wwPDB X-ray Structure Validation Summary Report (i)

Nov 8, 2022 – 05:47 pm GMT

PDB ID	:	7PX0
Title	:	Drosophila melanogaster Aldehyde Oxidase 1
Authors	:	Vilela-Alves, G.; Mota, C.; Romao, M.J.
Deposited on	:	2021-10-07
Resolution	:	2.20 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:

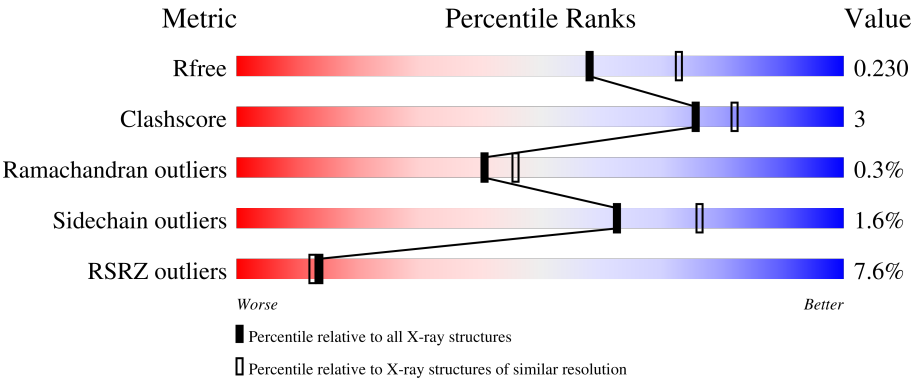
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	1273	3% 90% 7%
1	B	1273	7% 90% 8%
1	C	1273	5% 90% 8%
1	D	1273	15% 87% 9%

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	GOL	A	1310	-	-	X	-
7	PEG	A	1309	-	-	X	-

2 Entry composition (i)

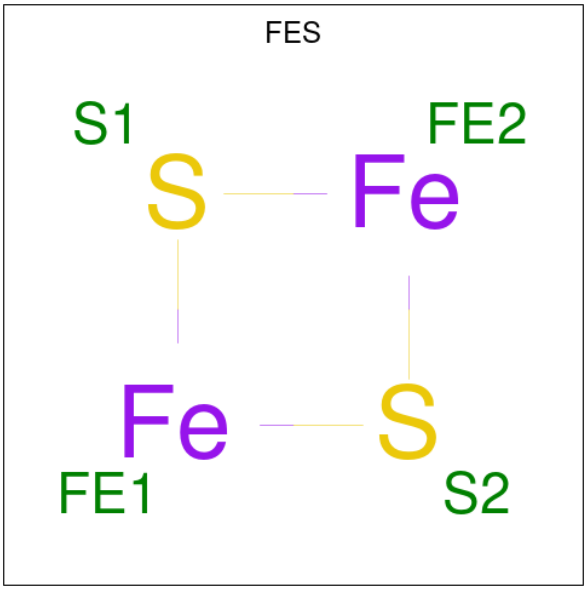
There are 9 unique types of molecules in this entry. The entry contains 41321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1249	Total	C	N	O	S	0	2	0
			9615	6082	1651	1823	59			
1	B	1253	Total	C	N	O	S	0	2	0
			9643	6097	1659	1829	58			
1	C	1252	Total	C	N	O	S	0	2	0
			9639	6096	1656	1830	57			
1	D	1236	Total	C	N	O	S	0	1	0
			9513	6019	1638	1800	56			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			4	2	2			
2	A	1	Total	Fe	S		0	0
			4	2	2			

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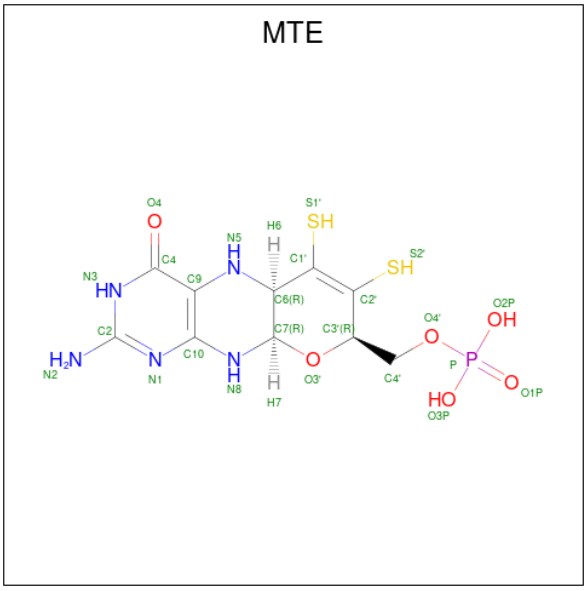
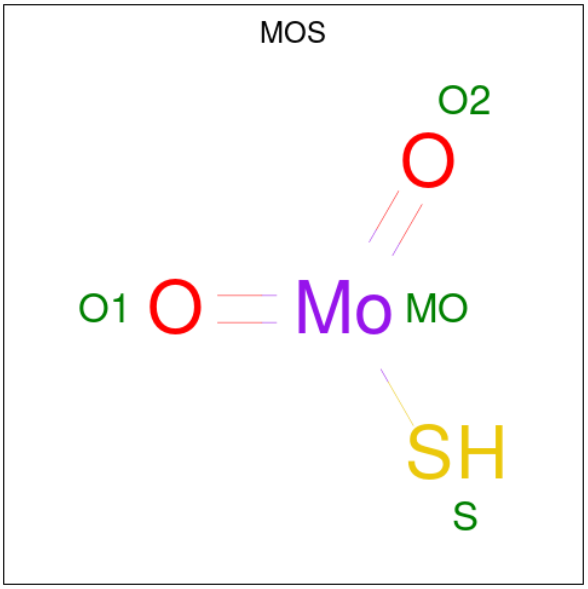
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	C	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0
2	D	1	Total Fe S 4 2 2	0	0

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A,9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL)ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$) (labeled as "Ligand of Interest" by depositor).



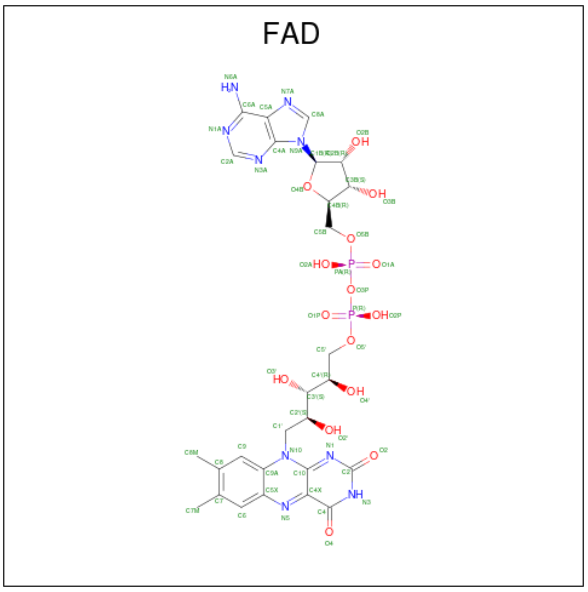
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 24 10 5 6 1 2	0	0
3	B	1	Total C N O P S 24 10 5 6 1 2	0	0
3	C	1	Total C N O P S 24 10 5 6 1 2	0	0
3	D	1	Total C N O P S 24 10 5 6 1 2	0	0

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$) (labeled as "Ligand of Interest" by depositor).



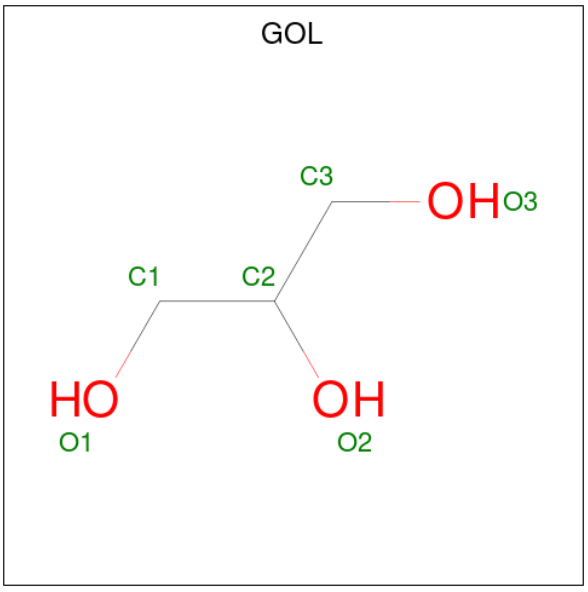
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	D	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



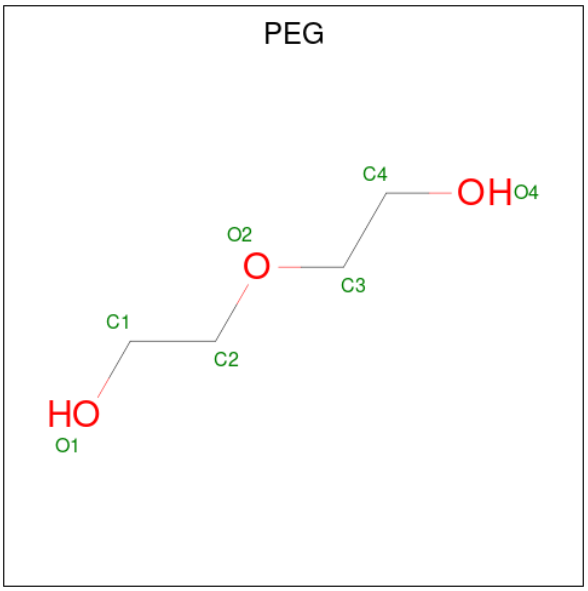
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



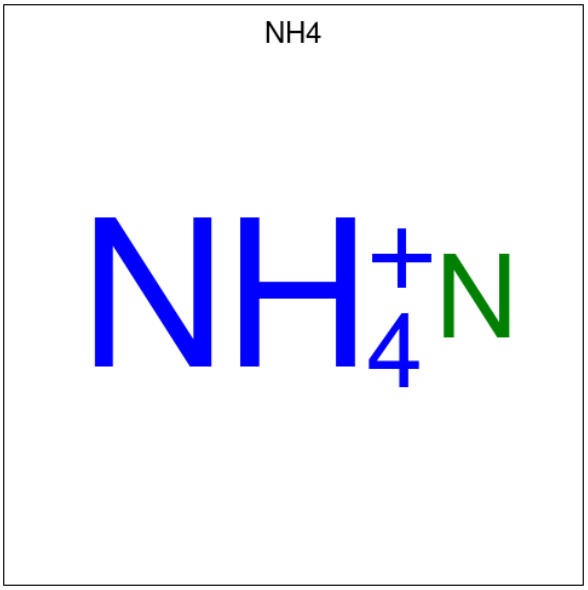
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total N 1 1	0	0

- Molecule 9 is water.

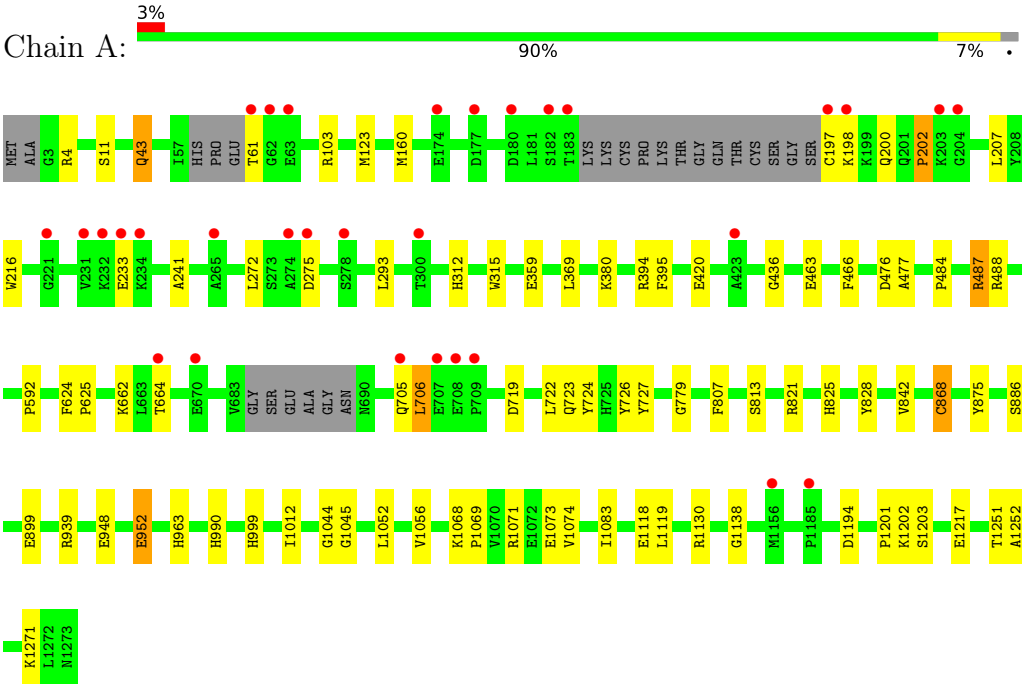
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	776	Total O 776 776	0	0
9	B	619	Total O 619 619	0	0
9	C	607	Total O 607 607	0	0
9	D	461	Total O 461 461	0	0

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.

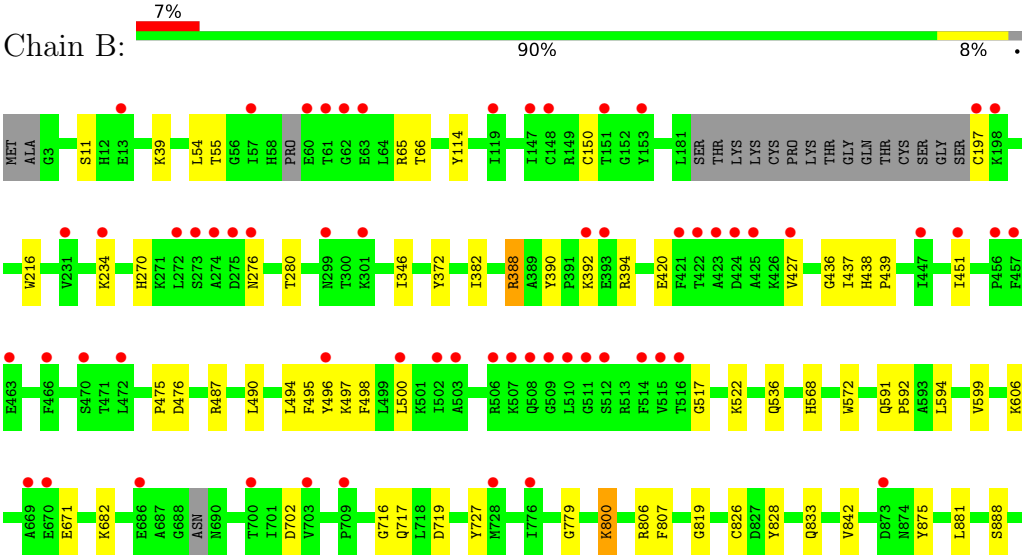
• Molecule 1: Aldehyde oxidase 1

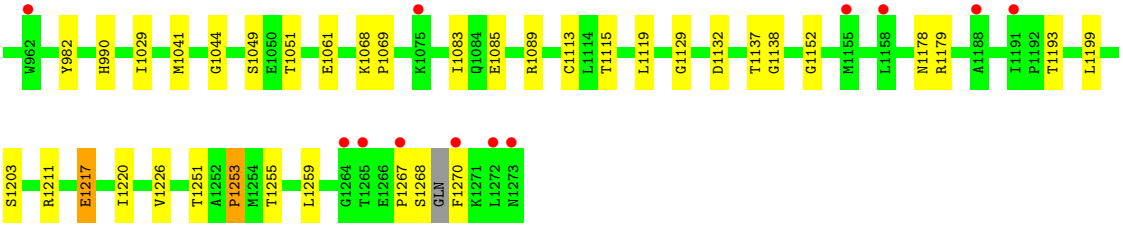
Chain A:



• Molecule 1: Aldehyde oxidase 1

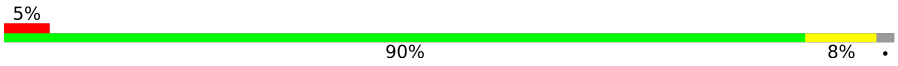
Chain B:

