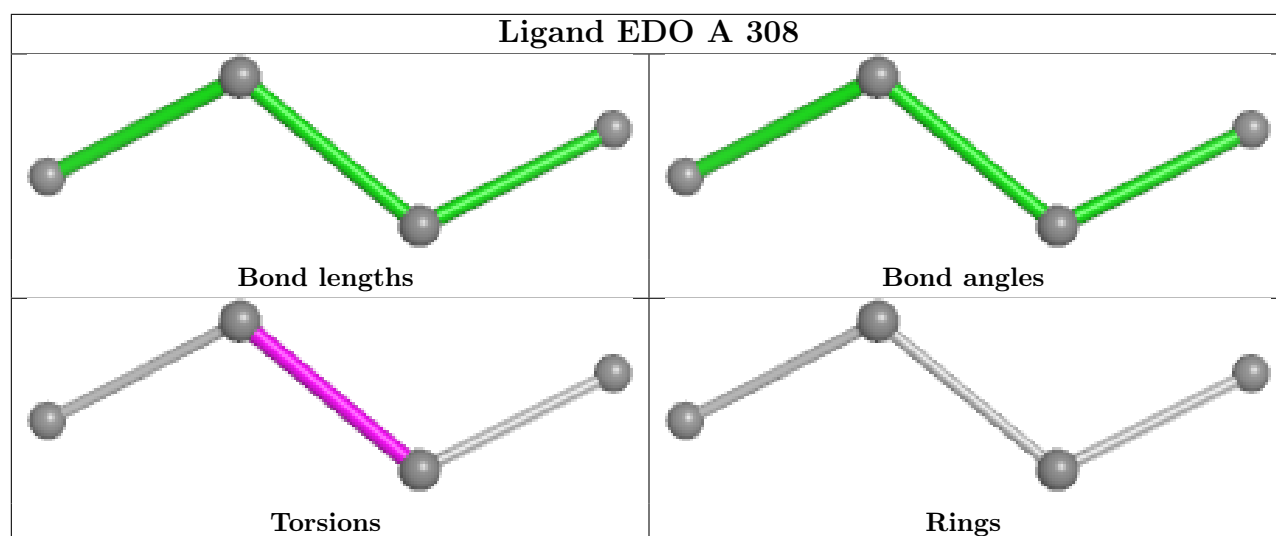
Torsions

Rings

Ligand SO4 D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand A1I52 C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 309

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 303

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT B 304

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 311

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT C 307

Bond lengths

Bond angles

Torsions

Rings

Ligand A1I52 A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 305

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand A1I52 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 304