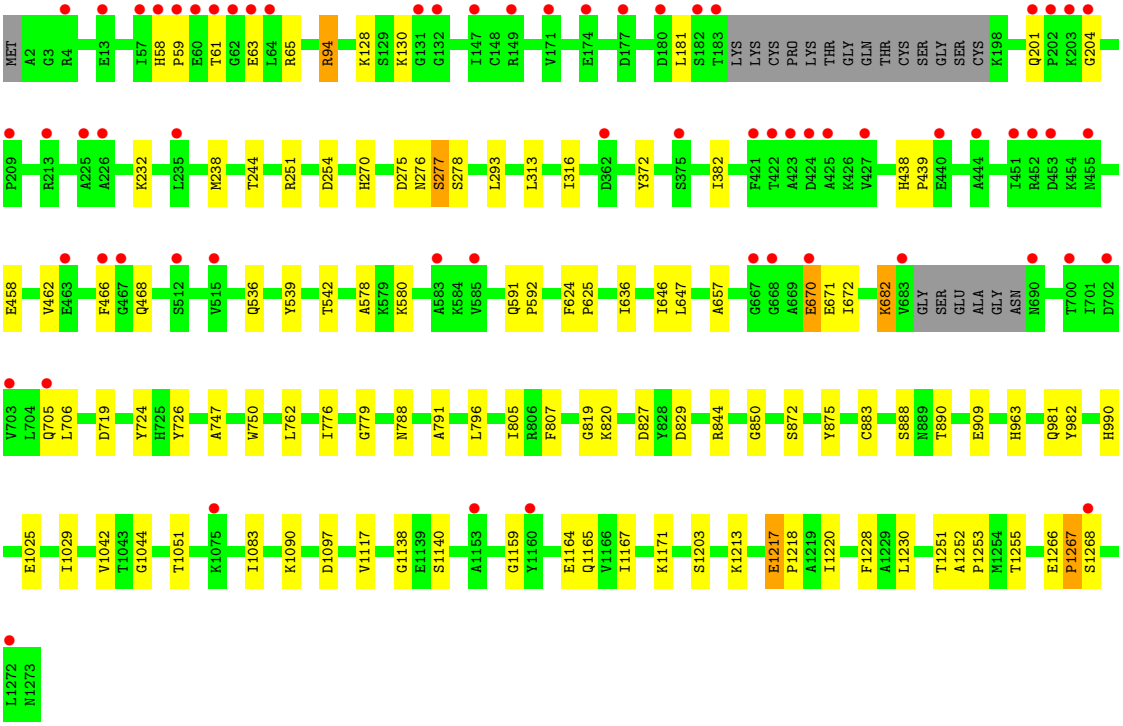




• Molecule 1: Aldehyde oxidase 1

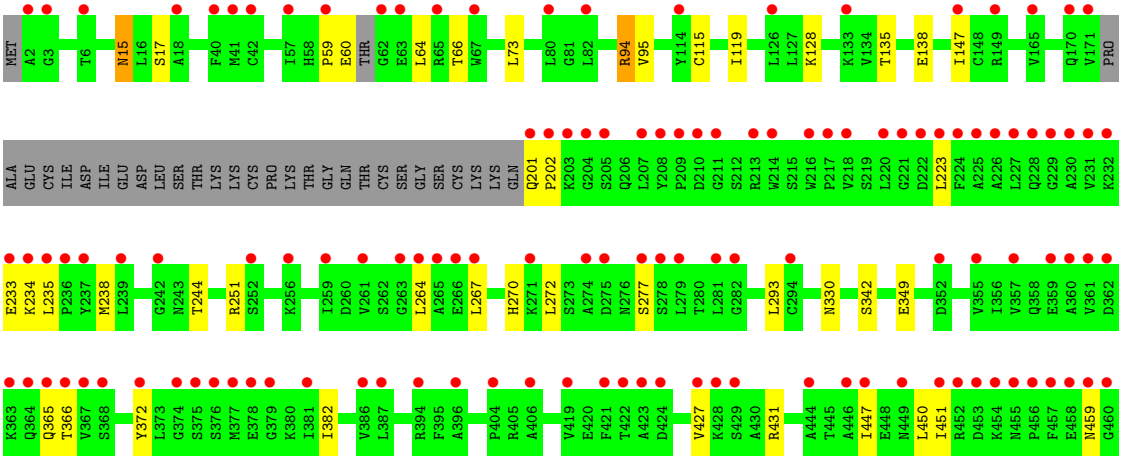
Chain C:

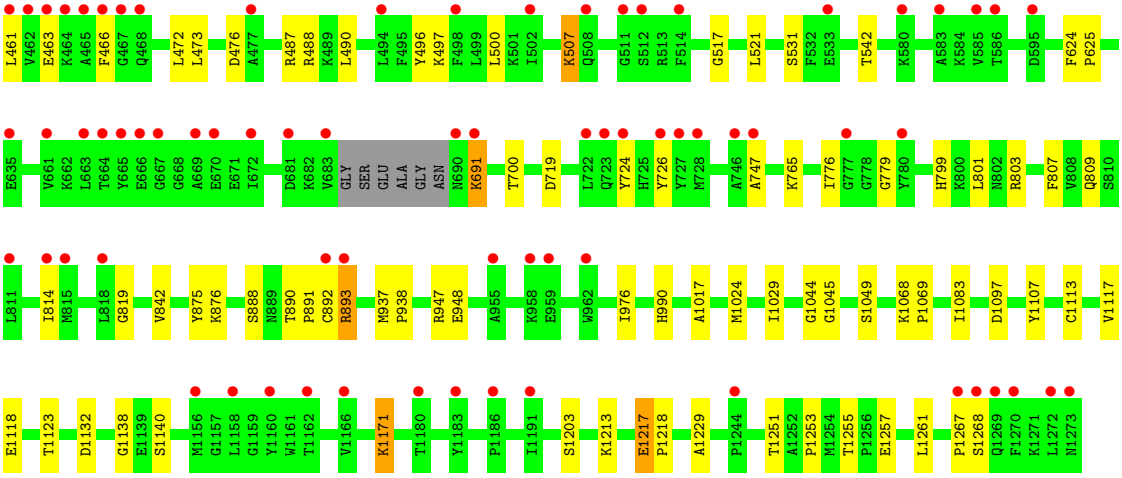




• Molecule 1: Aldehyde oxidase 1

Chain D:




L461 V462 E463 K464 A465 F466 G467 Q468 L472 L473 D476 A477 R487 R488 K489 L490 L494 F495 Y496 K497 F498 L499 L500 K501 I502 K507 Q508 G511 S512 R513 F514 G517 L521 S531 F532 E533 T542 K580 A583 K584 V585 T586 D595 F624 P625
E635 V661 K662 L663 T664 Y665 E666 G667 G668 A669 E670 E671 I672 D681 K682 V683 GLY SER GLU ALA GLY ASN N690 K691 T700 D719 L722 Q723 Y724 H725 Y726 Y727 M728 A746 A747 K765 I776 G777 G778 G779 Y780 H799 K800 L801 N802 R803 F807 V808 Q809 S810
L811 I814 M815 L818 G819 V842 Y875 K876 S888 N889 T890 P891 C892 R893 M937 P938 R947 E948 A955 K958 E959 W962 I976 H990 A1017 M1024 I1029 G1044 G1045 S1049 K1068 P1069 I1083 D1097 Y1107 C1113 V1117
E1118 T1123 D1132 G1138 E1139 S1140 M1156 G1157 L1158 G1159 Y1160 W1161 T1162 V1166 K1171 T1180 Y1183 P1186 I1191 S1203 K1213 E1217 P1218 A1229 P1244 T1251 A1252 P1253 M1254 T1255 P1256 E1257 L1261 P1267 S1268 Q1269 F1270 K1271 L1272 N1273

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.66Å 127.91Å 152.55Å 90.00° 110.63° 90.00°	Depositor
Resolution (Å)	48.66 – 2.20 48.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.66-2.20) 97.8 (48.66-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.175 , 0.220 0.184 , 0.230	Depositor DCC
R_{free} test set	12900 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41321	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: FES, GOL, FAD, PEG, MTE, NH4, MOS

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	0.69	0/9816	0.84	3/13297 (0.0%)
1	B	0.68	0/9844	0.81	0/13333
1	C	0.69	0/9842	0.82	1/13335 (0.0%)
1	D	0.68	0/9711	0.80	0/13156
All	All	0.68	0/39213	0.82	4/53121 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	487	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	59	PRO	N-CA-CB	5.96	110.45	103.30
1	A	868	CYS	CB-CA-C	-5.93	98.53	110.40
1	A	103	ARG	NE-CZ-NH1	5.46	123.03	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	9615	0	9569	62	0
1	B	9643	0	9587	56	0
1	C	9639	0	9581	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	9513	0	9463	69	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	24	0	10	2	0
3	B	24	0	10	2	0
3	C	24	0	10	1	0
3	D	24	0	10	3	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	0	0
5	C	53	0	31	1	0
5	D	53	0	31	0	0
6	A	30	0	40	11	0
6	B	30	0	40	1	0
6	C	12	0	16	0	0
6	D	12	0	16	1	0
7	A	7	0	10	4	0
8	D	1	0	0	0	0
9	A	776	0	0	6	1
9	B	619	0	0	3	1
9	C	607	0	0	3	0
9	D	461	0	0	3	0
All	All	41321	0	38486	238	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 3.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HD11	7:A:1309:PEG:H21	1.49	0.94
1:A:723:GLN:HE21	1:A:821:ARG:HE	1.33	0.73
1:B:833:GLN:NE2	9:B:1402:HOH:O	2.20	0.73
1:D:1268:SER:HB3	9:D:1631:HOH:O	1.89	0.71
1:A:952:GLU:HA	6:A:1310:GOL:H2	1.73	0.71

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)
9:A:1527:HOH:O	9:B:1934:HOH:O[2_746]	2.03	0.17

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	1243/1273 (98%)	1200 (96%)	39 (3%)	4 (0%)	41	46
1	B	1245/1273 (98%)	1200 (96%)	41 (3%)	4 (0%)	41	46
1	C	1248/1273 (98%)	1206 (97%)	40 (3%)	2 (0%)	47	55
1	D	1229/1273 (96%)	1185 (96%)	38 (3%)	6 (0%)	29	31
All	All	4965/5092 (98%)	4791 (96%)	158 (3%)	16 (0%)	41	46

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	893	ARG
1	A	706	LEU
1	A	893	ARG
1	B	893	ARG
1	B	1267	PRO

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	1037/1053 (98%)	1020 (98%)	17 (2%)	62	76
1	B	1038/1053 (99%)	1023 (99%)	15 (1%)	67	80
1	C	1038/1053 (99%)	1015 (98%)	23 (2%)	52	65
1	D	1023/1053 (97%)	1010 (99%)	13 (1%)	69	81
All	All	4136/4212 (98%)	4068 (98%)	68 (2%)	62	76

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	277	SER
1	D	507	LYS
1	D	948	GLU
1	B	536	GLN
1	B	522	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	568	HIS
1	C	296	GLN
1	D	365	GLN
1	C	981	GLN
1	D	15	ASN

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 36 ligands modelled in this entry, 1 is modelled with single atom - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FES	B	1302	1	0,4,4	-	-	-		
6	GOL	B	1310	-	5,5,5	0.18	0	5,5,5	0.45	0
5	FAD	B	1305	-	53,58,58	0.72	1 (1%)	68,89,89	0.76	1 (1%)
5	FAD	D	1305	-	53,58,58	0.64	0	68,89,89	0.77	1 (1%)
3	MTE	A	1303	4	21,26,26	1.08	1 (4%)	21,40,40	2.30	7 (33%)
4	MOS	B	1304	3	0,3,3	-	-	-		
4	MOS	D	1304	3	0,3,3	-	-	-		
2	FES	D	1302	1	0,4,4	-	-	-		
6	GOL	B	1308	-	5,5,5	0.14	0	5,5,5	0.56	0
6	GOL	D	1306	-	5,5,5	0.11	0	5,5,5	0.29	0
2	FES	B	1301	1	0,4,4	-	-	-		
6	GOL	B	1309	-	5,5,5	0.08	0	5,5,5	0.21	0
6	GOL	C	1306	-	5,5,5	0.17	0	5,5,5	0.35	0
3	MTE	B	1303	4	21,26,26	1.14	1 (4%)	21,40,40	2.14	9 (42%)
3	MTE	C	1303	4	21,26,26	1.08	1 (4%)	21,40,40	2.12	8 (38%)
4	MOS	A	1304	3	0,3,3	-	-	-		
6	GOL	A	1308	-	5,5,5	0.38	0	5,5,5	0.58	0
6	GOL	A	1310	-	5,5,5	0.36	0	5,5,5	0.75	0
2	FES	A	1301	1	0,4,4	-	-	-		
2	FES	C	1302	1	0,4,4	-	-	-		
6	GOL	A	1306	-	5,5,5	0.14	0	5,5,5	0.62	0
6	GOL	C	1307	-	5,5,5	0.12	0	5,5,5	0.39	0
2	FES	D	1301	1	0,4,4	-	-	-		
6	GOL	B	1306	-	5,5,5	0.06	0	5,5,5	0.32	0
3	MTE	D	1303	4	21,26,26	1.20	1 (4%)	21,40,40	2.11	7 (33%)
2	FES	A	1302	1	0,4,4	-	-	-		
7	PEG	A	1309	-	6,6,6	0.76	0	5,5,5	0.70	0
6	GOL	A	1311	-	5,5,5	0.22	0	5,5,5	0.44	0
5	FAD	A	1305	-	53,58,58	0.63	0	68,89,89	0.82	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	B	1307	-	5,5,5	0.11	0	5,5,5	0.29	0
6	GOL	D	1307	-	5,5,5	0.13	0	5,5,5	0.43	0
5	FAD	C	1305	-	53,58,58	0.61	0	68,89,89	0.83	2 (2%)
4	MOS	C	1304	3	0,3,3	-	-	-		
2	FES	C	1301	1	0,4,4	-	-	-		
6	GOL	A	1307	-	5,5,5	0.06	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	B	1302	1	-	-	0/1/1/1
6	GOL	B	1310	-	-	2/4/4/4	-
5	FAD	B	1305	-	-	0/30/50/50	0/6/6/6
5	FAD	D	1305	-	-	0/30/50/50	0/6/6/6
3	MTE	A	1303	4	-	3/6/34/34	0/3/3/3
6	GOL	B	1308	-	-	2/4/4/4	-
2	FES	D	1302	1	-	-	0/1/1/1
6	GOL	D	1306	-	-	0/4/4/4	-
6	GOL	B	1309	-	-	0/4/4/4	-
2	FES	B	1301	1	-	-	0/1/1/1
6	GOL	C	1306	-	-	0/4/4/4	-
3	MTE	B	1303	4	-	3/6/34/34	0/3/3/3
3	MTE	C	1303	4	-	4/6/34/34	0/3/3/3
6	GOL	A	1308	-	-	2/4/4/4	-
6	GOL	A	1310	-	-	4/4/4/4	-
2	FES	A	1301	1	-	-	0/1/1/1
2	FES	C	1302	1	-	-	0/1/1/1
6	GOL	A	1306	-	-	2/4/4/4	-
6	GOL	C	1307	-	-	0/4/4/4	-
2	FES	D	1301	1	-	-	0/1/1/1
6	GOL	B	1306	-	-	4/4/4/4	-
3	MTE	D	1303	4	-	3/6/34/34	0/3/3/3
2	FES	A	1302	1	-	-	0/1/1/1
7	PEG	A	1309	-	-	2/4/4/4	-
6	GOL	A	1311	-	-	2/4/4/4	-
5	FAD	A	1305	-	-	0/30/50/50	0/6/6/6
6	GOL	B	1307	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	1307	-	-	0/4/4/4	-
5	FAD	C	1305	-	-	0/30/50/50	0/6/6/6
2	FES	C	1301	1	-	-	0/1/1/1
6	GOL	A	1307	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1303	MTE	C4-N3	4.10	1.40	1.33
3	C	1303	MTE	C4-N3	3.83	1.39	1.33
3	A	1303	MTE	C4-N3	3.70	1.39	1.33
3	B	1303	MTE	C4-N3	3.53	1.39	1.33
5	B	1305	FAD	C1'-C2'	-2.96	1.48	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1303	MTE	C10-C9-C4	5.07	119.08	114.57
3	B	1303	MTE	C10-C9-C4	4.90	118.92	114.57
3	C	1303	MTE	C10-C9-C4	4.83	118.86	114.57
3	A	1303	MTE	C10-C9-C4	4.60	118.65	114.57
3	A	1303	MTE	O3'-C7-C6	4.25	111.80	108.96

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	MTE	C3'-C4'-O4'-P
3	A	1303	MTE	C4'-O4'-P-O1P
3	B	1303	MTE	C3'-C4'-O4'-P
3	B	1303	MTE	C4'-O4'-P-O2P
3	B	1303	MTE	C4'-O4'-P-O3P

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1310	GOL	1	0
3	A	1303	MTE	2	0
3	B	1303	MTE	2	0
3	C	1303	MTE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1308	GOL	3	0
6	A	1310	GOL	7	0
6	A	1306	GOL	1	0
3	D	1303	MTE	3	0
7	A	1309	PEG	4	0
5	A	1305	FAD	1	0
6	D	1307	GOL	1	0
5	C	1305	FAD	1	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.