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 306

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 305

Bond lengths

Bond angles

Torsions

Rings

Ligand A1I52 D 301 (B)	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	243/243 (100%)	-1.37	0	100	100	14, 29, 44, 62	12 (4%)
1	B	243/243 (100%)	-1.28	0	100	100	16, 32, 51, 77	12 (4%)
1	C	243/243 (100%)	-1.30	0	100	100	16, 32, 51, 64	12 (4%)
1	D	243/243 (100%)	-1.37	0	100	100	14, 29, 45, 60	17 (6%)
All	All	972/972 (100%)	-1.33	0	100	100	14, 30, 49, 77	53 (5%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å²)	Q<0.9
3	SO4	D	305	5/5	0.96	0.07	95,102,117,119	0
5	EDO	D	310	4/4	0.96	0.07	51,62,65,70	0
3	SO4	D	302	5/5	0.97	0.05	71,75,81,83	0
3	SO4	A	302	5/5	0.97	0.04	67,72,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	306	4/4	0.97	0.06	61,63,64,65	0
5	EDO	C	306	4/4	0.97	0.08	61,62,64,67	0
5	EDO	C	309	4/4	0.97	0.06	70,72,72,85	0
3	SO4	A	304	5/5	0.97	0.08	85,94,112,118	0
6	ACT	B	304	4/4	0.97	0.07	53,56,61,62	0
6	ACT	C	307	4/4	0.97	0.06	54,55,56,61	0
3	SO4	B	307	5/5	0.98	0.06	70,88,97,99	0
3	SO4	C	302	5/5	0.98	0.05	88,97,100,103	0
3	SO4	C	303	5/5	0.98	0.06	80,84,91,95	0
3	SO4	C	304	5/5	0.98	0.04	75,79,88,92	0
3	SO4	C	305	5/5	0.98	0.05	74,76,84,89	0
3	SO4	C	308	5/5	0.98	0.04	62,66,73,94	0
2	A1I52	C	301	41/41	0.98	0.05	25,48,71,96	0
3	SO4	D	303	5/5	0.98	0.06	70,75,78,93	0
2	A1I52	D	301[A]	41/41	0.98	0.05	25,40,53,86	5
4	PEG	A	306	7/7	0.98	0.07	56,58,63,66	0
4	PEG	D	308	7/7	0.98	0.05	48,52,57,58	0
5	EDO	A	307	4/4	0.98	0.06	63,65,69,69	0
5	EDO	A	308	4/4	0.98	0.05	50,52,54,55	0
2	A1I52	D	301[B]	41/41	0.98	0.05	25,40,54,86	5
5	EDO	B	308	4/4	0.98	0.06	59,63,64,73	0
5	EDO	B	309	4/4	0.98	0.06	54,56,58,59	0