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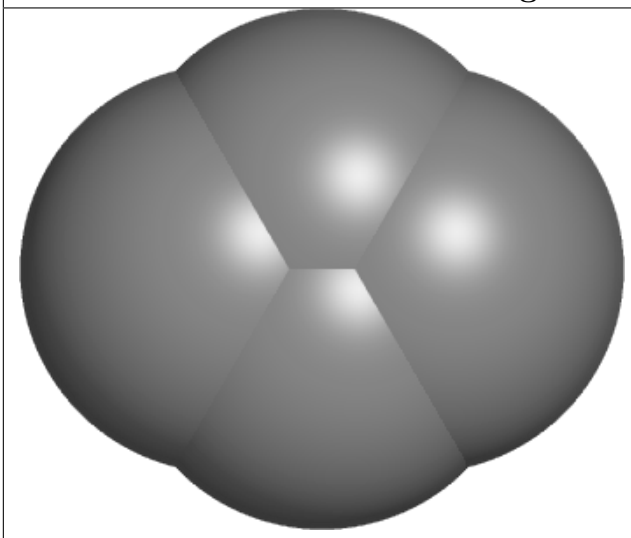
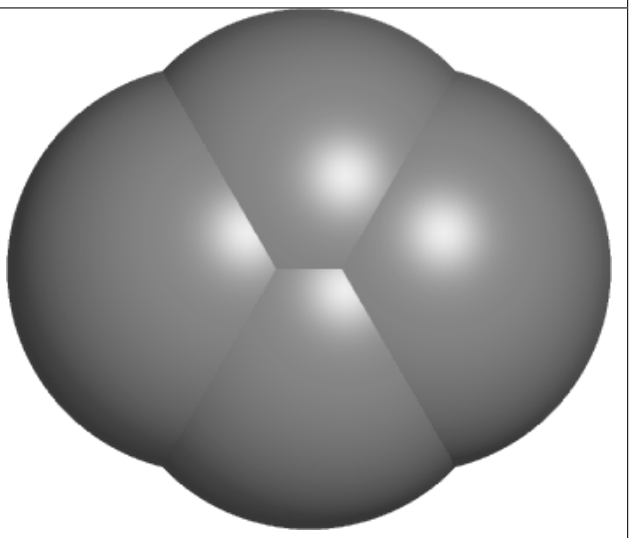
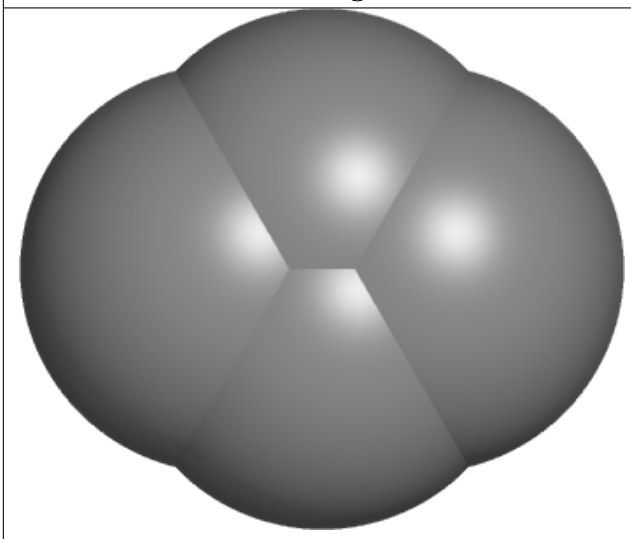
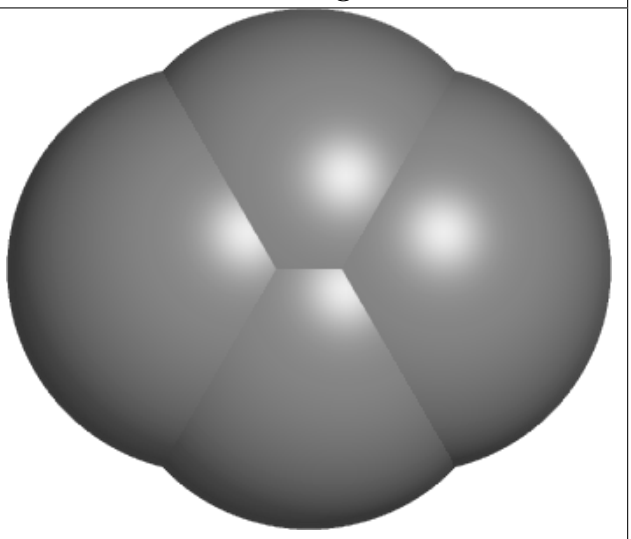
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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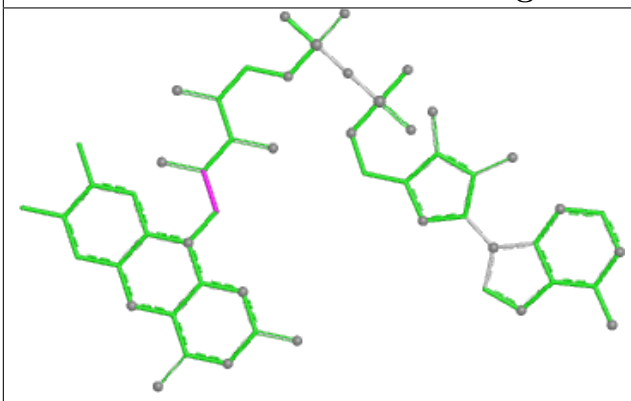

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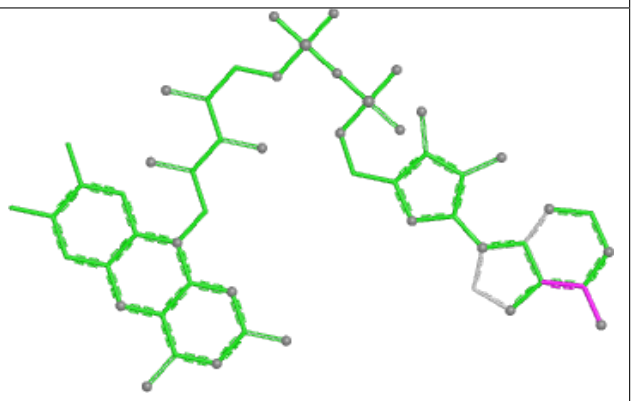
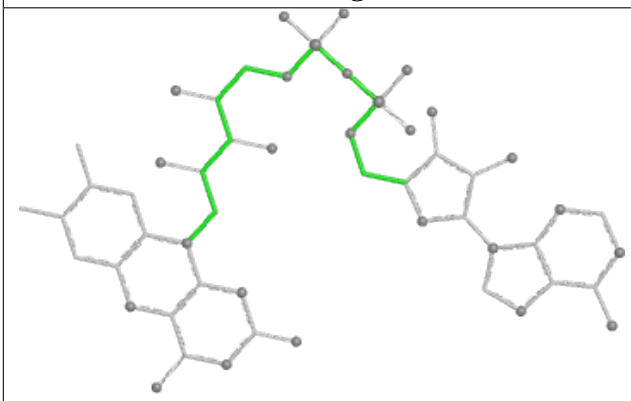
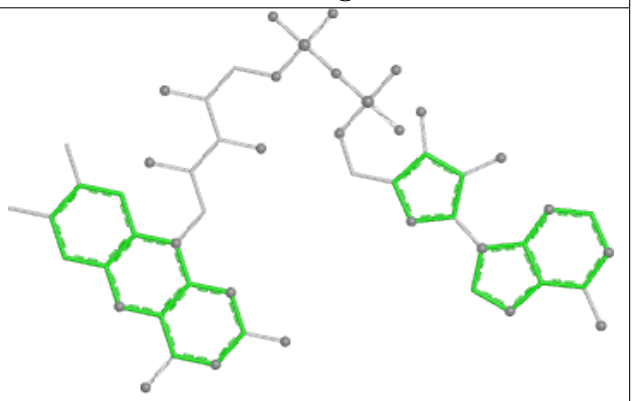


Bond angles



Torsions



Rings

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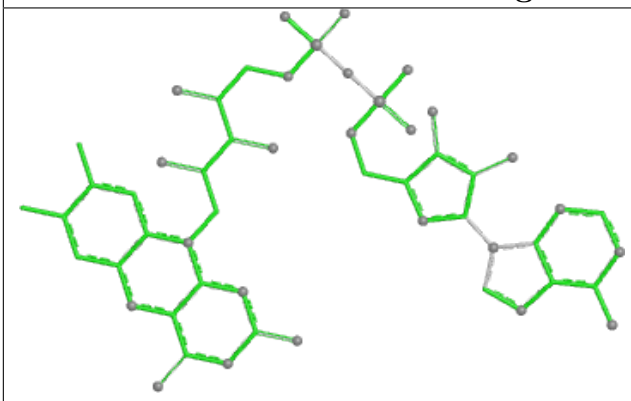
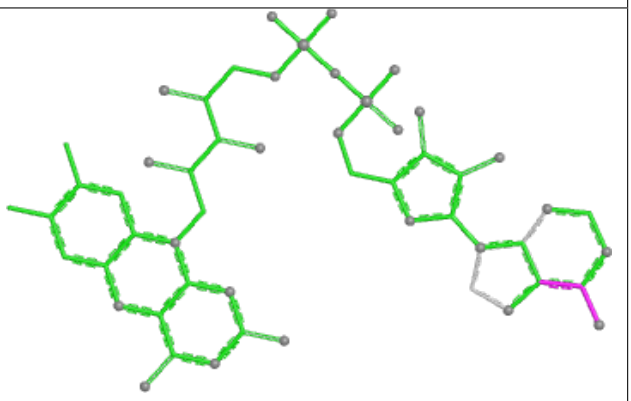
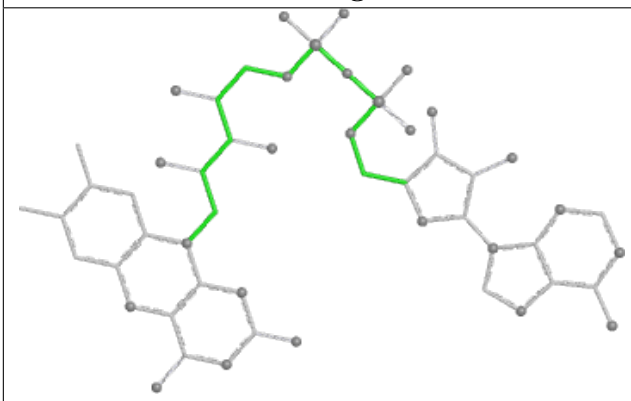
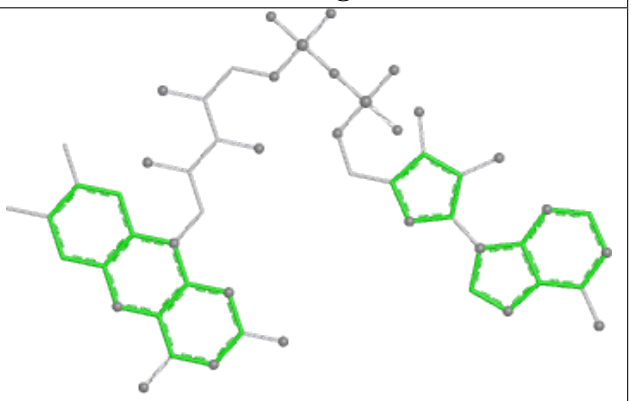
 Bond lengths	 Bond angles
 Torsions	 Rings

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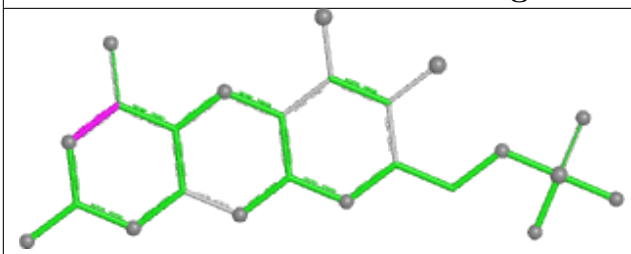
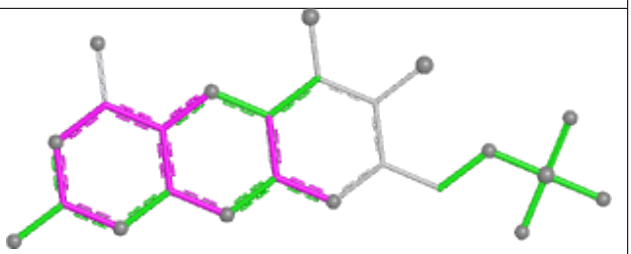
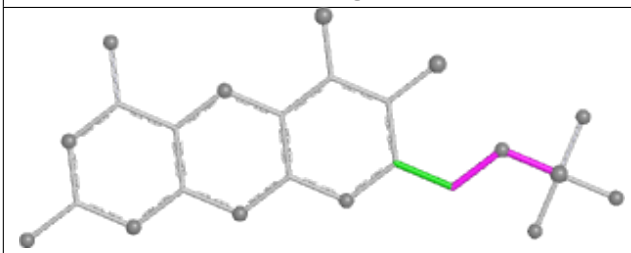
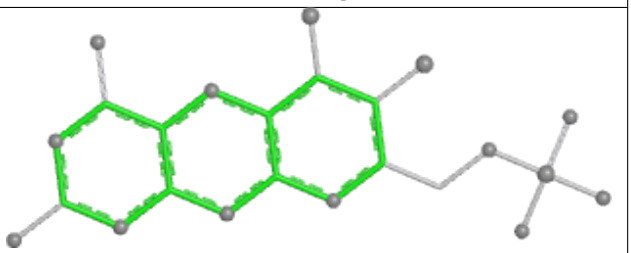
 Bond lengths	 Bond angles
 Torsions	 Rings

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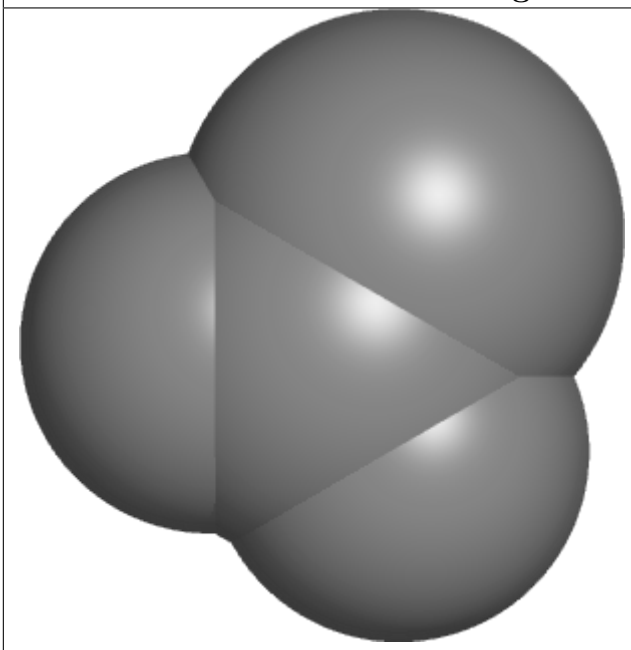
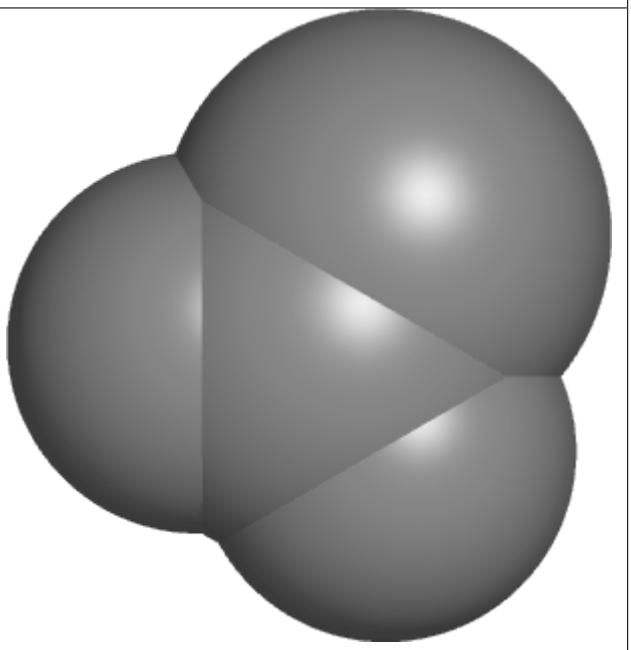
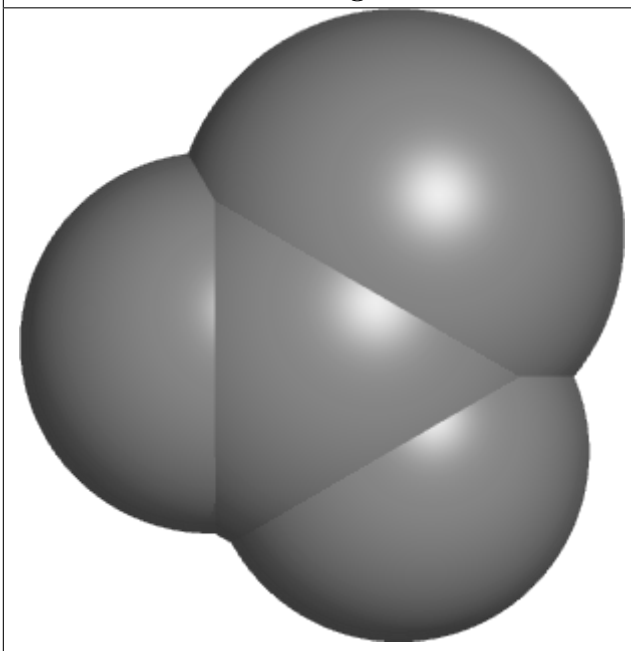


Bond lengths



Bond angles



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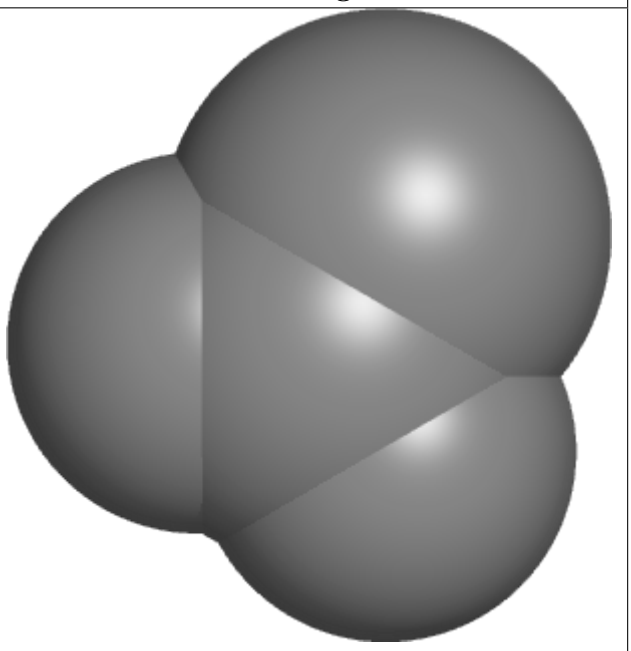
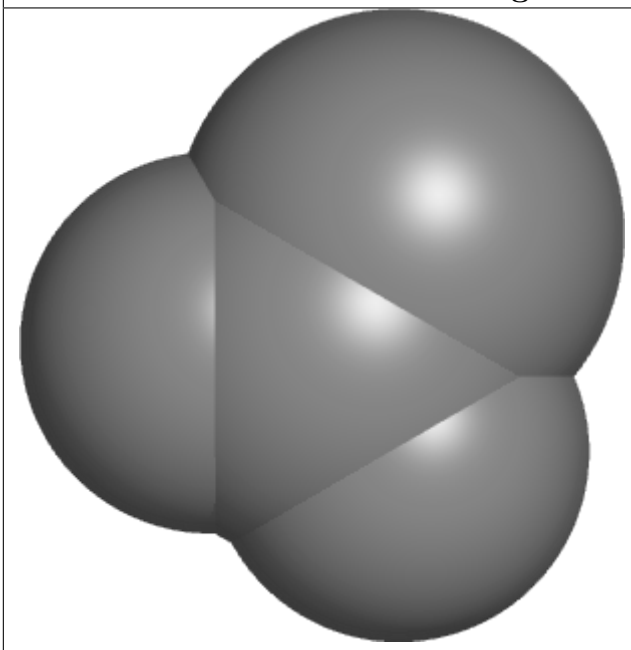


Rings

Ligand MOS D 1304



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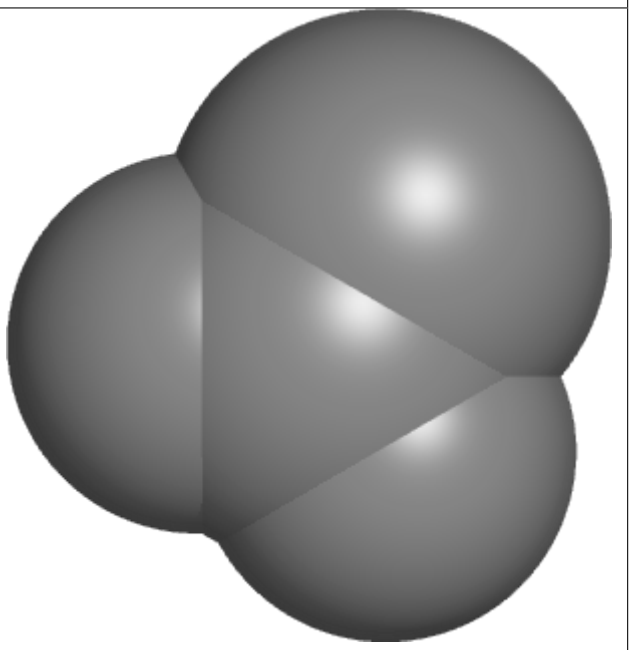

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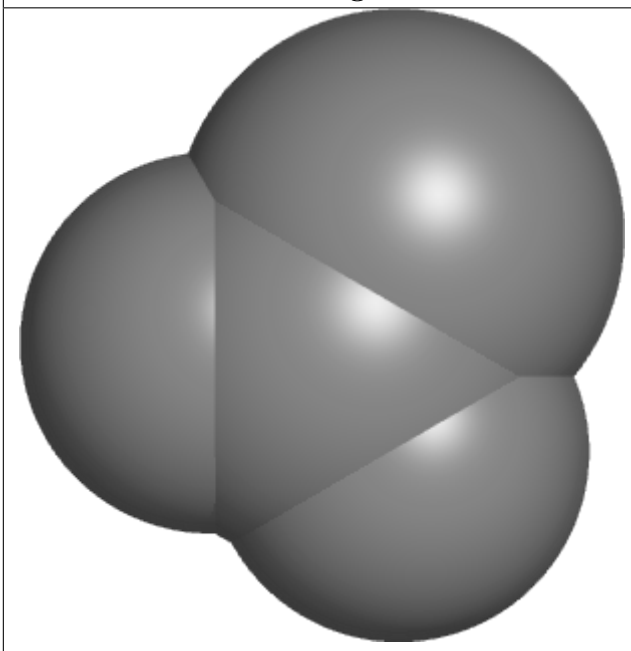
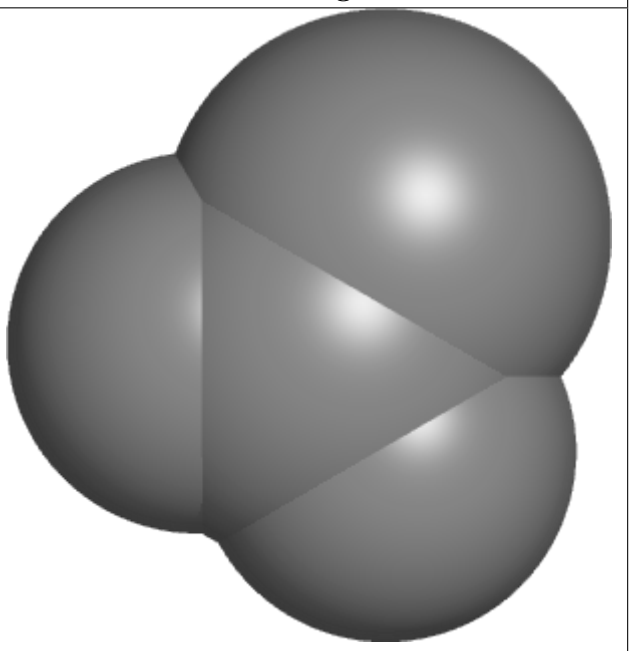


Torsions



Rings

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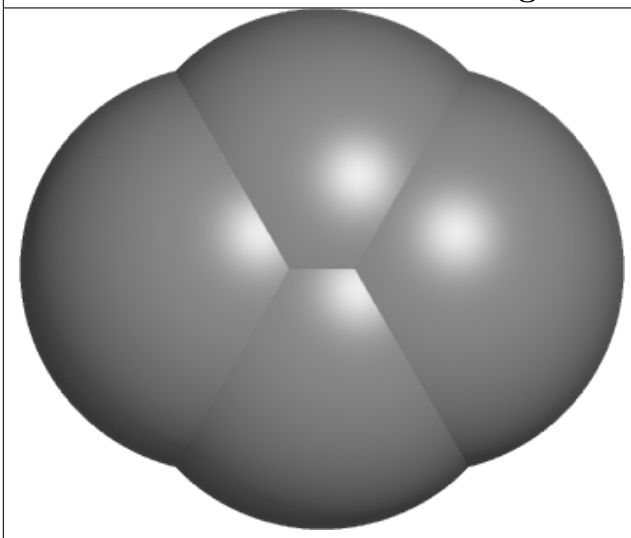
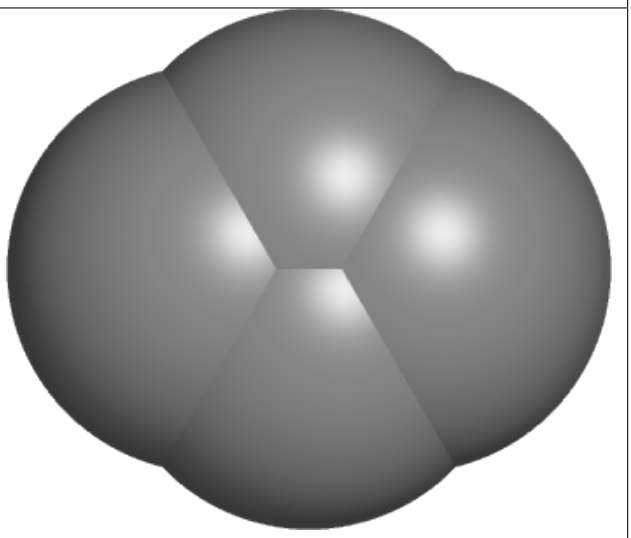
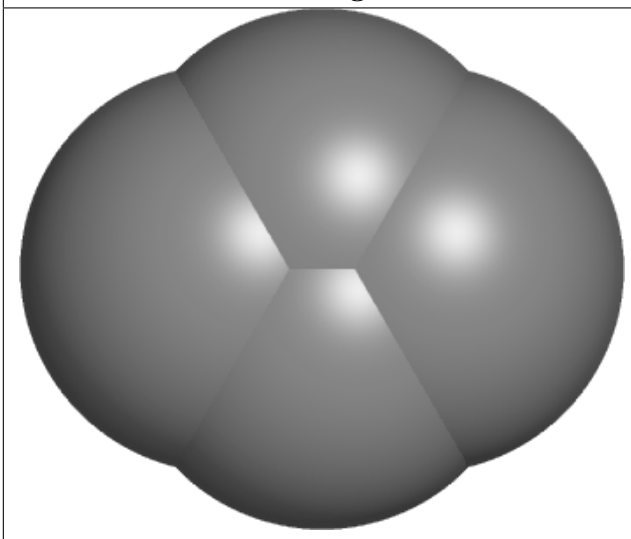
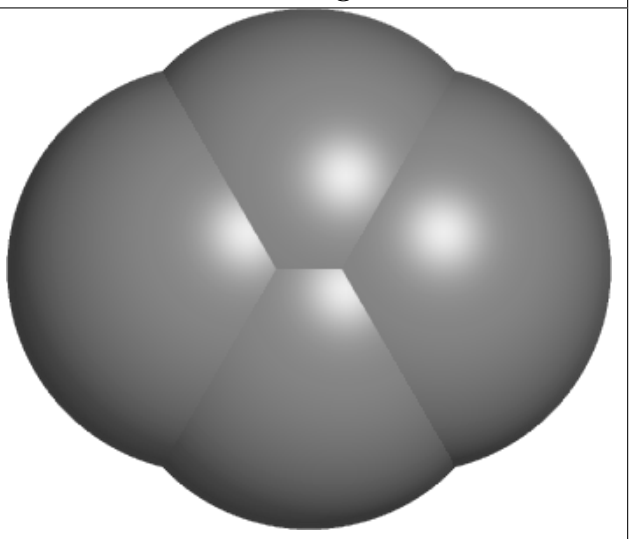
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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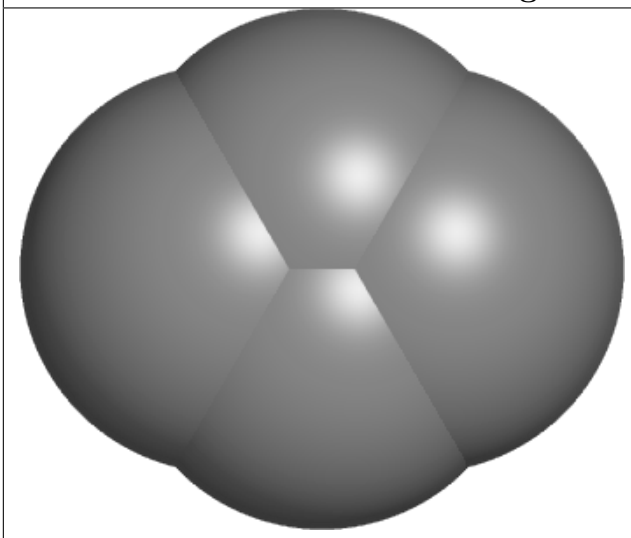
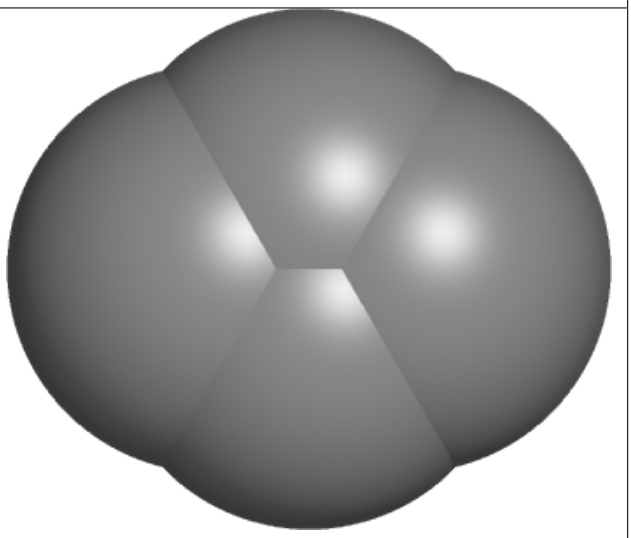
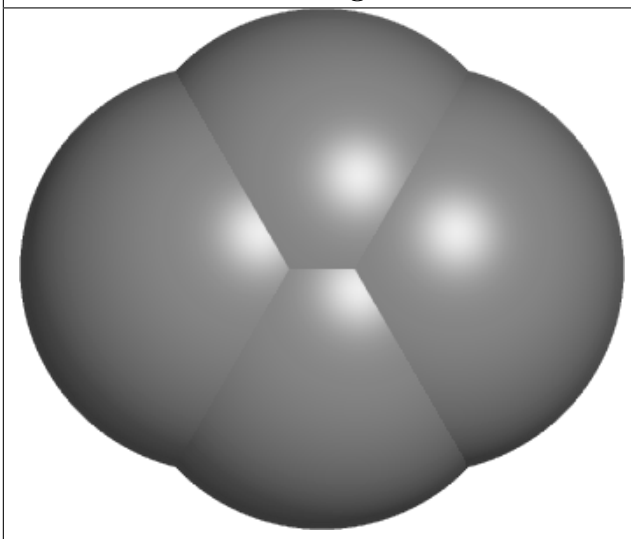
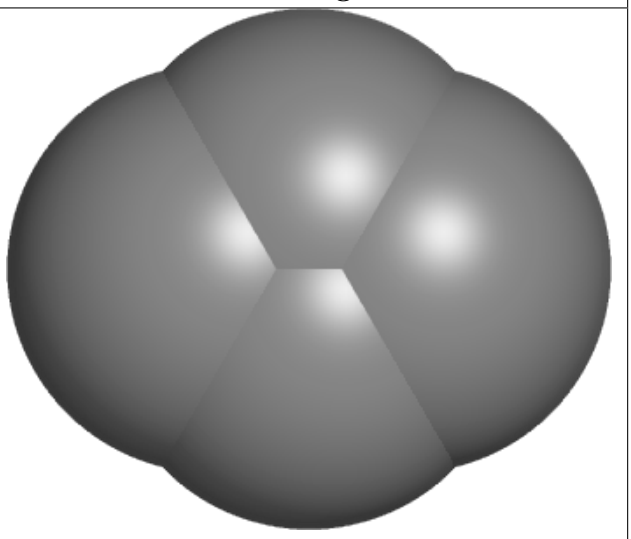
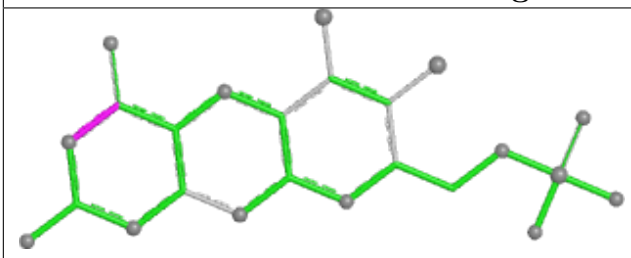
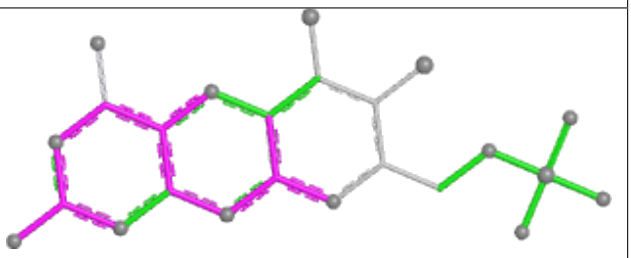
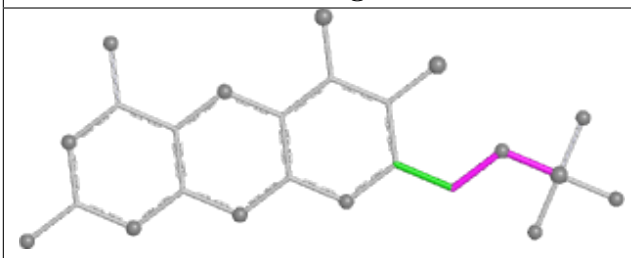
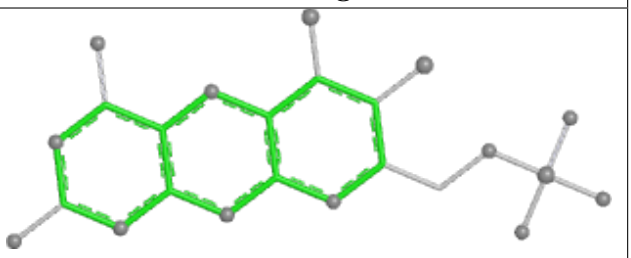
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand MTE B 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