2	A1I52	A	301	41/41	0.98	0.05	25,42,61,91	0
3	SO4	A	303	5/5	0.98	0.06	67,67,80,89	0
5	EDO	C	311	4/4	0.98	0.05	55,57,60,61	0
5	EDO	D	304	4/4	0.98	0.07	47,64,65,70	0
5	EDO	D	307	4/4	0.98	0.05	59,61,63,66	0
5	EDO	D	309	4/4	0.98	0.05	48,50,51,52	0
2	A1I52	B	301	41/41	0.98	0.06	26,48,72,108	0
3	SO4	B	302	5/5	0.98	0.04	83,89,90,99	0
3	SO4	B	303	5/5	0.98	0.06	69,95,105,113	0
3	SO4	D	306	5/5	0.99	0.05	55,56,76,80	0
5	EDO	C	310	4/4	0.99	0.05	59,65,66,67	0
5	EDO	A	309	4/4	0.99	0.05	58,59,59,63	0
6	ACT	A	310	4/4	0.99	0.05	40,51,54,56	0
5	EDO	C	312	4/4	0.99	0.08	61,62,74,84	0
3	SO4	A	305	5/5	0.99	0.04	53,55,77,83	0
7	GOL	B	305	6/6	0.99	0.05	48,54,57,58	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 D 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
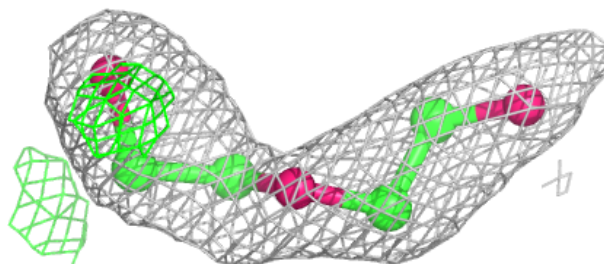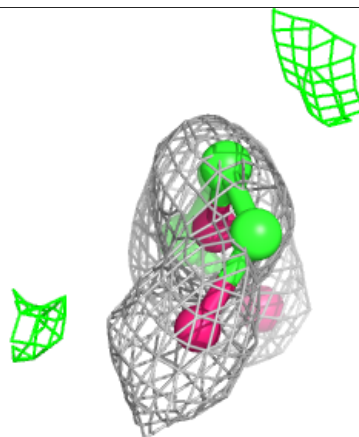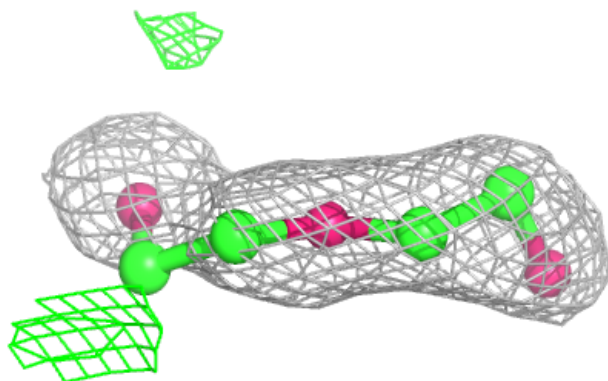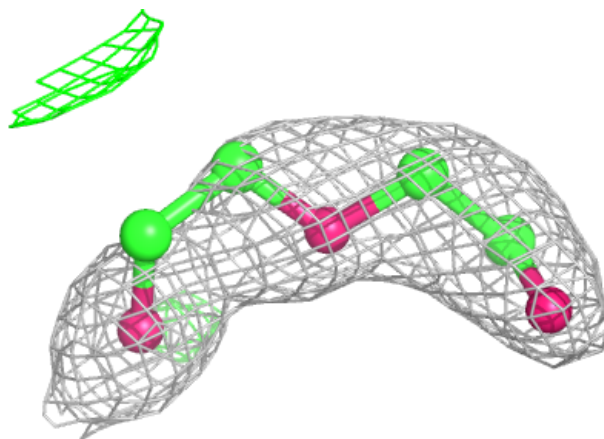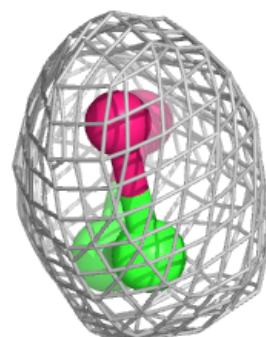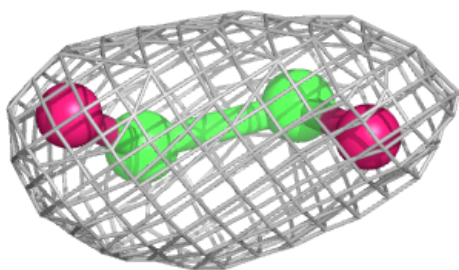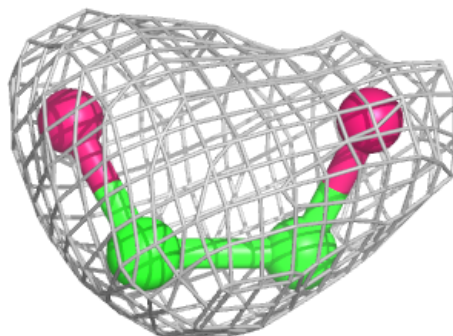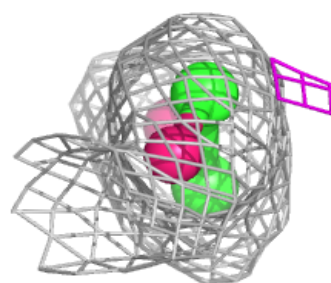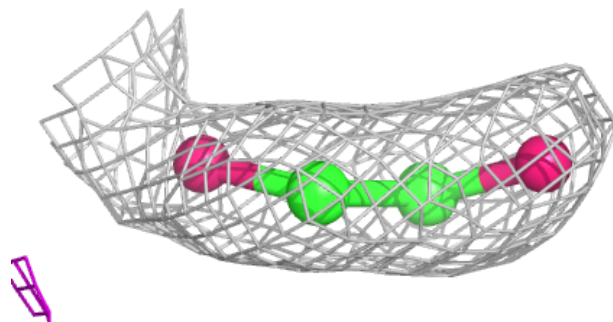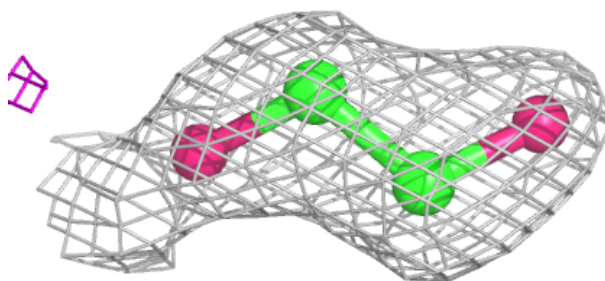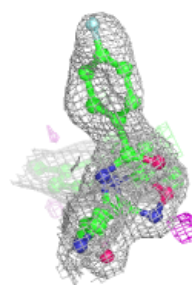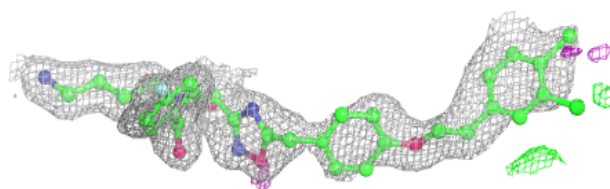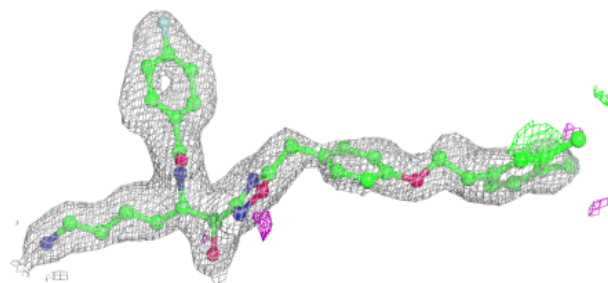mF_o-DF_c (at 3 rmsd) in purple (negative)
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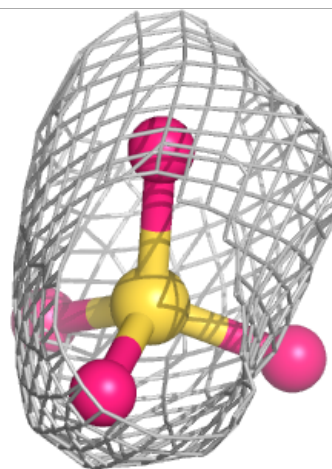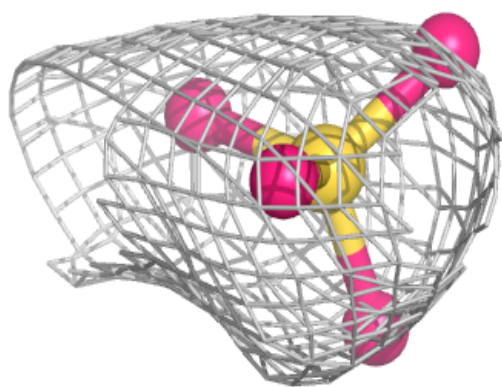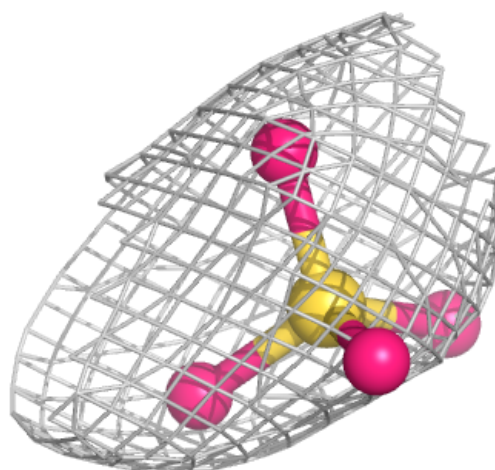
Electron density around EDO D 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