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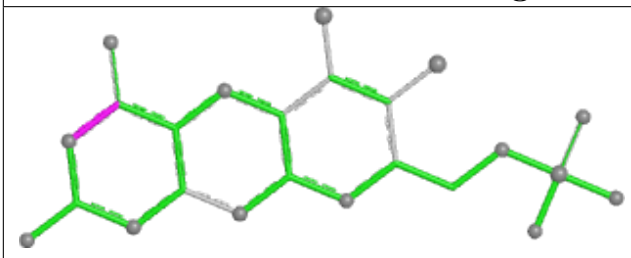
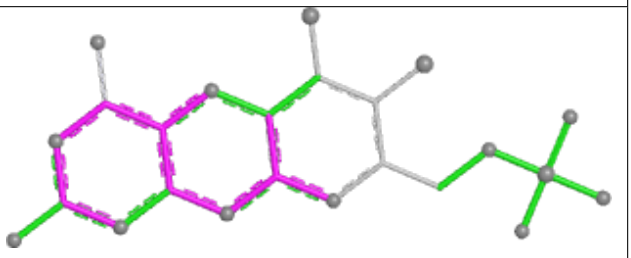
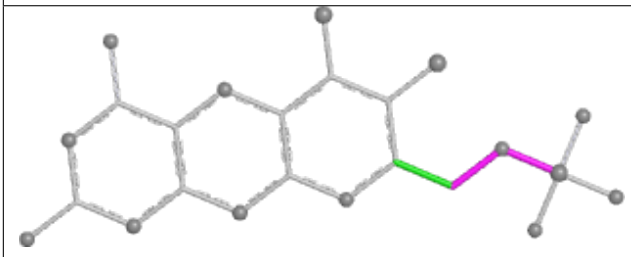
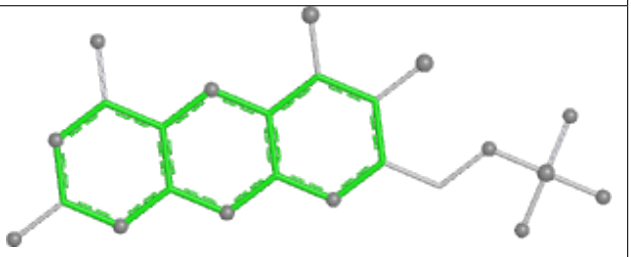
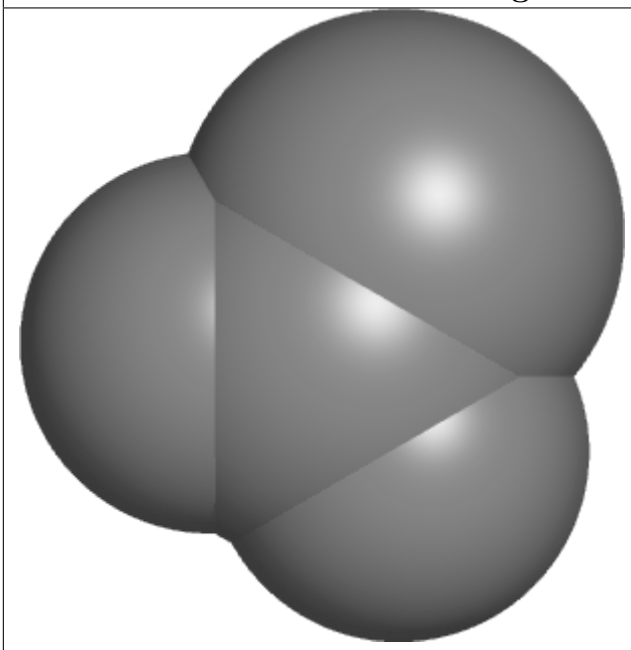
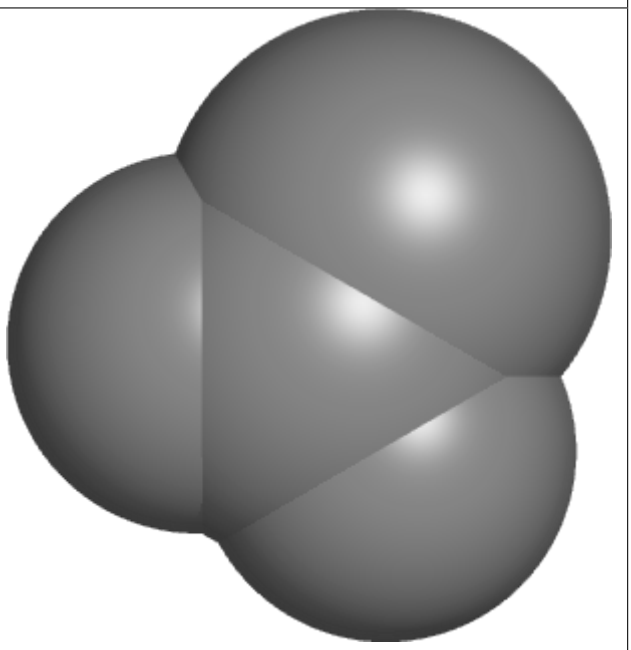
	
Bond lengths	Bond angles
	
Torsions	Rings

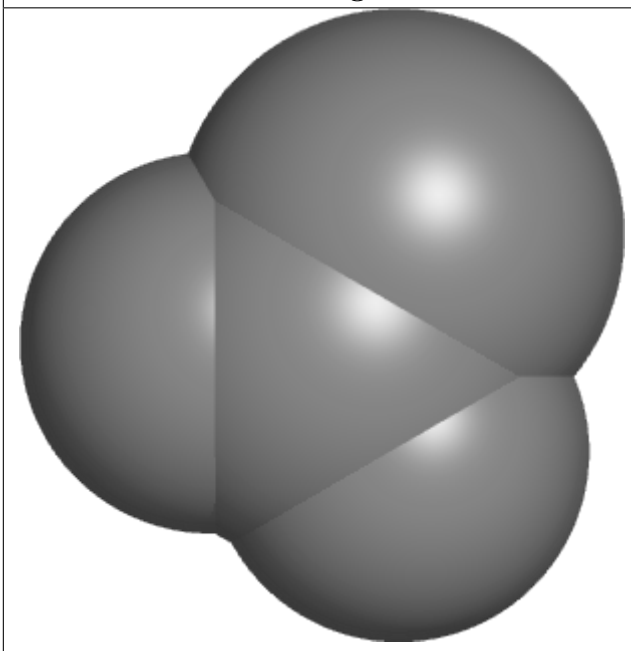
Ligand MOS A 1304



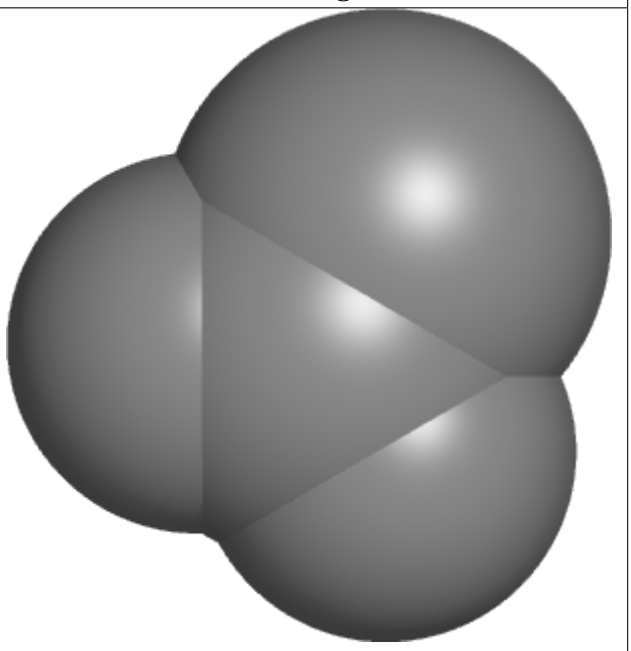
Bond lengths



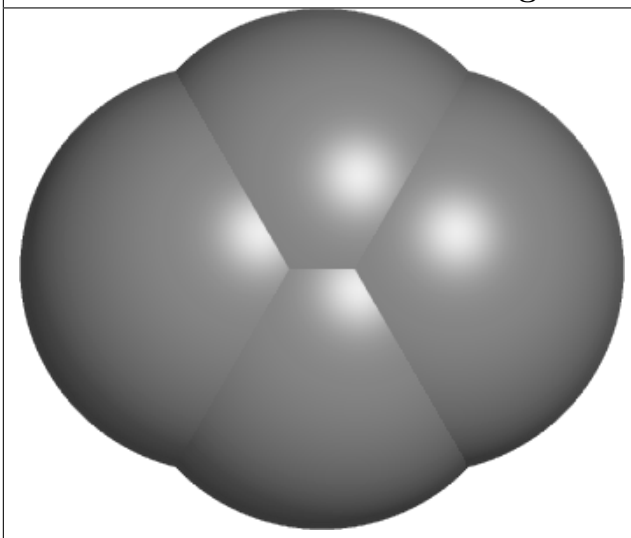
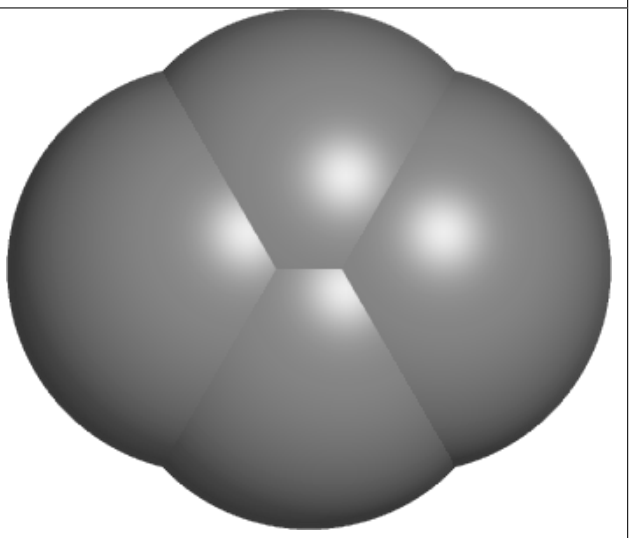
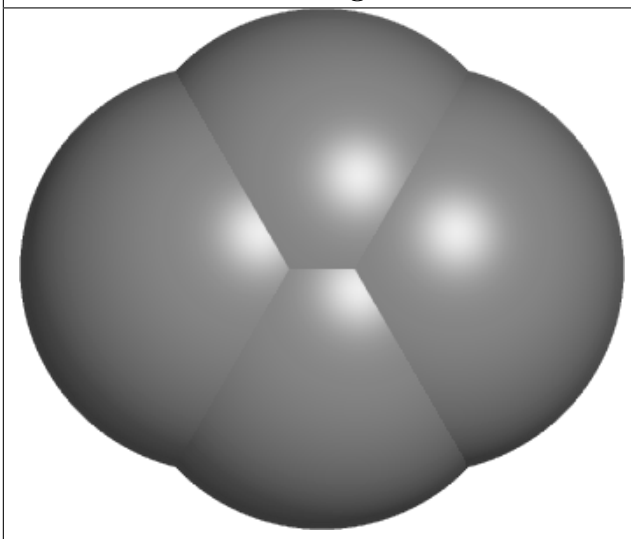
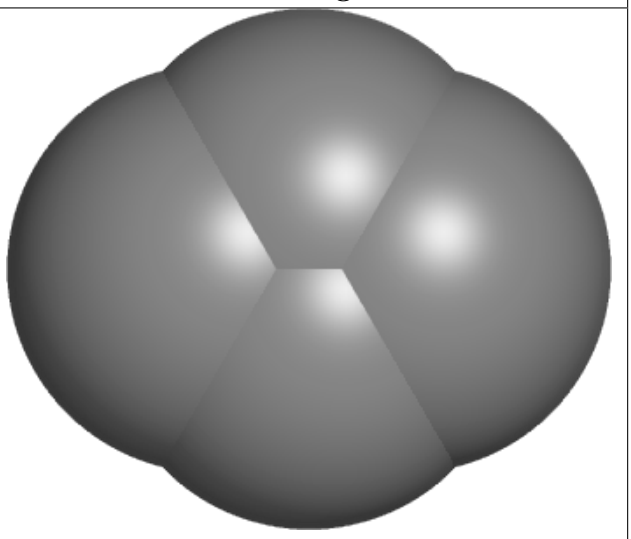
Bond angles



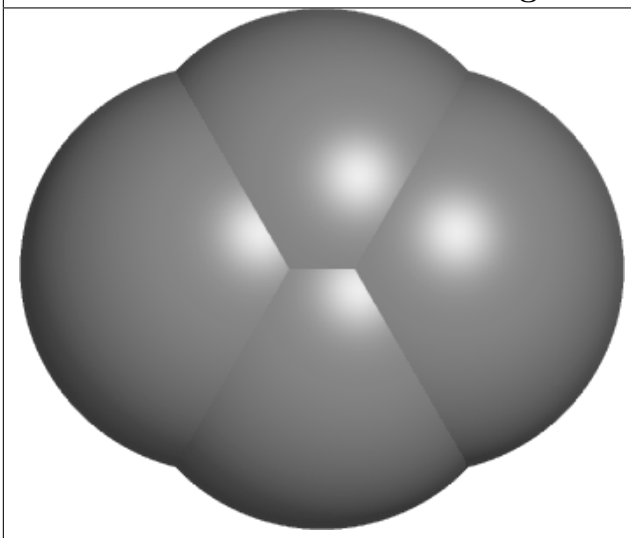
Torsions



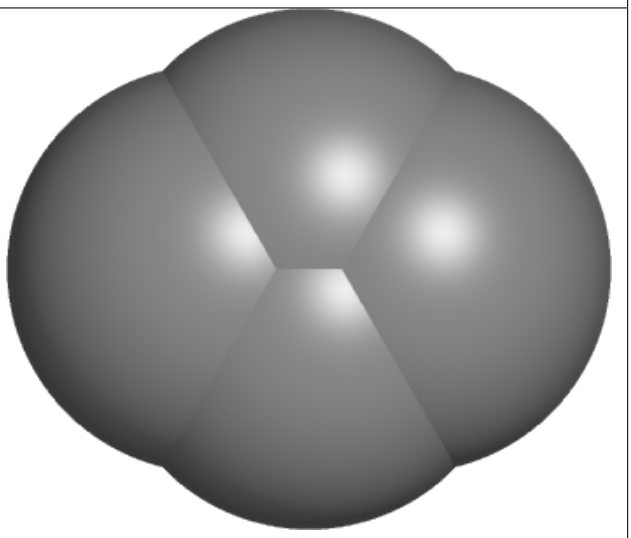
Rings

Ligand FES A 1301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

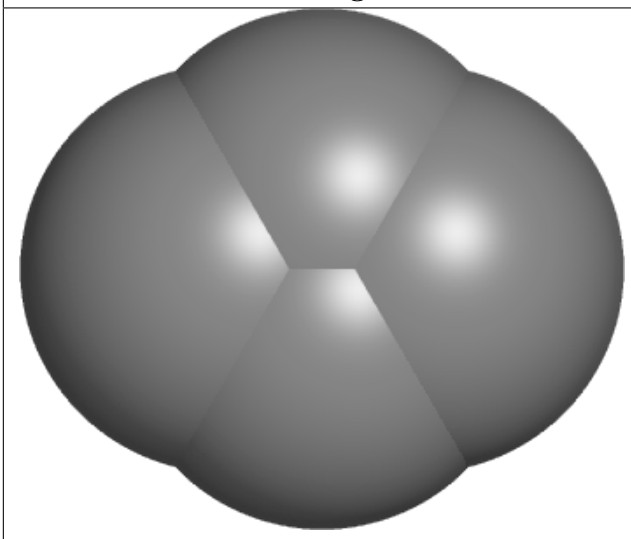
Ligand FES C 1302



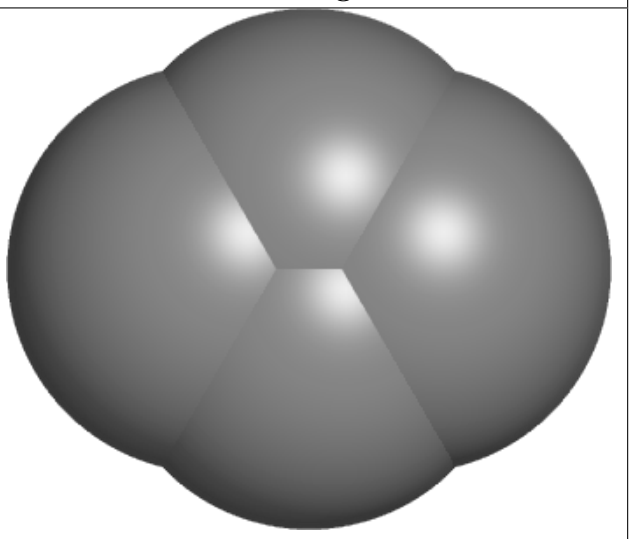
Bond lengths



Bond angles

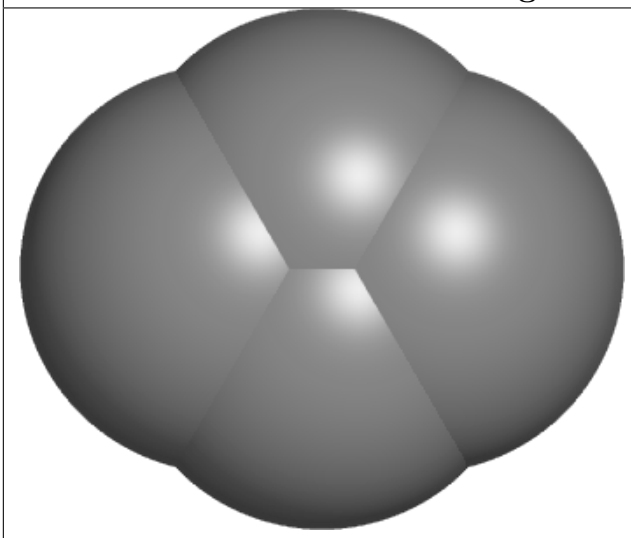


Torsions

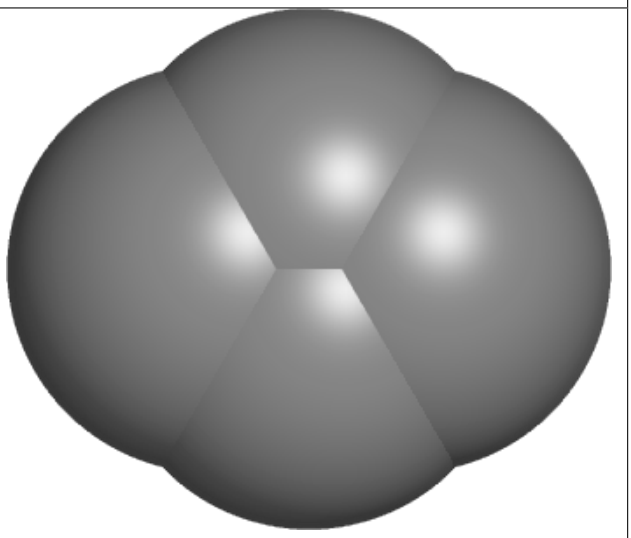


Rings

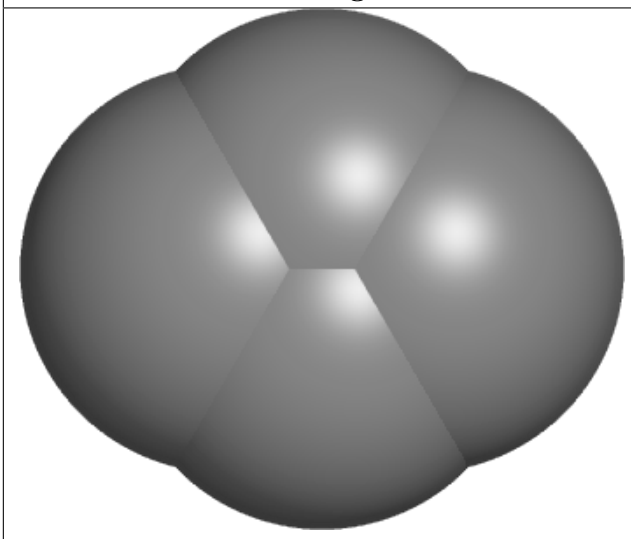
Ligand FES D 1301



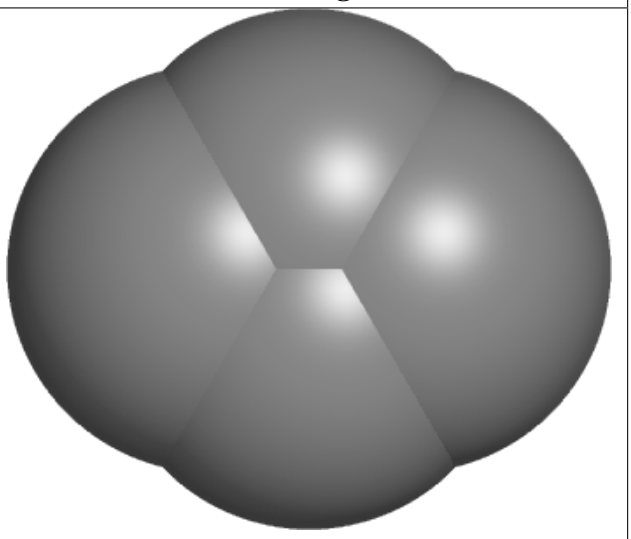
Bond lengths



Bond angles

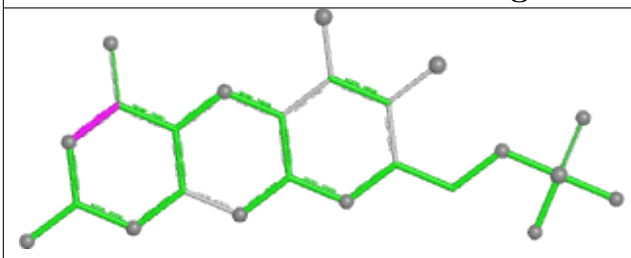


Torsions

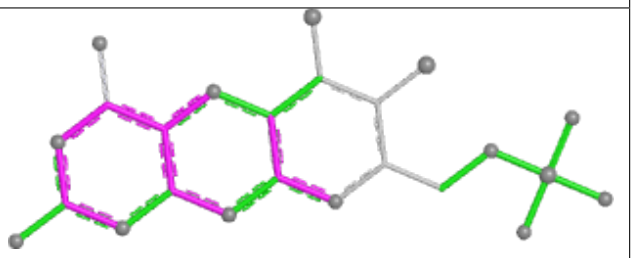


Rings

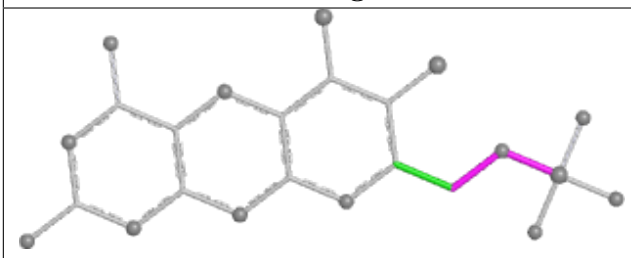
Ligand MTE D 1303



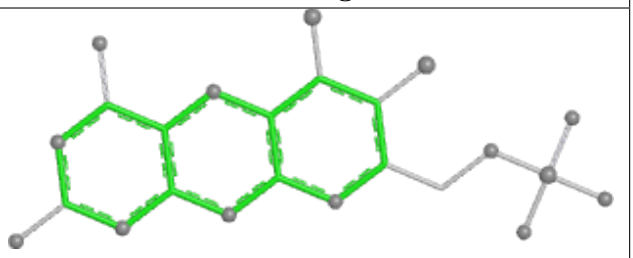
Bond lengths



Bond angles

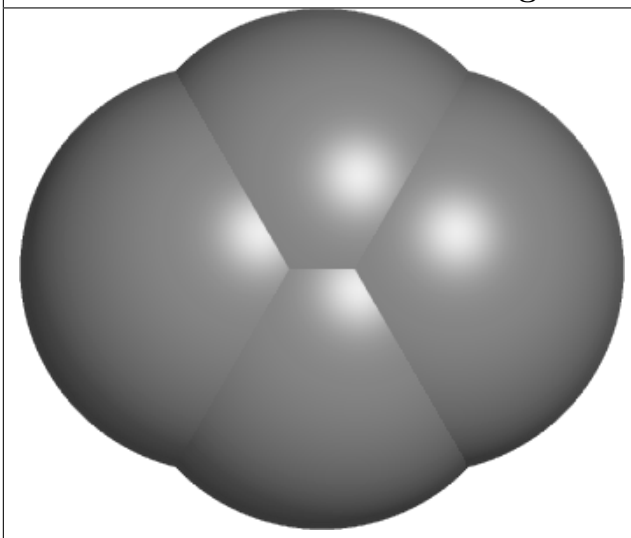


Torsions

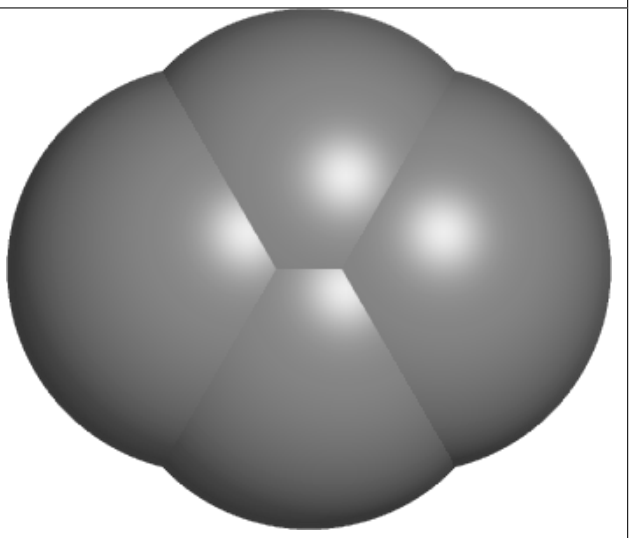


Rings

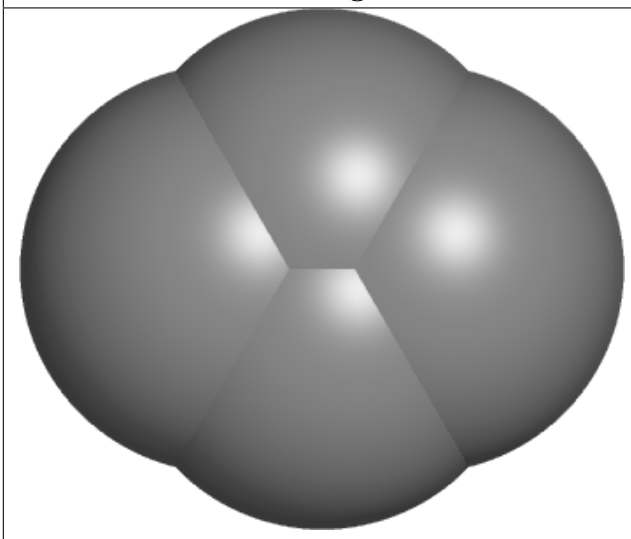
Ligand FES A 1302



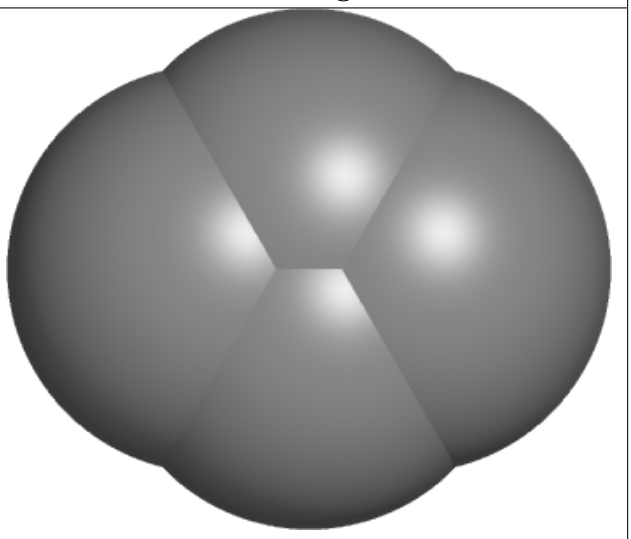
Bond lengths



Bond angles

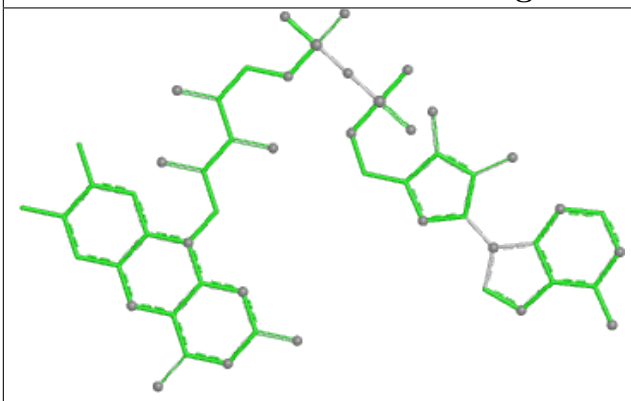


Torsions

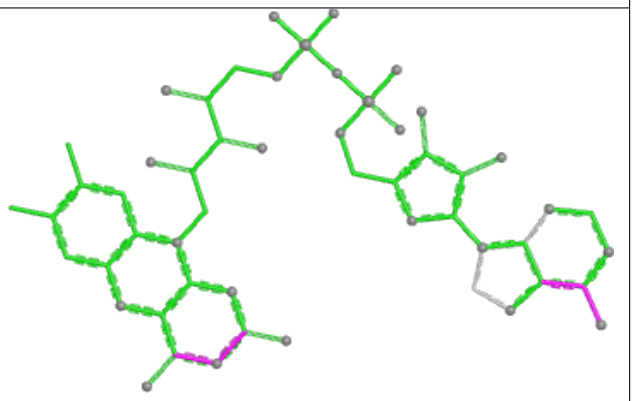


Rings

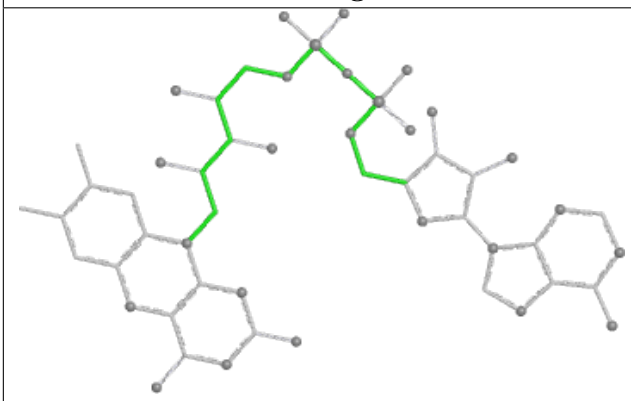
Ligand FAD A 1305



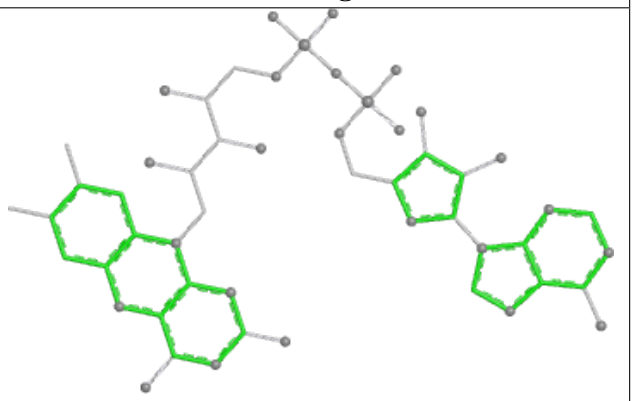
Bond lengths



Bond angles

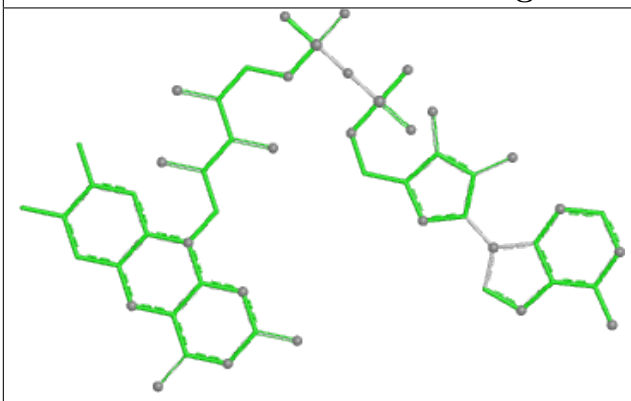


Torsions

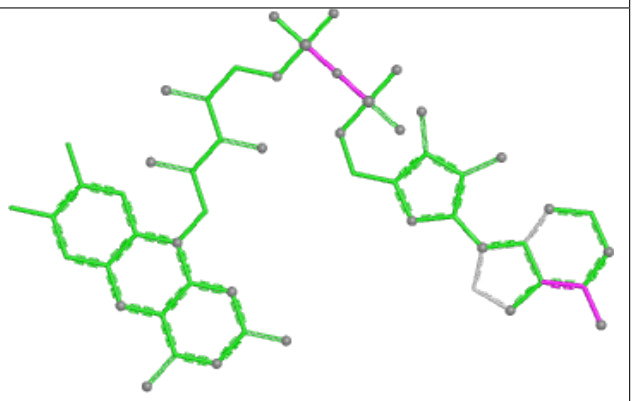


Rings

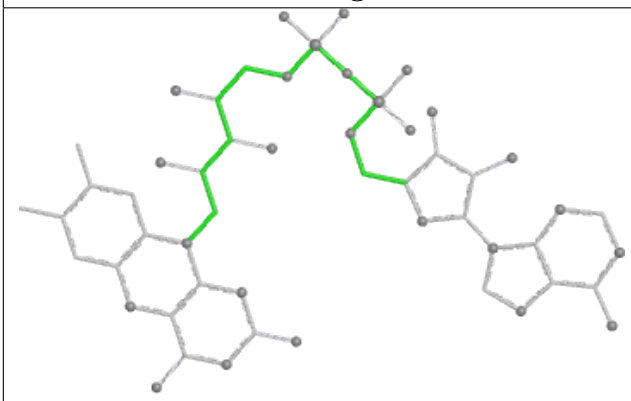
Ligand FAD C 1305



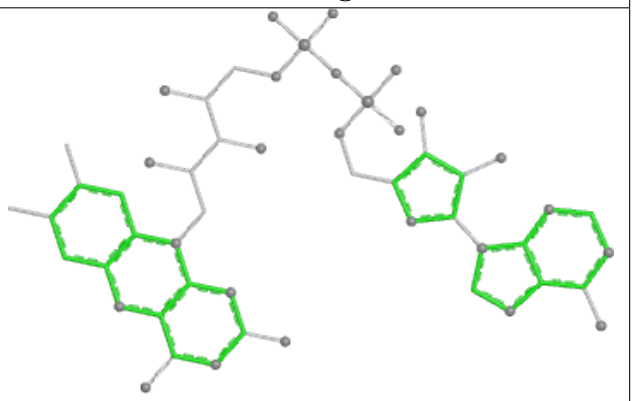
Bond lengths



Bond angles

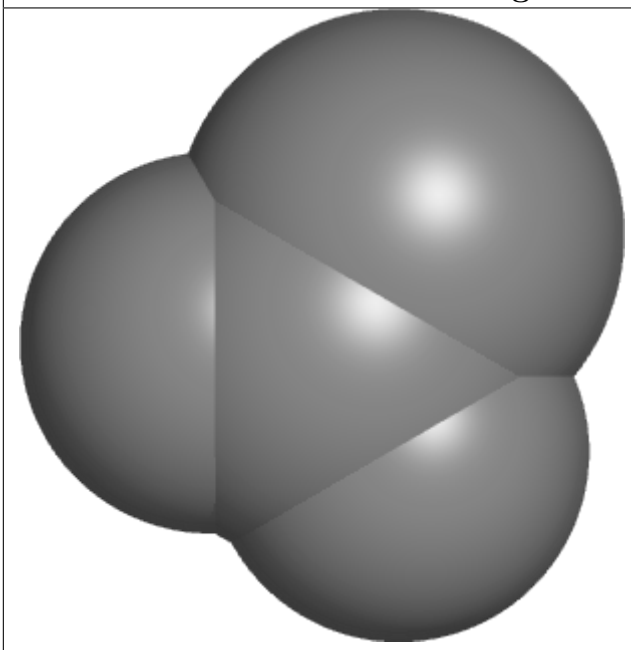


Torsions

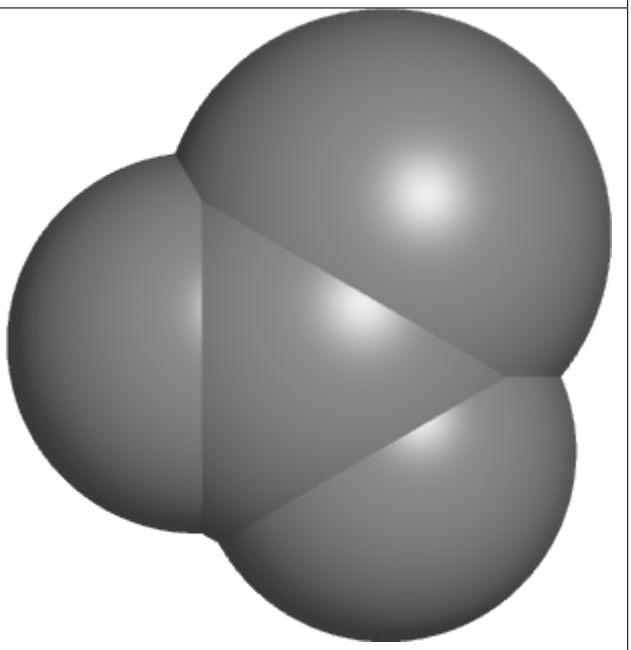


Rings

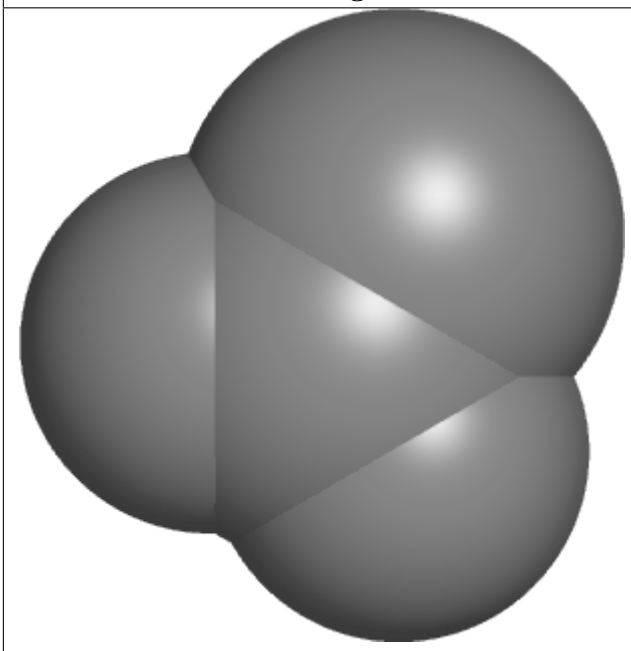
Ligand MOS C 1304



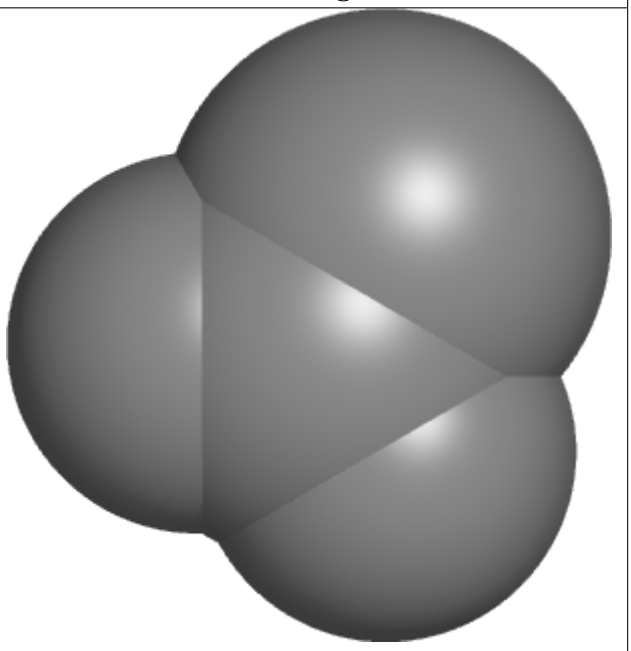
Bond lengths



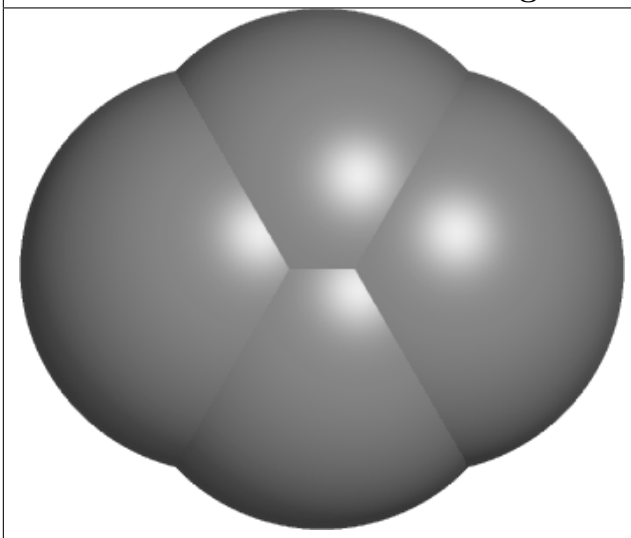
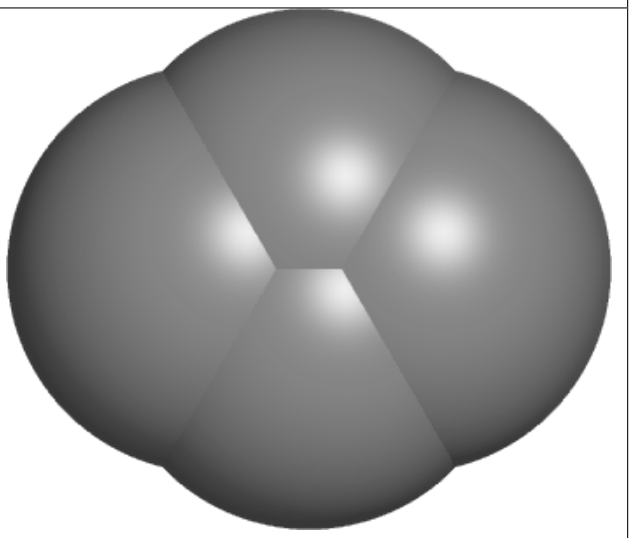
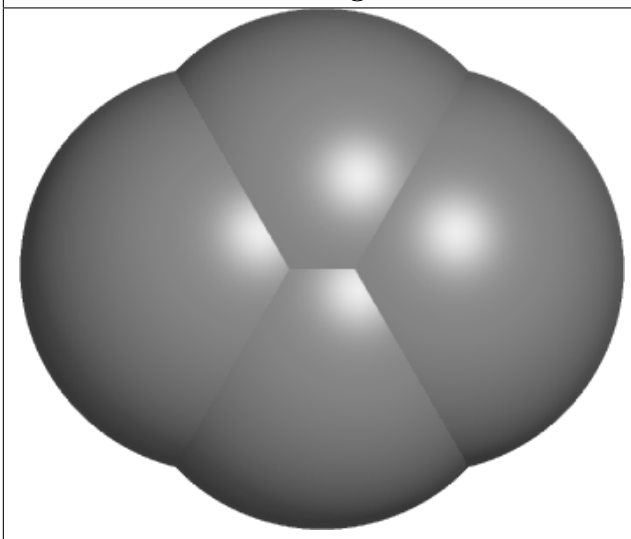
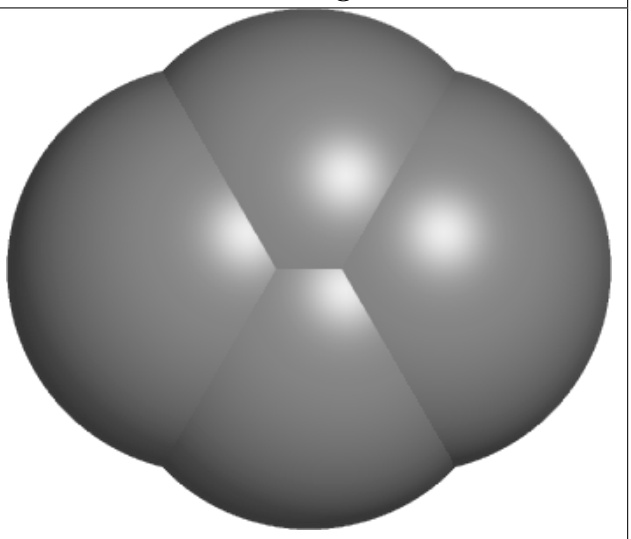
Bond angles



Torsions



Rings

Ligand FES C 1301	
 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	1249/1273 (98%)	0.22	33 (2%) 56 53	14, 23, 49, 85	0
1	B	1253/1273 (98%)	0.35	83 (6%) 18 17	15, 28, 61, 89	0