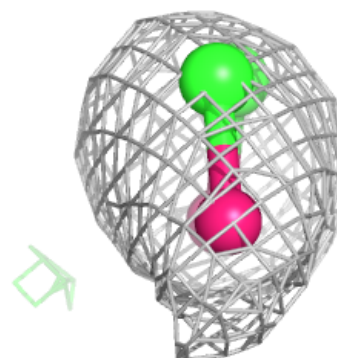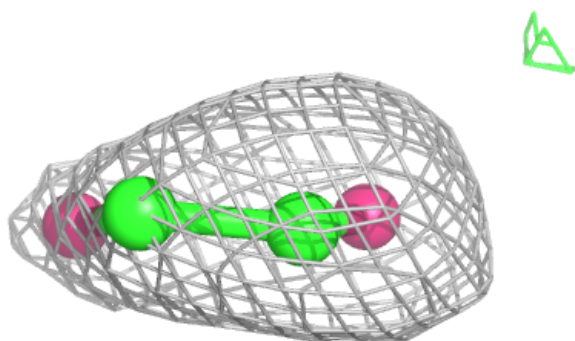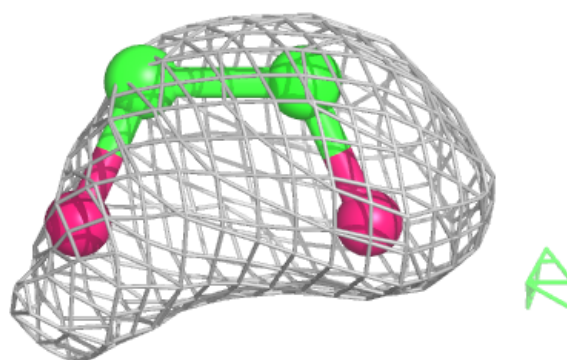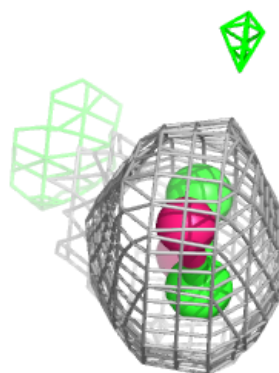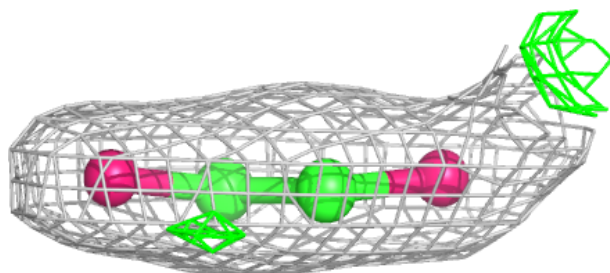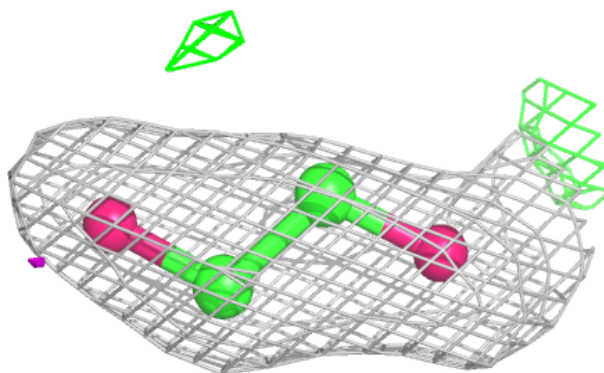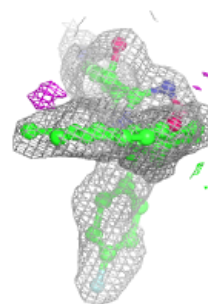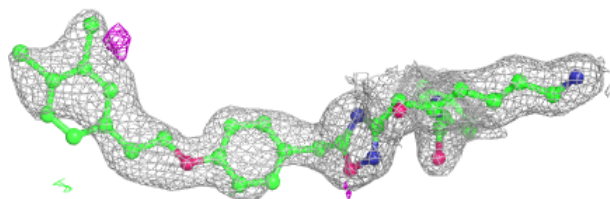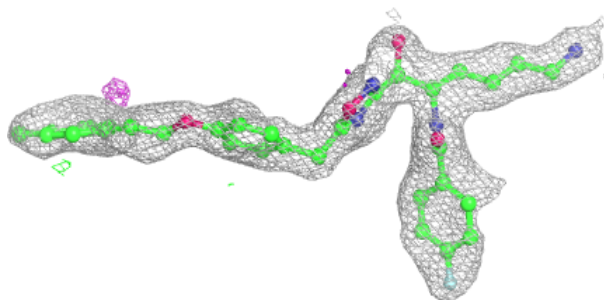mF_o-DF_c (at 3 rmsd) in purple (negative)
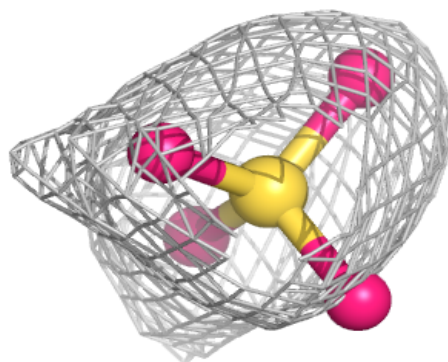and green (positive)
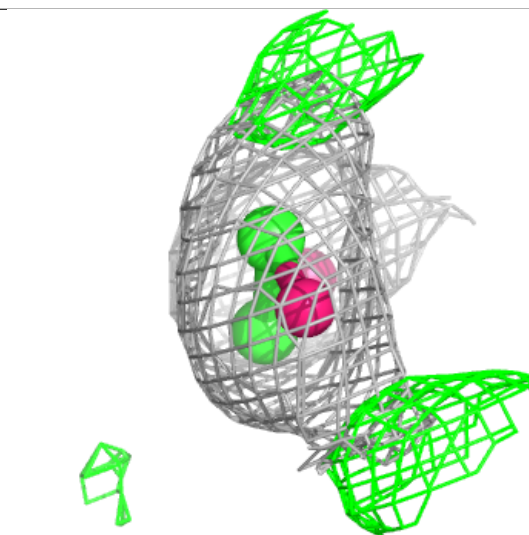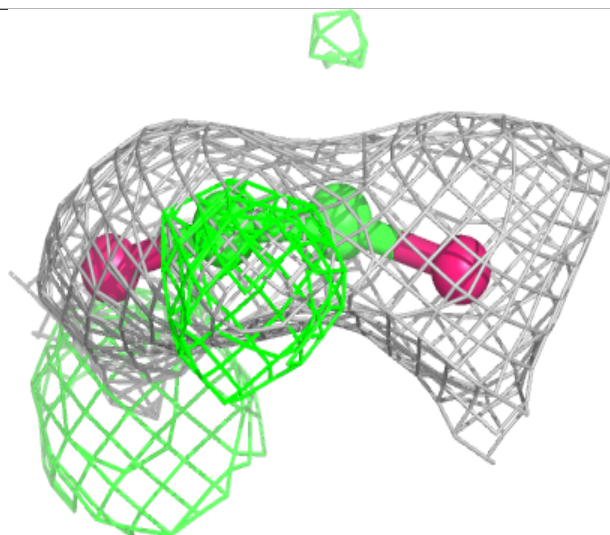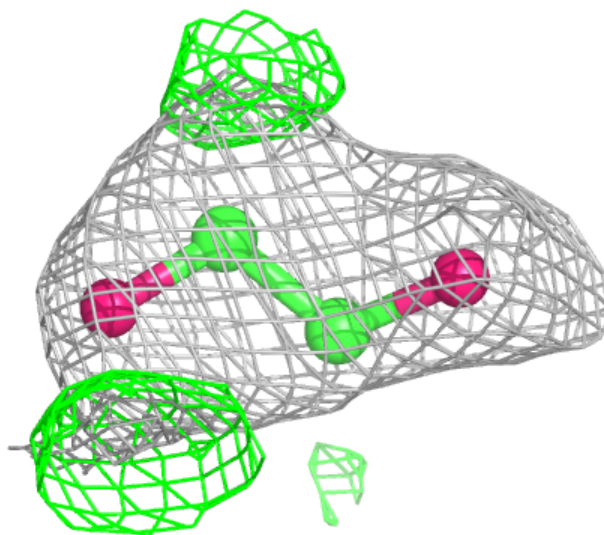
Electron density around SO4 D 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
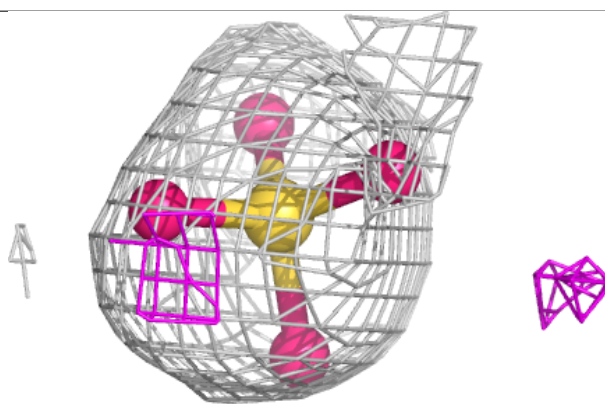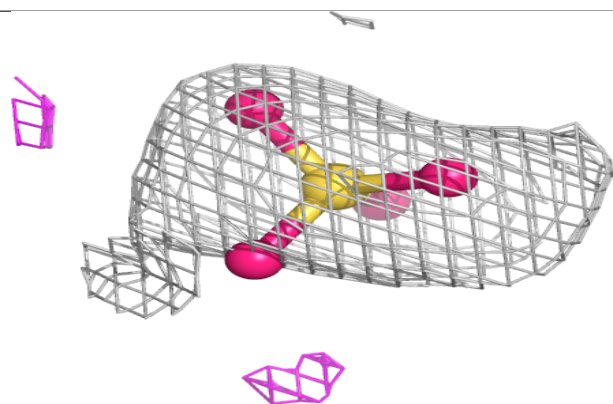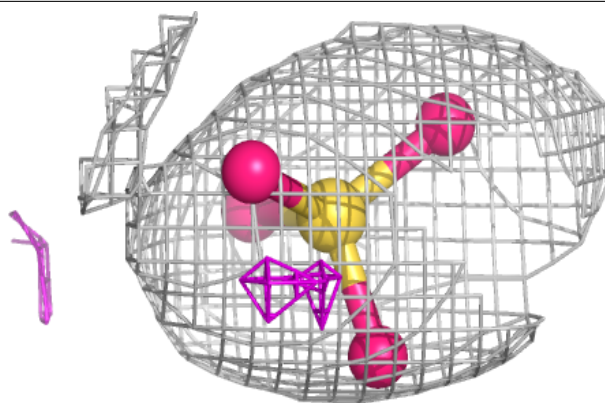
Electron density around SO4 A 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
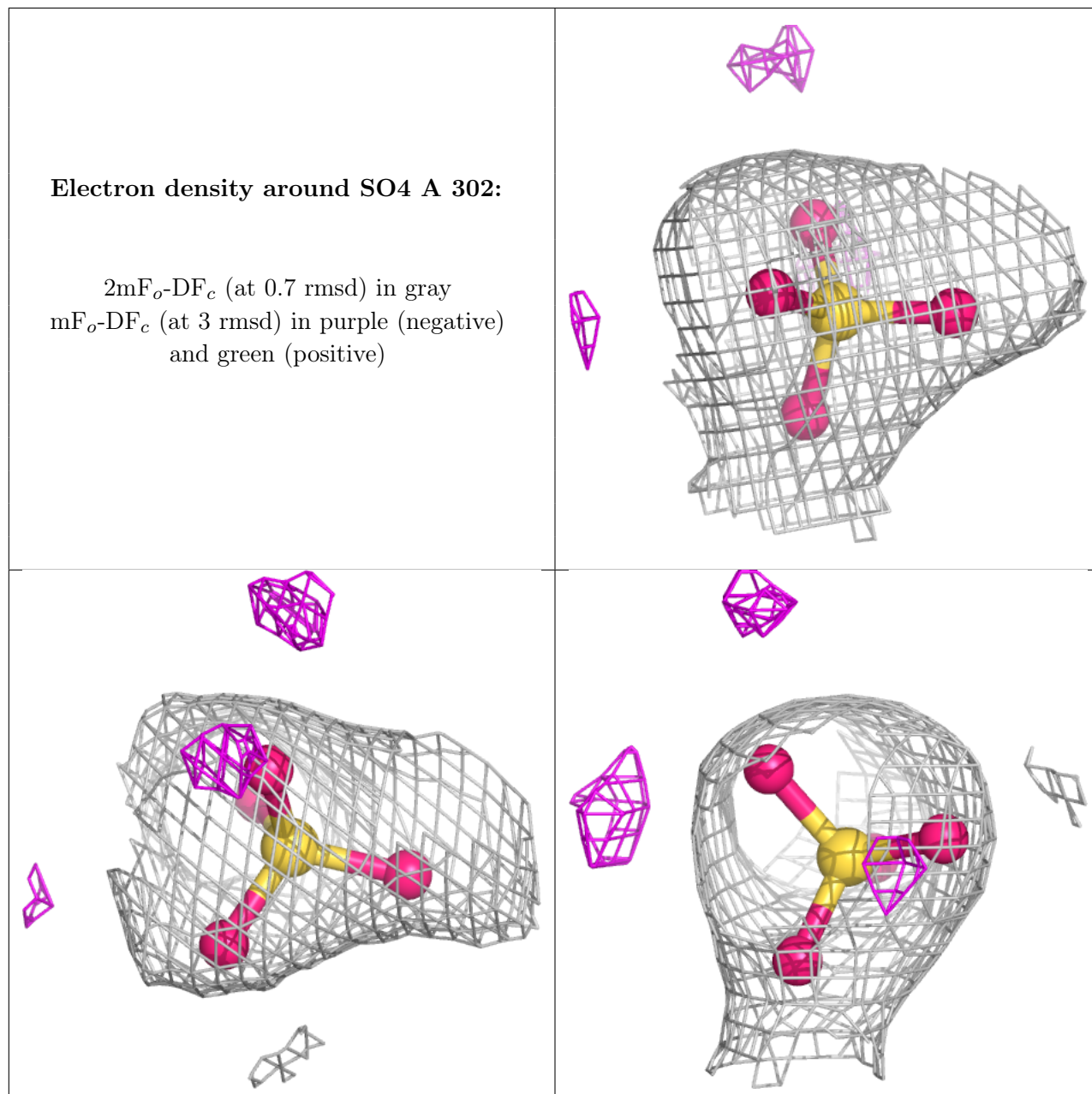
Electron density around EDO B 306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
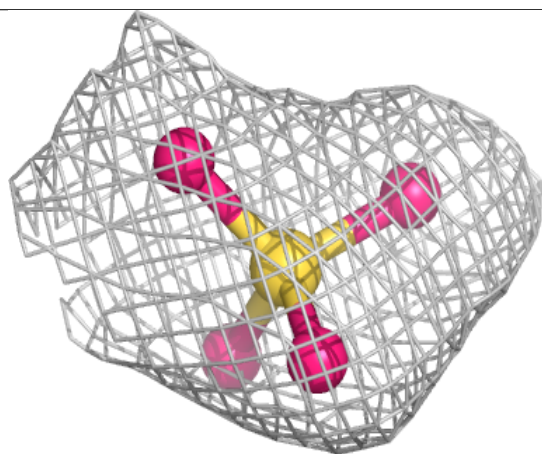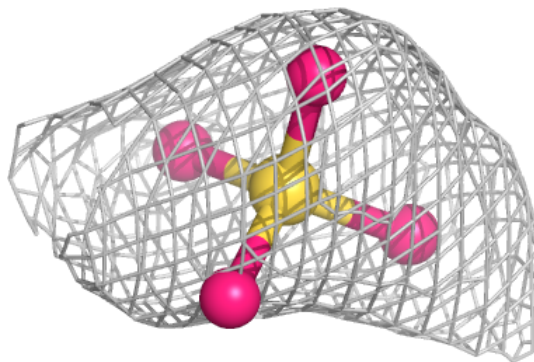$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
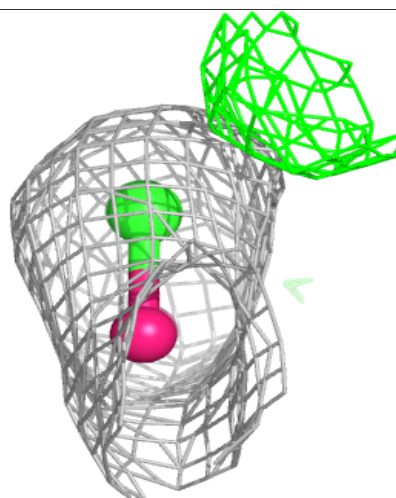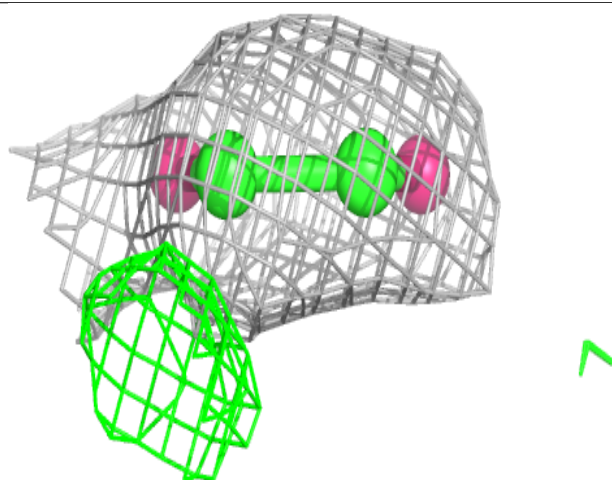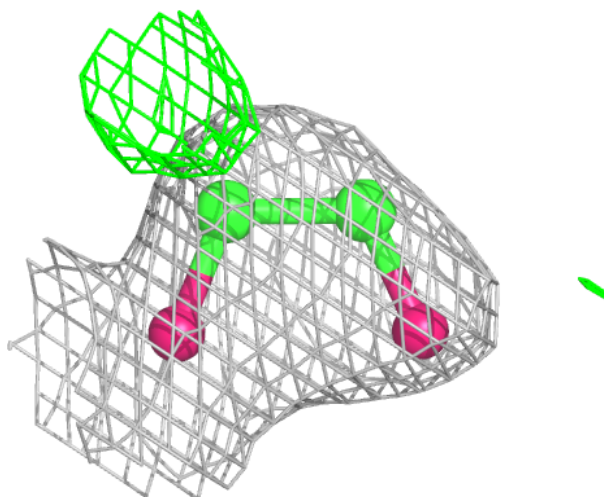
Electron density around EDO C 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
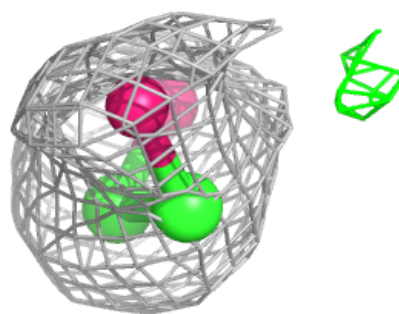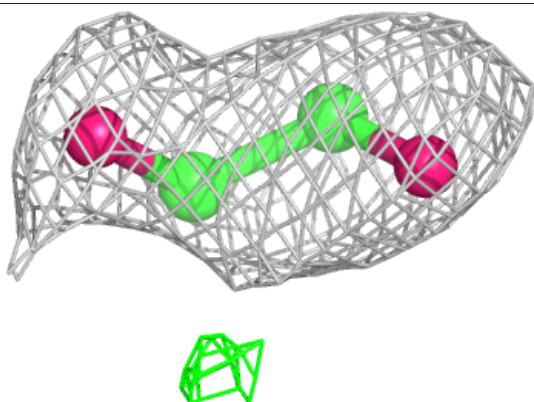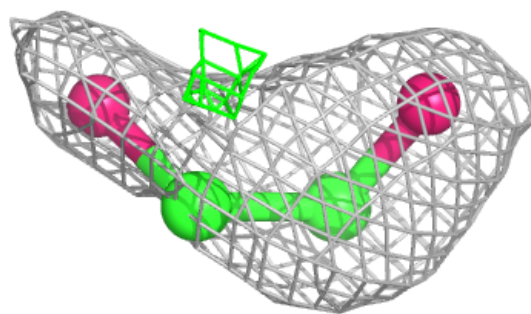
Electron density around EDO C 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
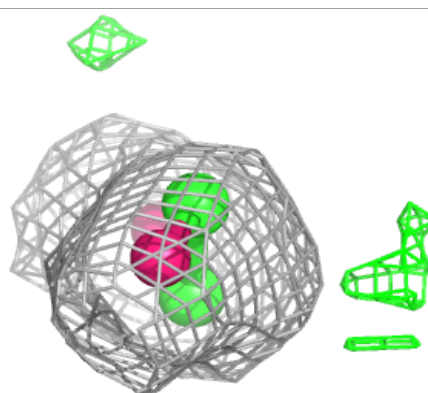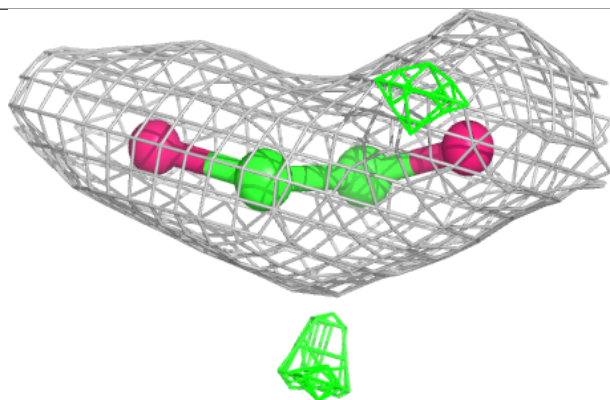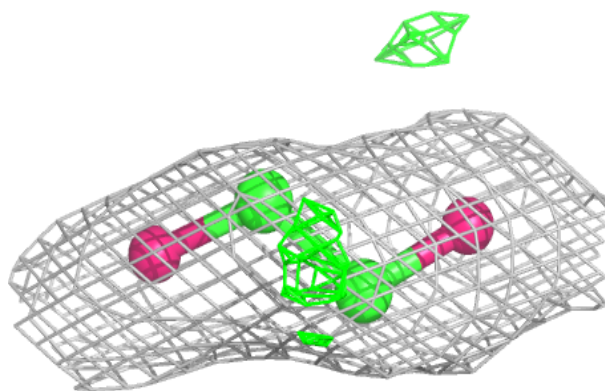and green (positive)
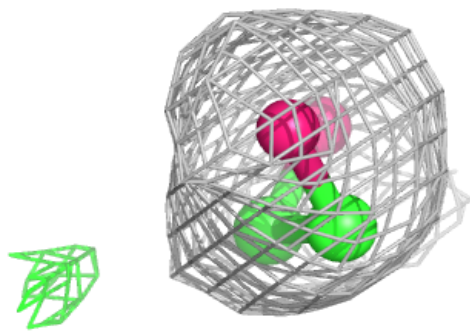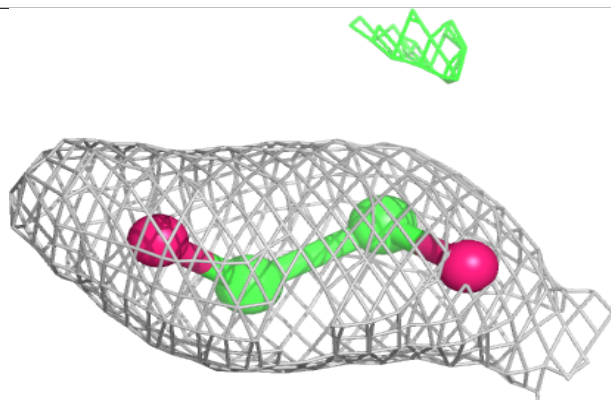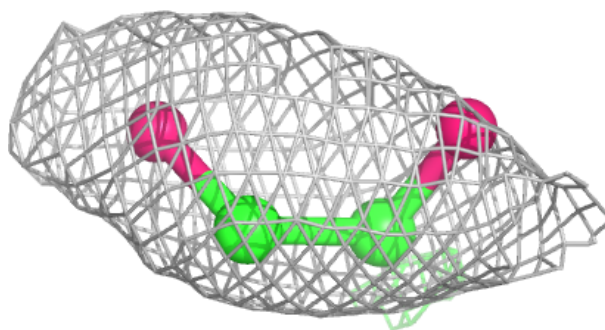