1	C	1252/1273 (98%)	0.39	64 (5%) 28 26	18, 30, 58, 105	0
1	D	1236/1273 (97%)	0.80	197 (15%) 1 1	20, 36, 72, 102	0
All	All	4990/5092 (97%)	0.44	377 (7%) 13 12	14, 29, 62, 105	0

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	LEU	7.7
1	D	231	VAL	7.6
1	D	274	ALA	6.6
1	D	263	GLY	6.1
1	D	464	LYS	6.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

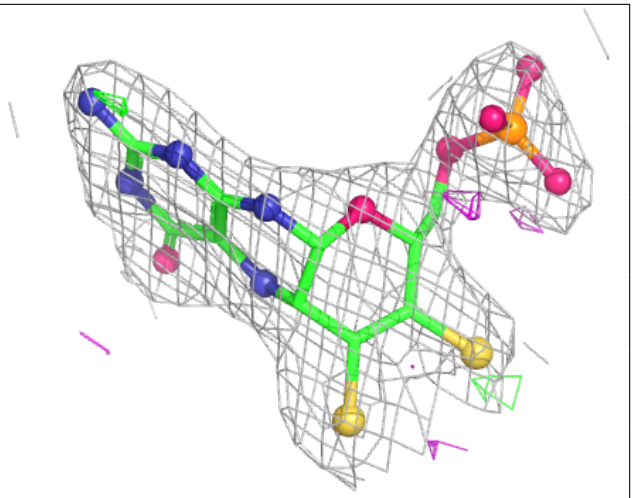
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

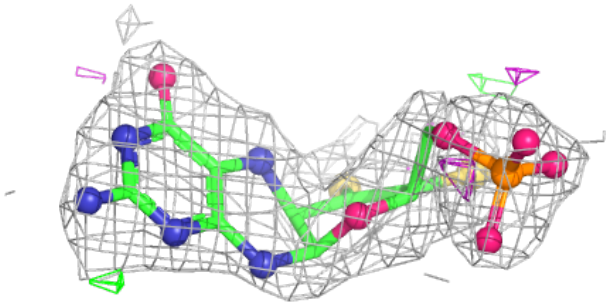
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	1310	6/6	0.59	0.22	54,60,62,62	0
6	GOL	A	1308	6/6	0.63	0.28	35,42,44,46	0
6	GOL	D	1307	6/6	0.64	0.31	45,49,50,51	6
7	PEG	A	1309	7/7	0.76	0.26	32,32,38,39	0
6	GOL	A	1311	6/6	0.79	0.23	43,46,49,51	0
6	GOL	B	1309	6/6	0.83	0.21	29,42,46,52	0
6	GOL	A	1310	6/6	0.83	0.34	34,41,43,48	0
3	MTE	D	1303	24/24	0.84	0.21	40,46,49,66	0
6	GOL	A	1307	6/6	0.85	0.21	45,50,50,52	0
6	GOL	C	1307	6/6	0.86	0.12	52,55,56,56	0
3	MTE	C	1303	24/24	0.88	0.17	33,47,55,58	0
6	GOL	D	1306	6/6	0.88	0.27	31,33,35,40	0
3	MTE	A	1303	24/24	0.88	0.19	35,41,50,52	0
6	GOL	C	1306	6/6	0.88	0.20	28,29,31,34	0
5	FAD	D	1305	53/53	0.89	0.18	37,45,51,56	0
6	GOL	B	1308	6/6	0.89	0.26	39,42,44,52	0
3	MTE	B	1303	24/24	0.89	0.18	30,42,52,56	0
6	GOL	B	1307	6/6	0.90	0.19	33,37,38,40	0
6	GOL	A	1306	6/6	0.93	0.22	25,30,32,33	0
5	FAD	C	1305	53/53	0.93	0.13	22,31,34,35	0
5	FAD	B	1305	53/53	0.94	0.12	20,25,29,30	0
5	FAD	A	1305	53/53	0.94	0.12	19,22,25,26	0
6	GOL	B	1306	6/6	0.94	0.18	29,32,34,36	0
8	NH4	D	1308	1/1	0.94	0.41	22,22,22,22	0
4	MOS	A	1304	4/4	0.95	0.21	22,23,27,28	4
2	FES	D	1302	4/4	0.96	0.06	31,31,31,35	0
2	FES	D	1301	4/4	0.96	0.09	27,28,29,32	0
4	MOS	B	1304	4/4	0.96	0.14	32,33,38,40	4
4	MOS	C	1304	4/4	0.96	0.16	31,31,34,38	4
4	MOS	D	1304	4/4	0.96	0.15	32,33,38,39	4
2	FES	A	1301	4/4	0.98	0.10	19,19,19,21	0
2	FES	A	1302	4/4	0.98	0.07	17,18,18,18	0
2	FES	B	1301	4/4	0.98	0.10	21,21,22,23	0
2	FES	B	1302	4/4	0.98	0.08	20,21,21,22	0
2	FES	C	1301	4/4	0.98	0.08	22,22,23,23	0
2	FES	C	1302	4/4	0.98	0.06	23,23,24,25	0