Electron density around SO4 A 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
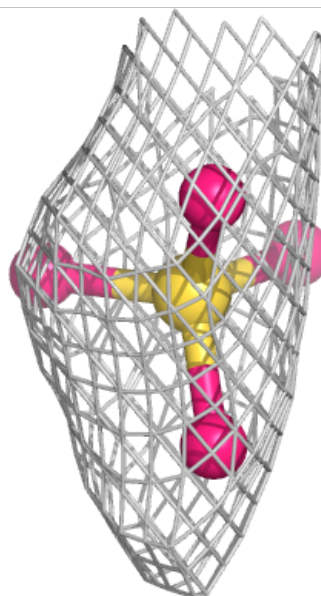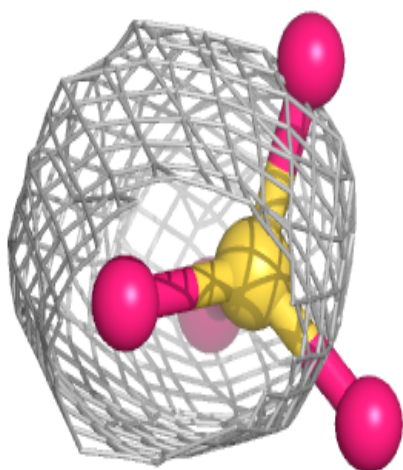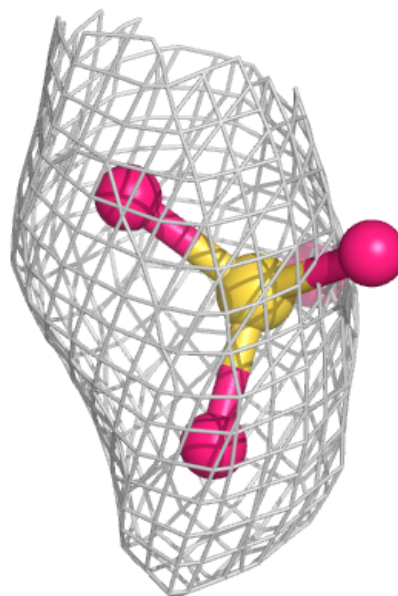
Electron density around ACT B 304:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
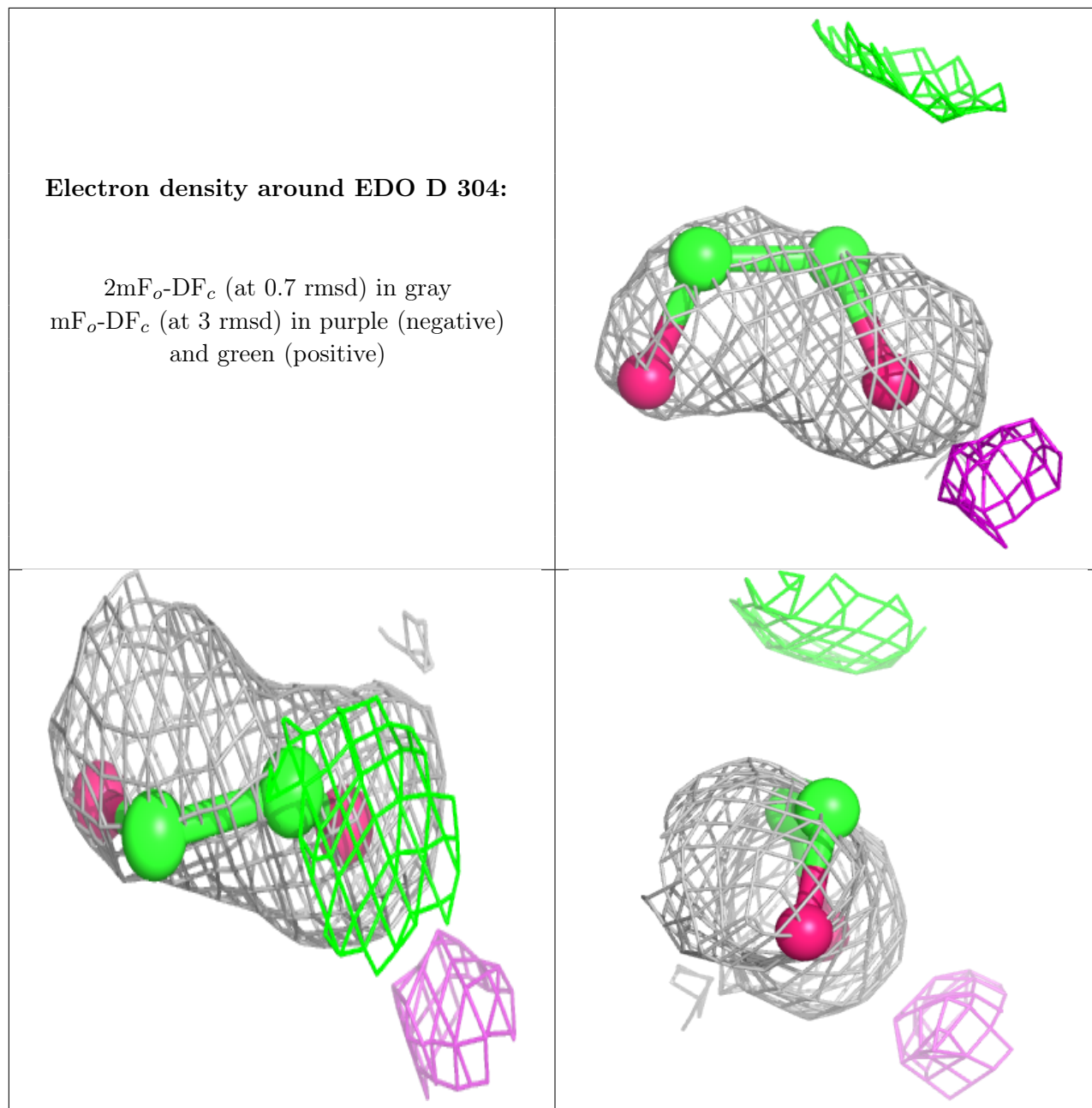and green (positive)
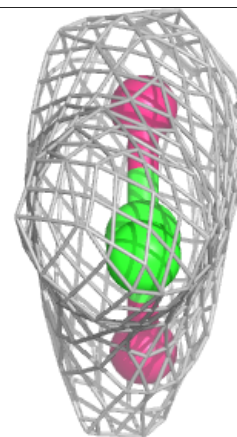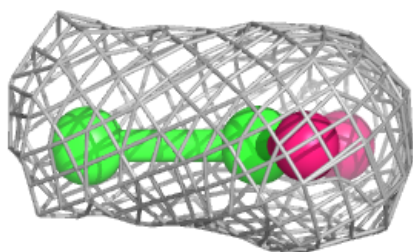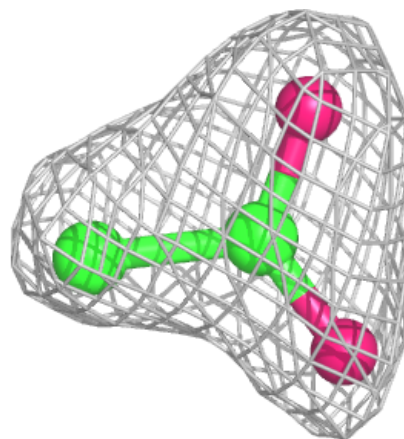
Electron density around ACT C 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
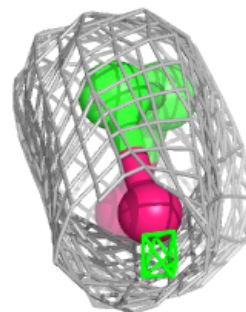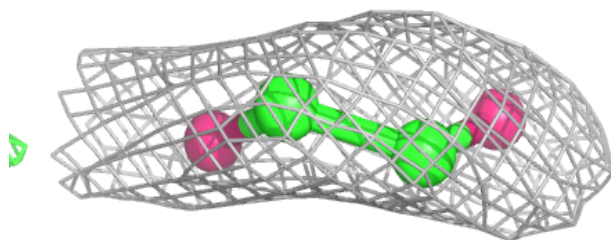and green (positive)
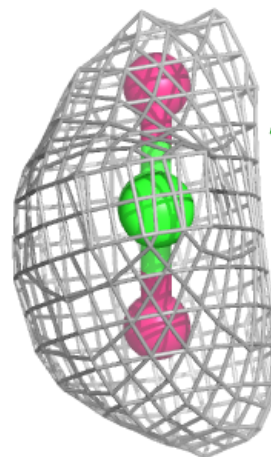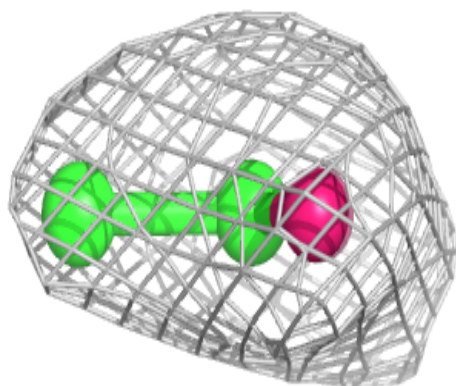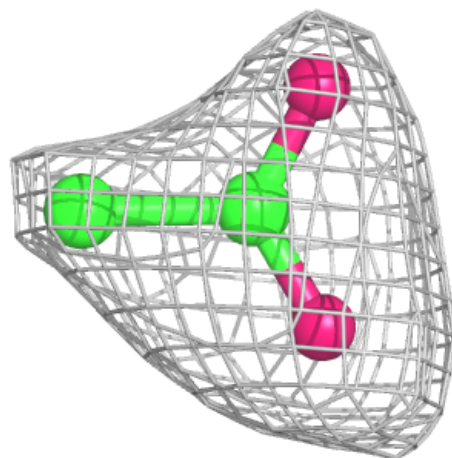
Electron density around SO4 B 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
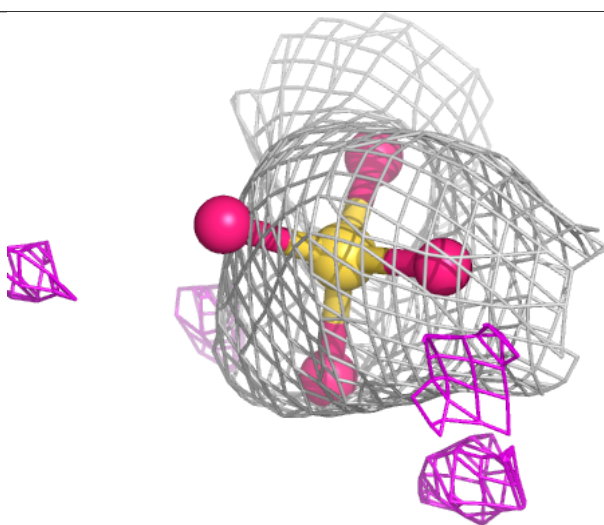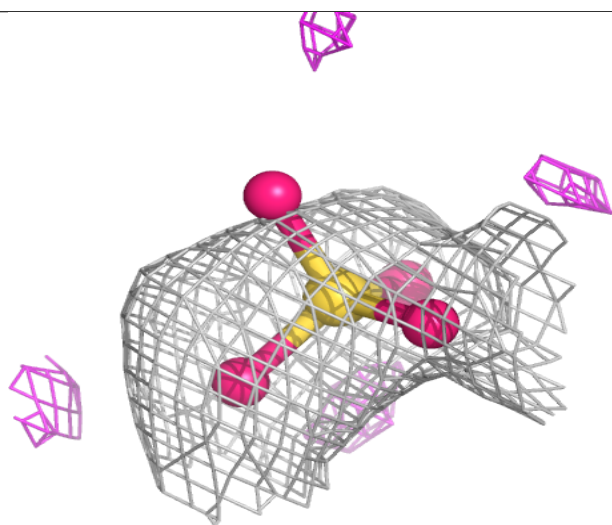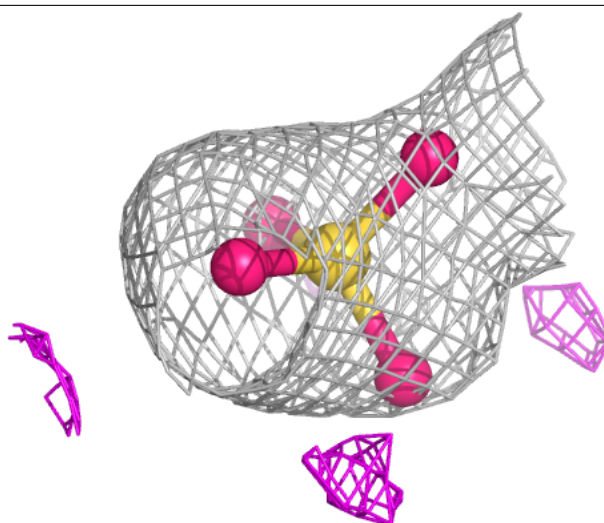
Electron density around SO4 C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
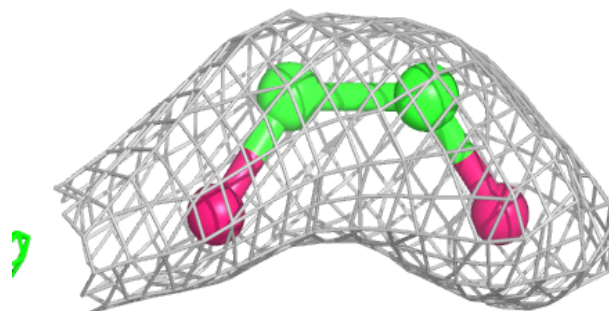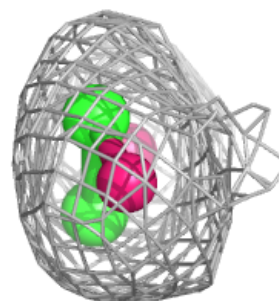and green (positive)
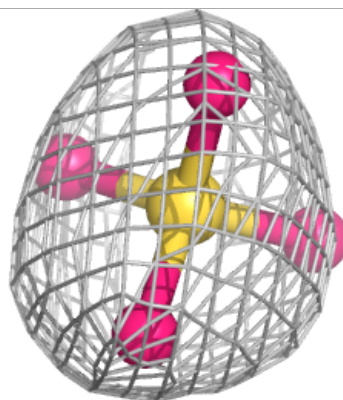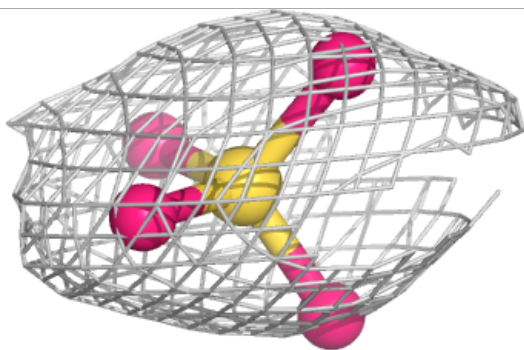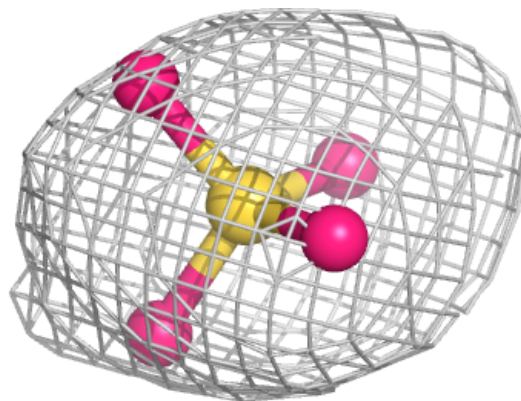
Electron density around SO4 C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
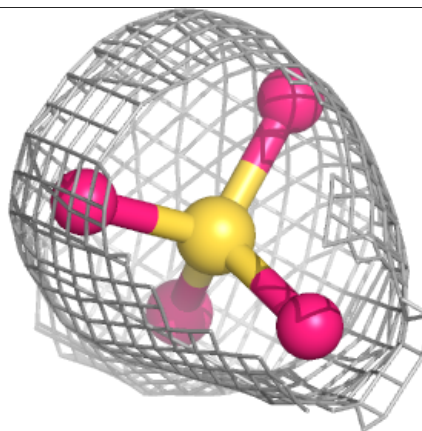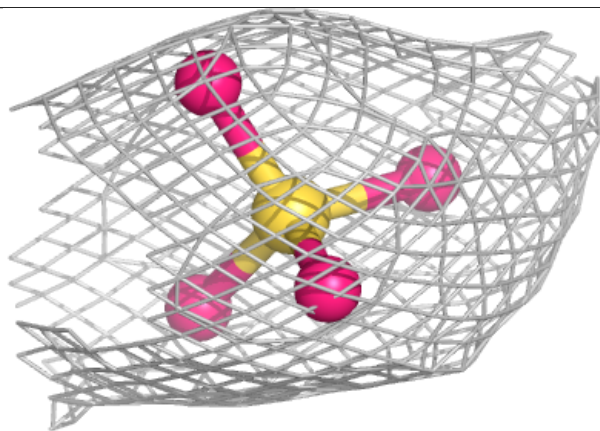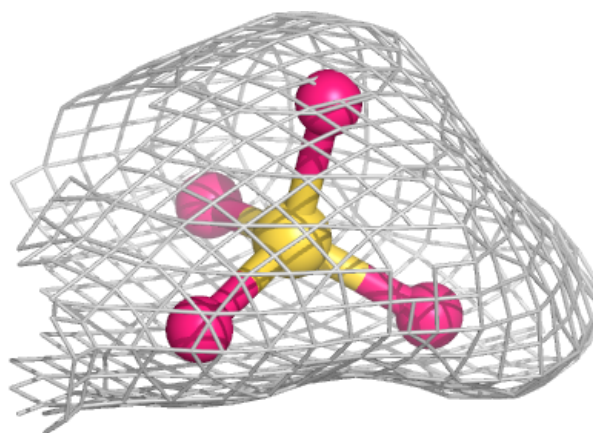
Electron density around SO4 C 304:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
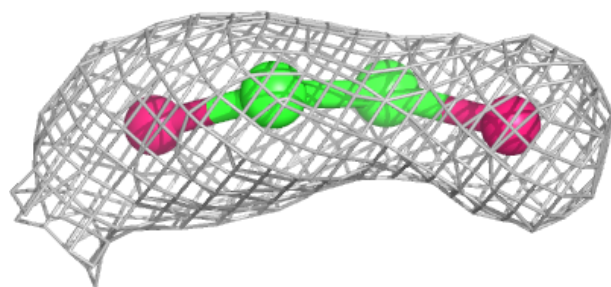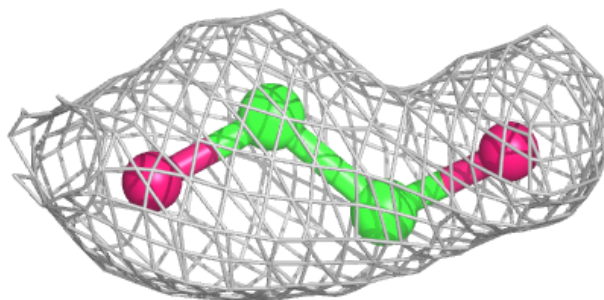and green (positive)
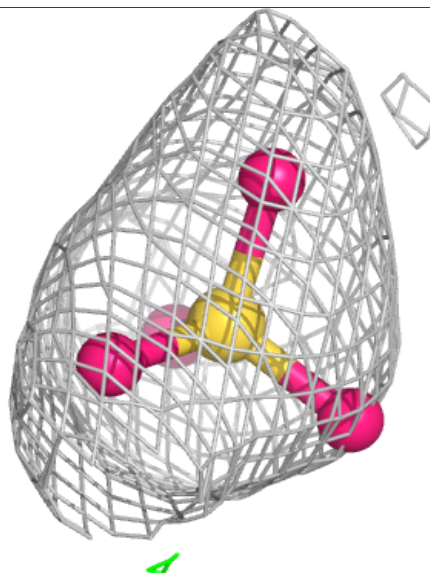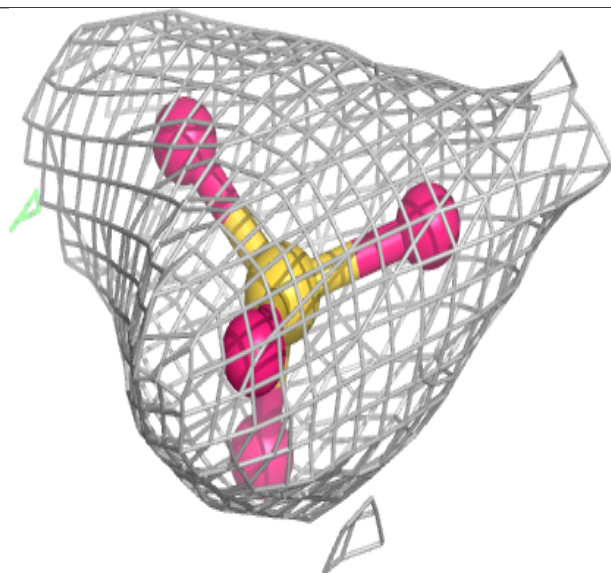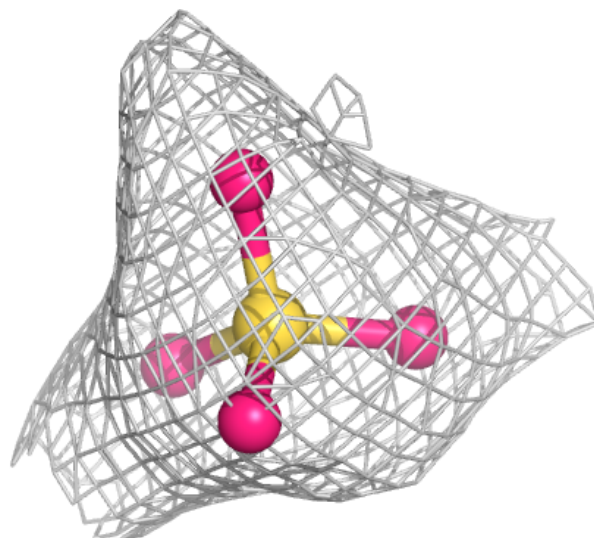
Electron density around SO4 C 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
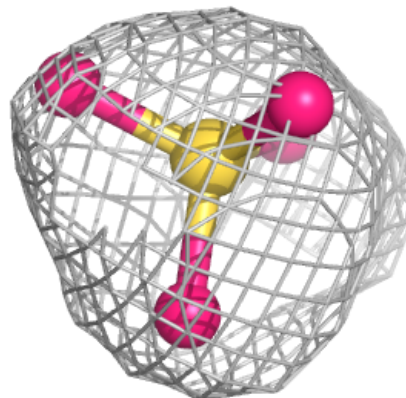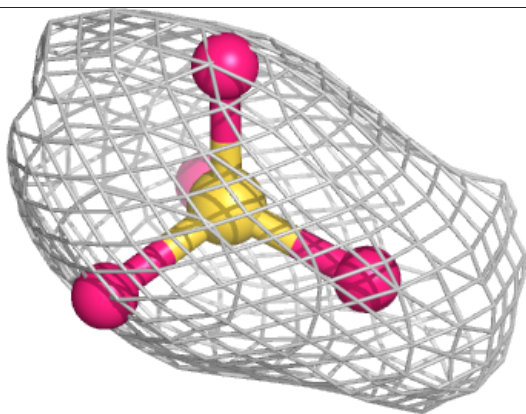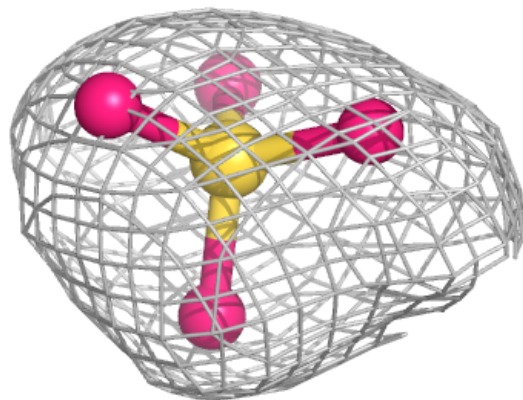
Electron density around SO4 C 308:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
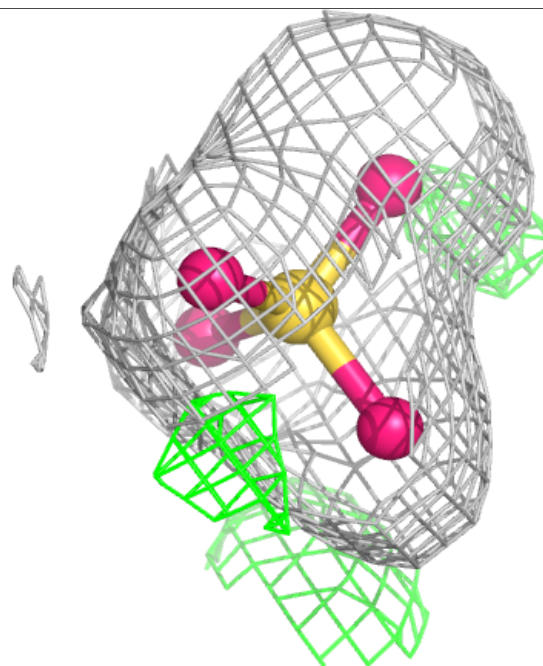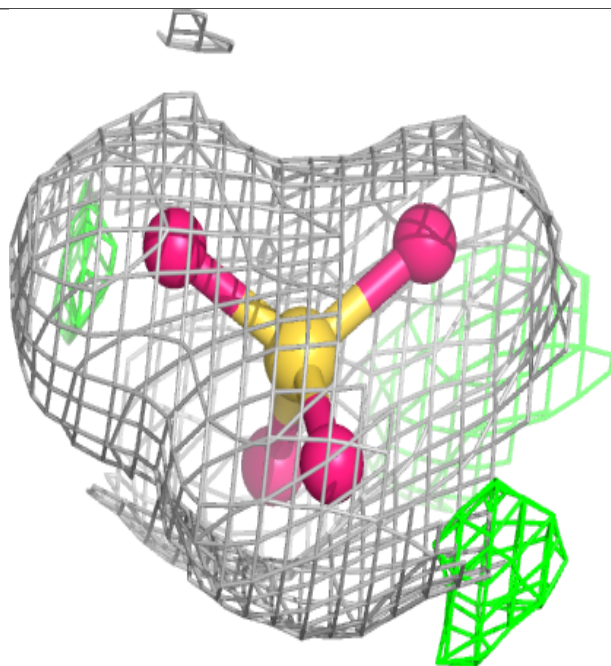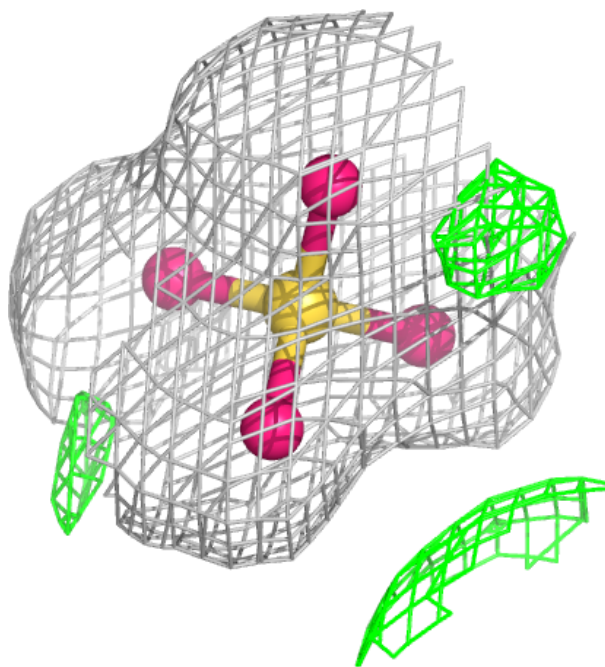
Electron density around A1I52 C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
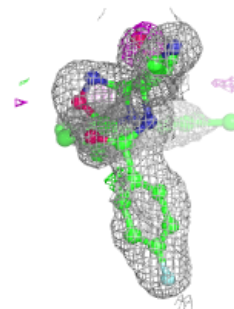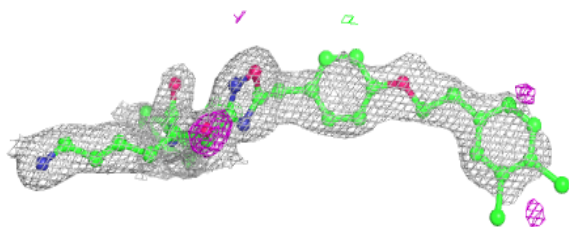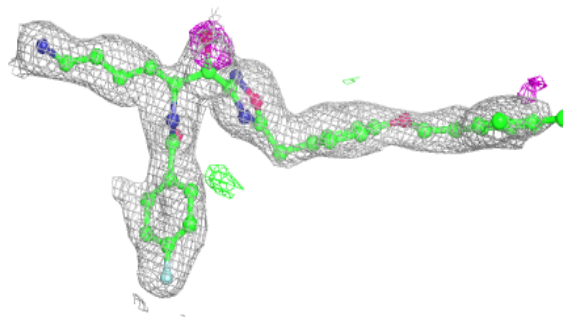and green (positive)
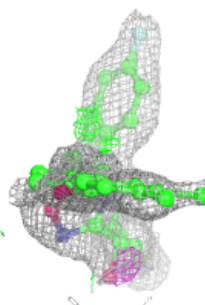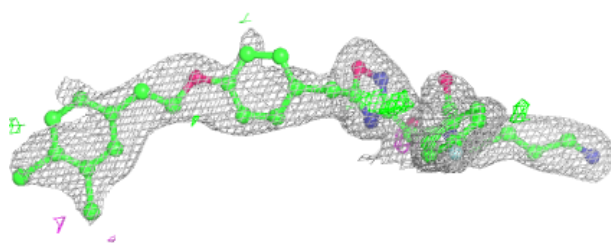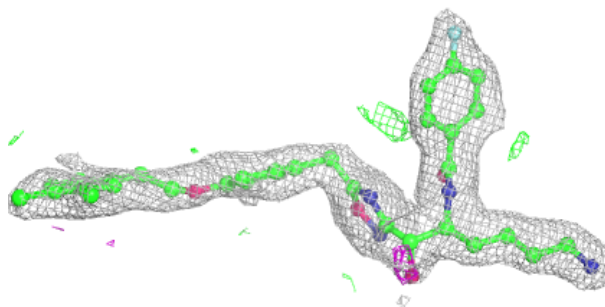
Electron density around SO4 D 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
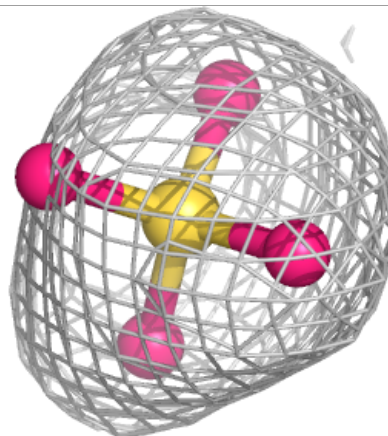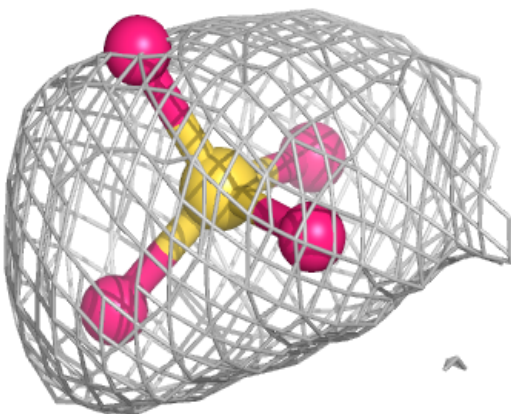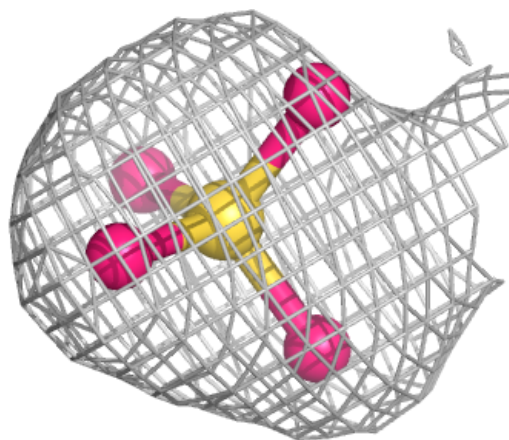and green (positive)
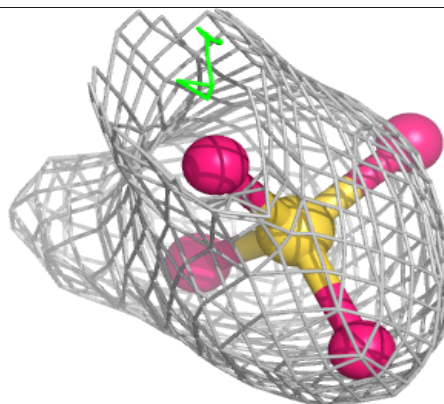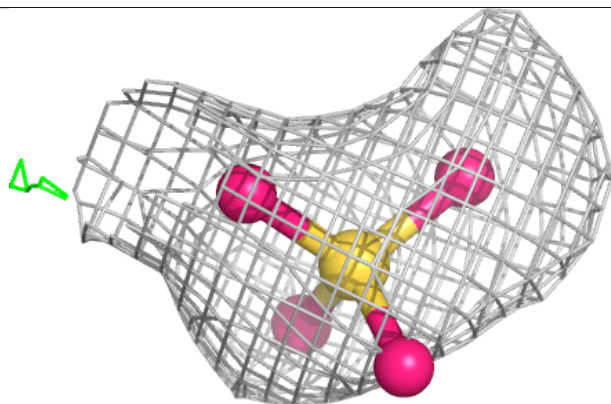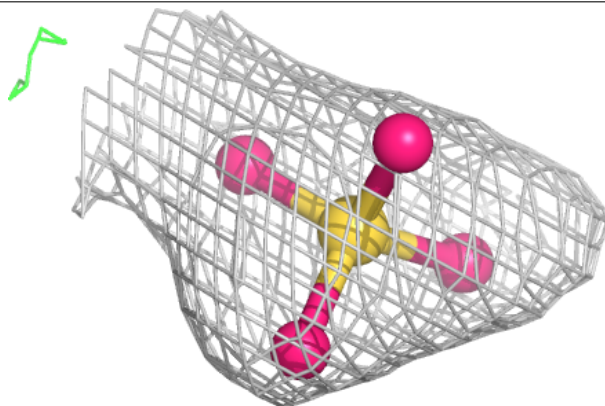
Electron density around A1I52 D 301 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
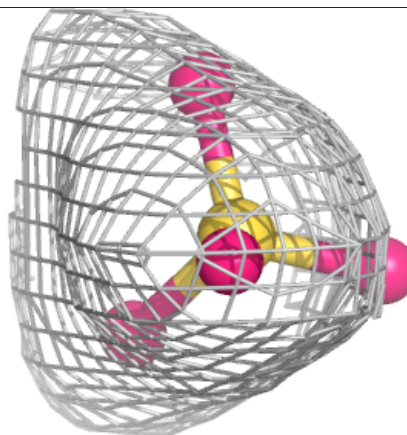and green (positive)
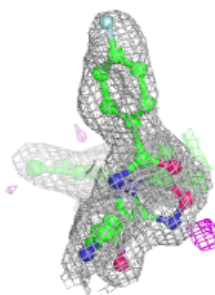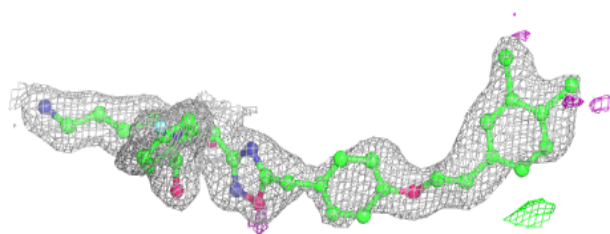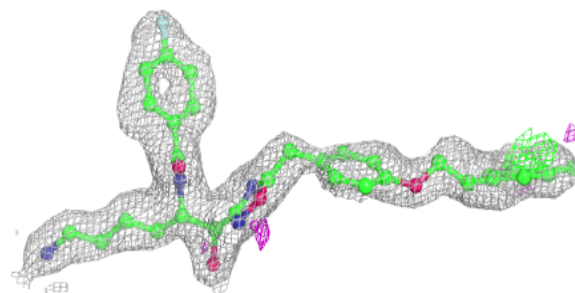
Electron density around PEG A 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
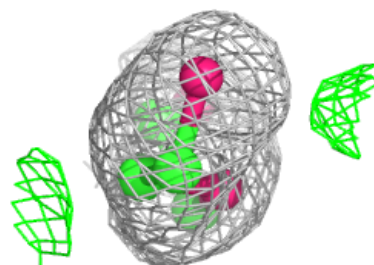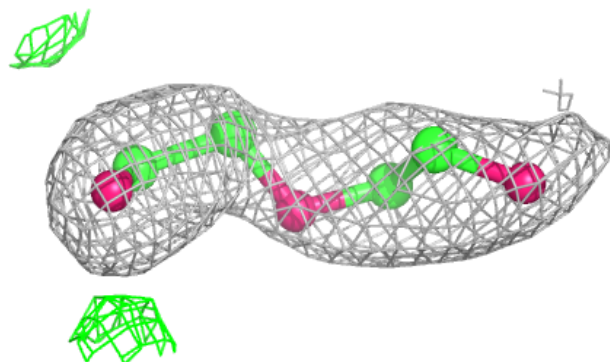
Electron density around PEG D 308:

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

Electron density around EDO A 307:

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

Electron density around EDO A 308:

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

Electron density around A1I52 D 301 (B):

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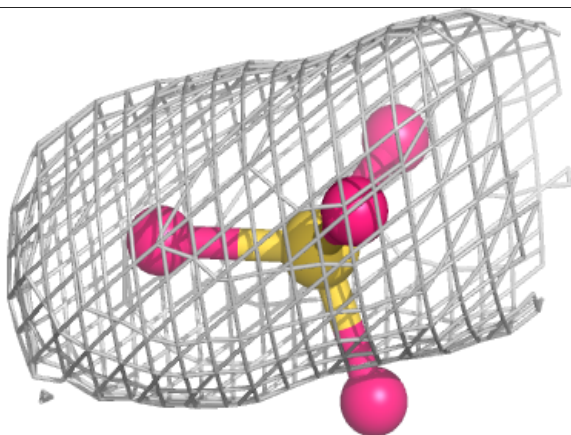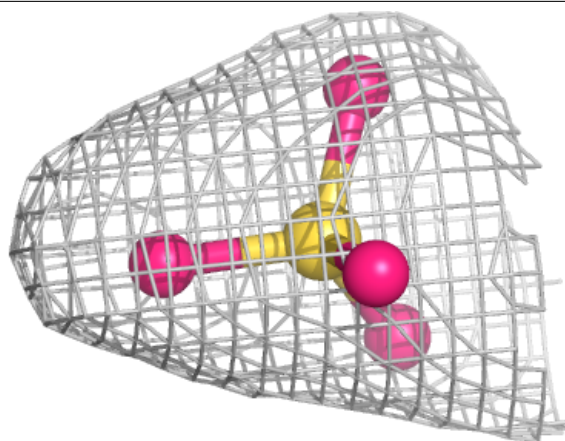mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO B 308:

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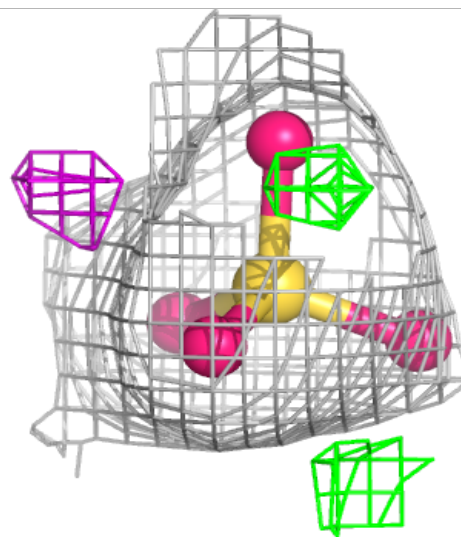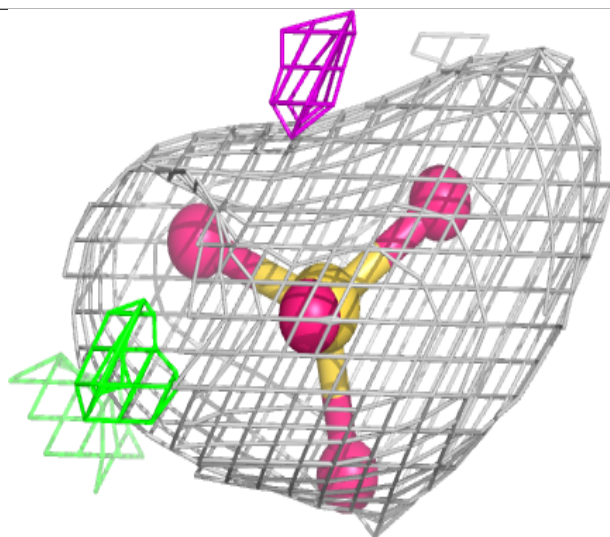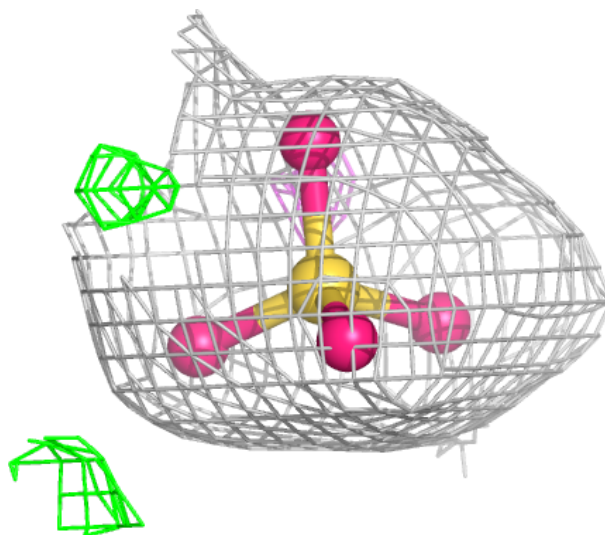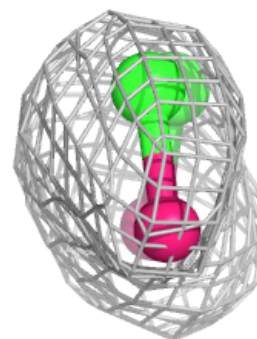mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around EDO B 309:

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

Electron density around A1I52 A 301:

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

Electron density around SO4 A 303:

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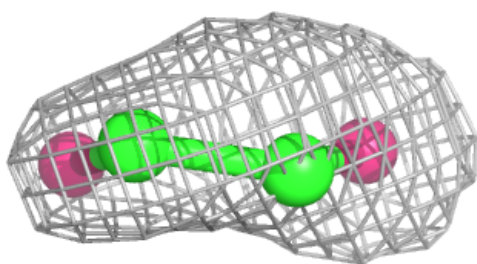and green (positive)

Electron density around EDO C 311:

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

Electron density around EDO D 304:

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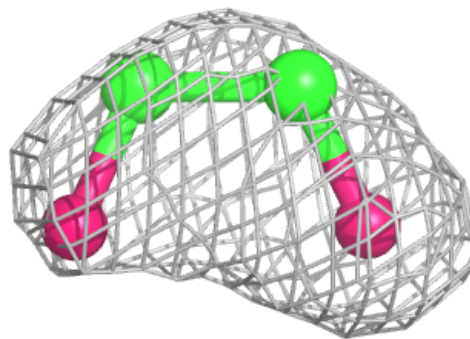$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
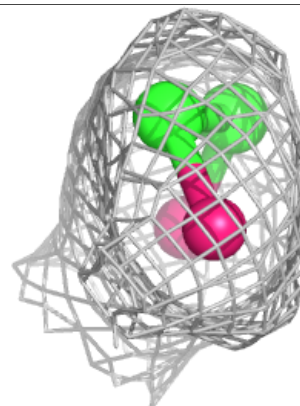and green (positive)

Electron density around EDO D 307:

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

Electron density around EDO D 309:

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

Electron density around A1I52 B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
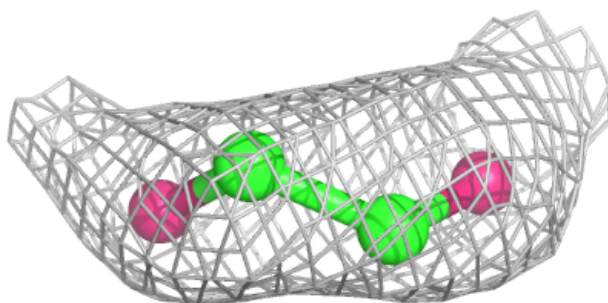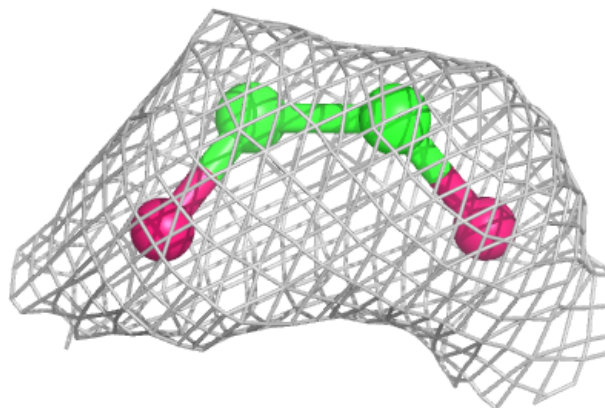mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
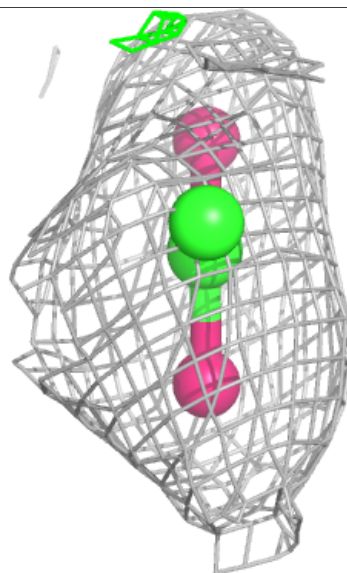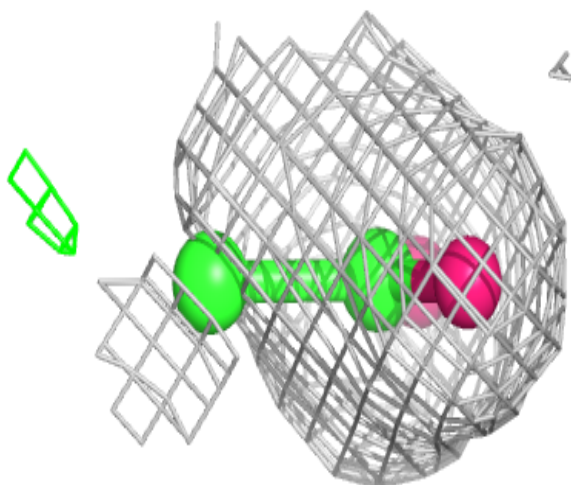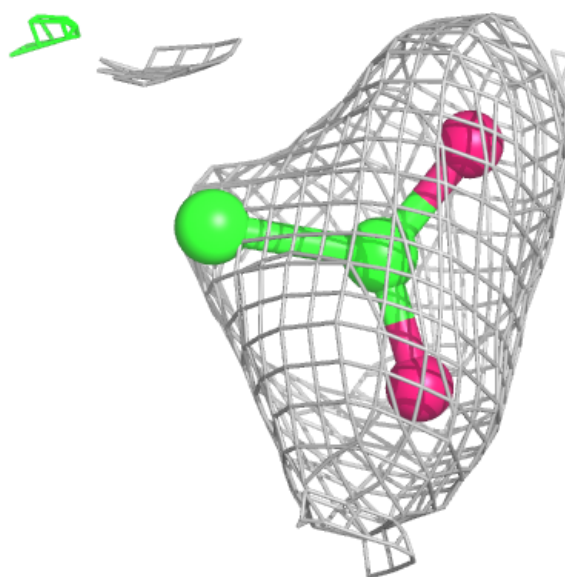and green (positive)

Electron density around SO4 B 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 B 303:

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

Electron density around SO4 D 306:

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

Electron density around EDO C 310:

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 A 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
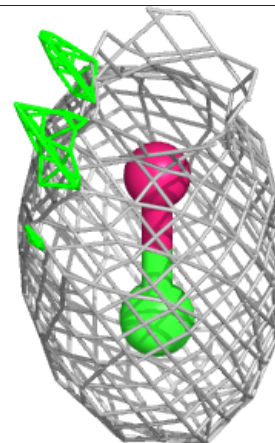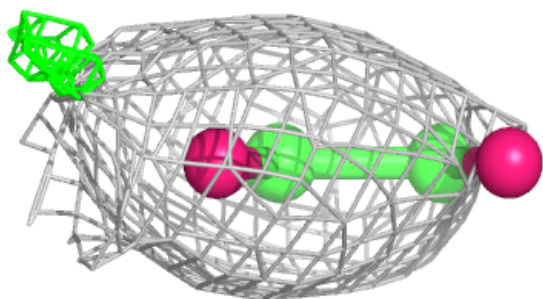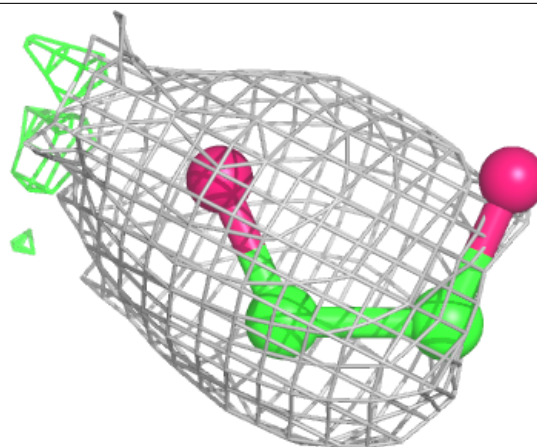mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ACT A 310:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
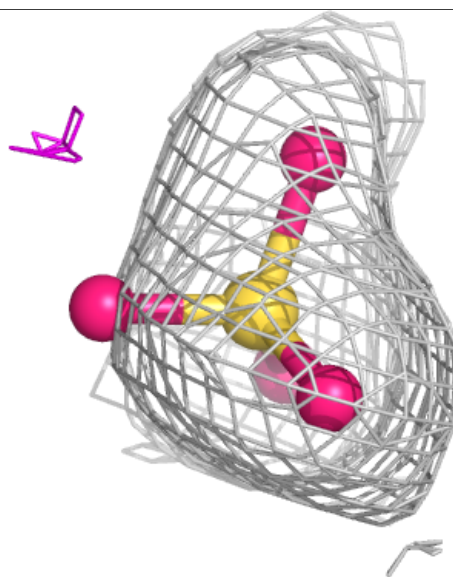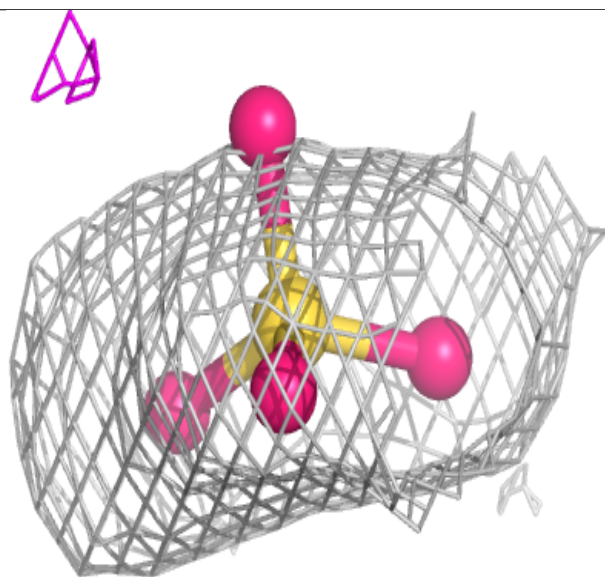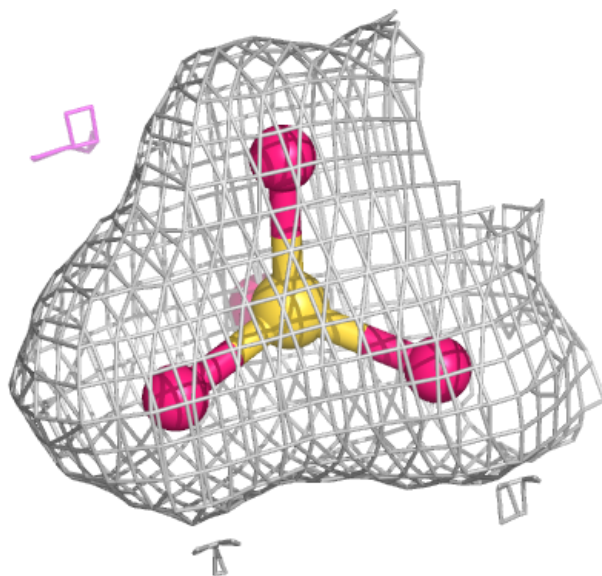and green (positive)
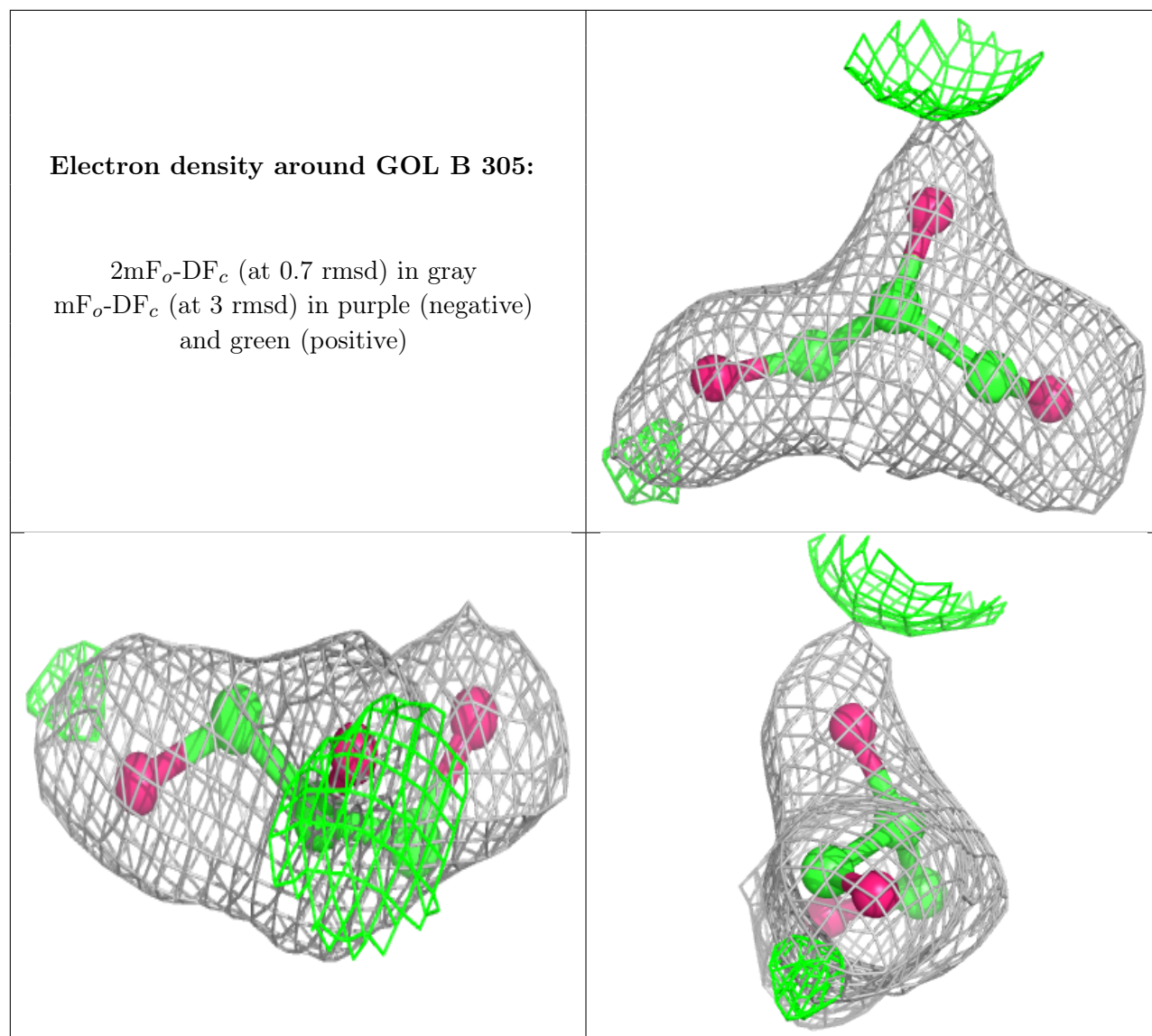
Electron density around EDO C 312:

$2mF_o$-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 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GOL B 305:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.