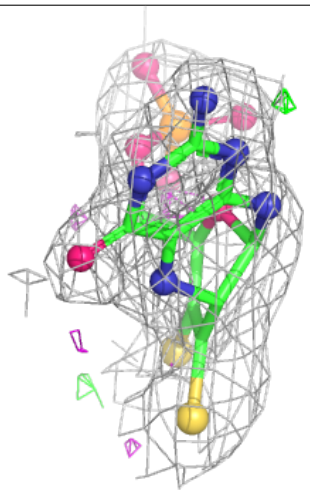
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTE D 1303:

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

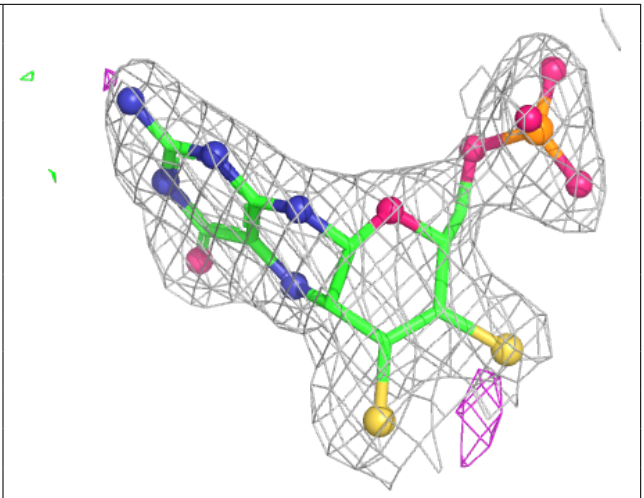


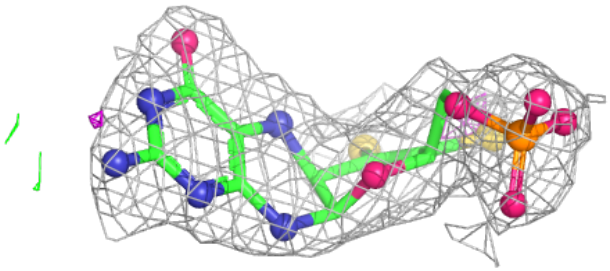


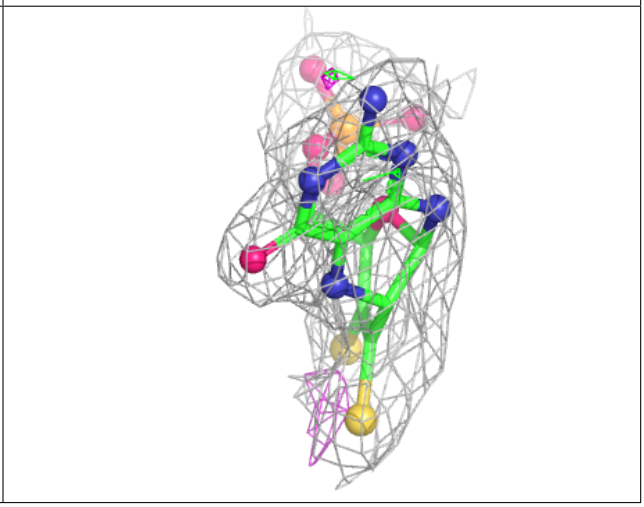


Electron density around MTE C 1303:

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

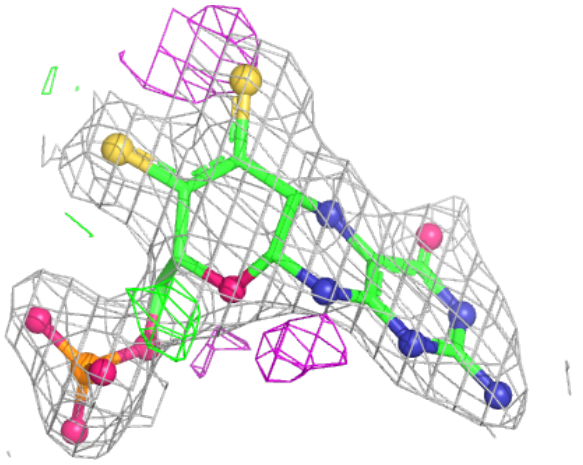


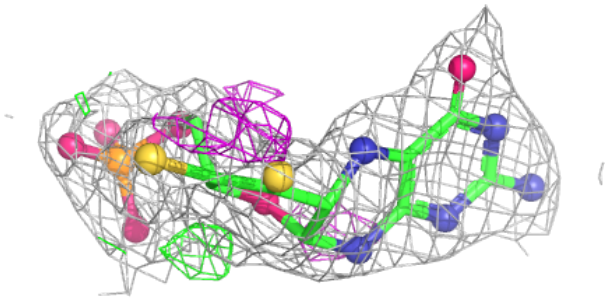


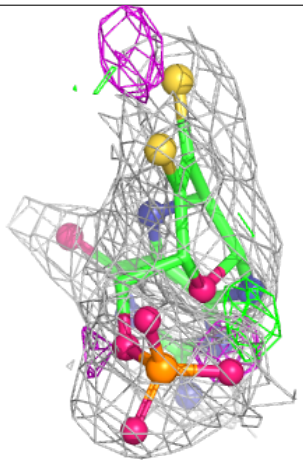


Electron density around MTE A 1303:

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

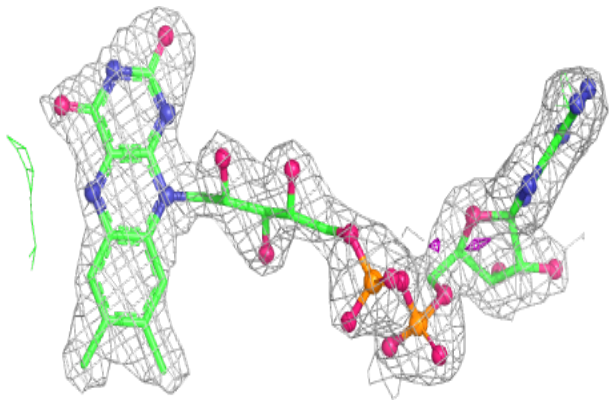


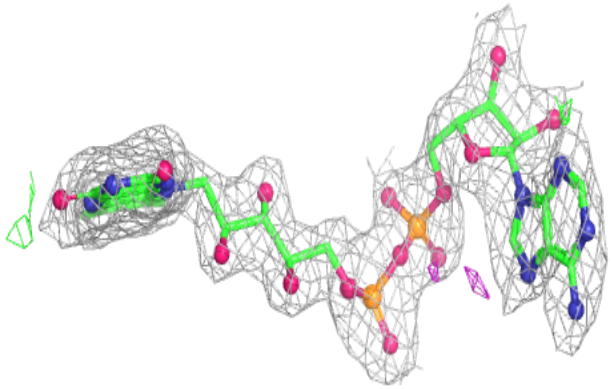


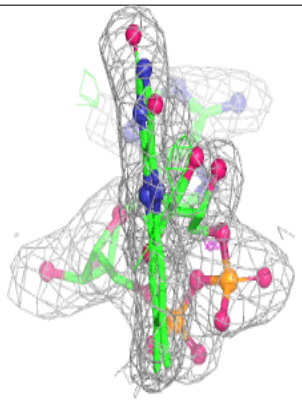


Electron density around FAD D 1305:

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

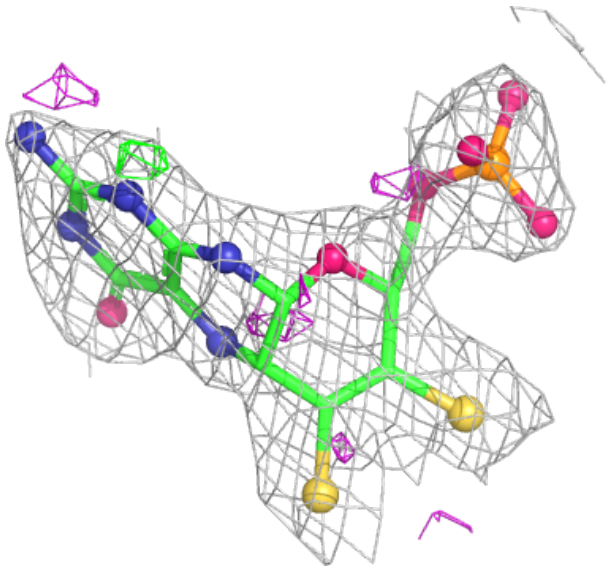


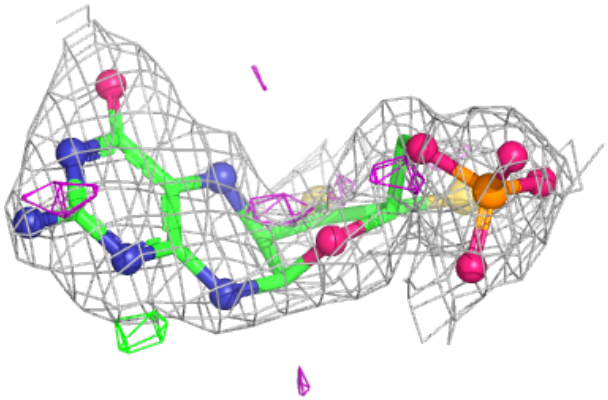


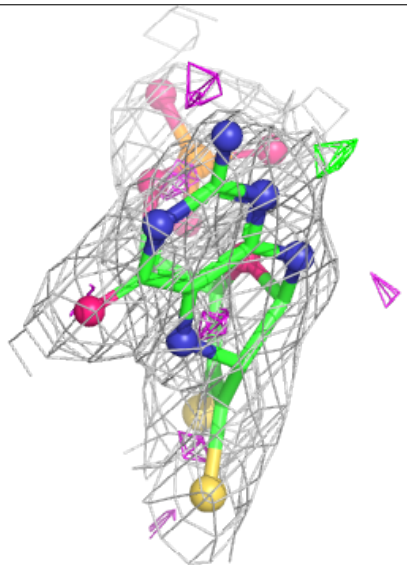


Electron density around MTE B 1303:

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

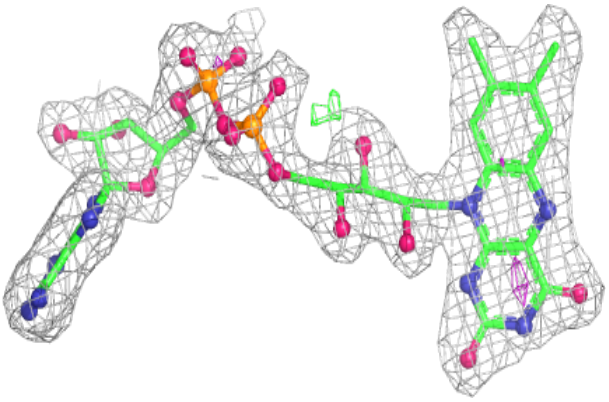


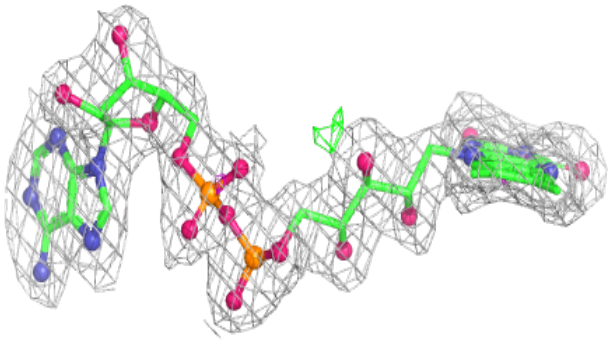


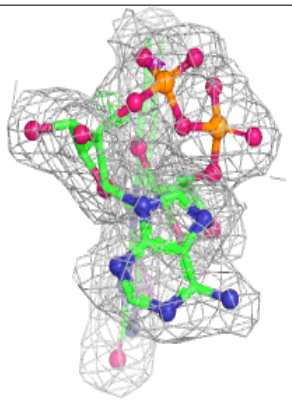


Electron density around FAD C 1305:

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

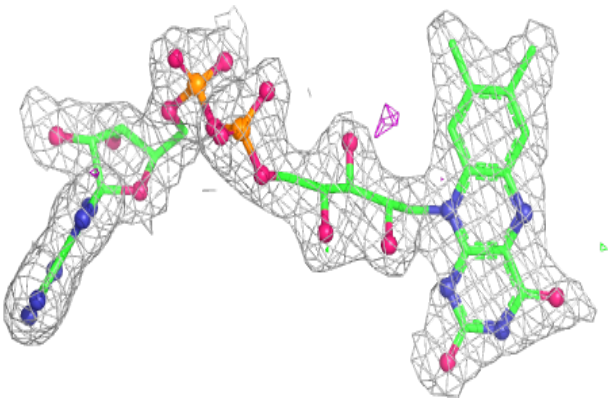


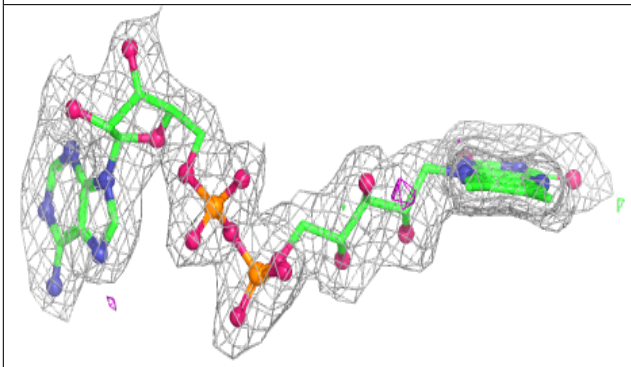


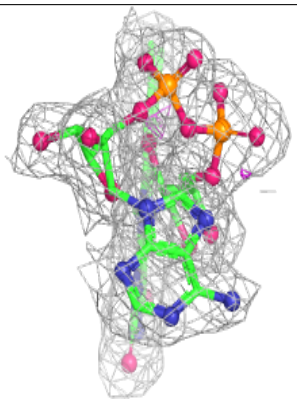


Electron density around FAD B 1305:

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

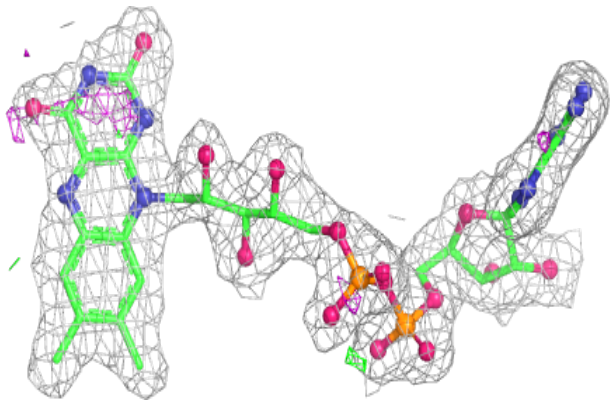


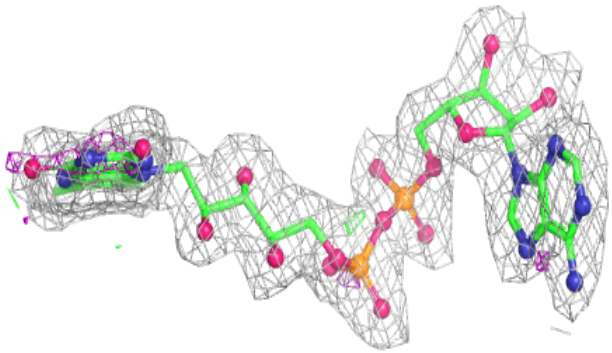


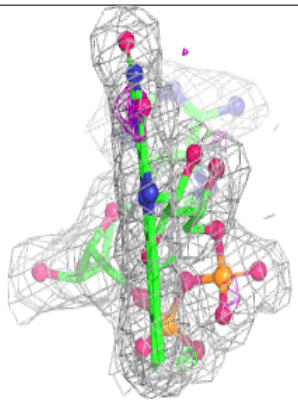


Electron density around FAD A 1305:

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

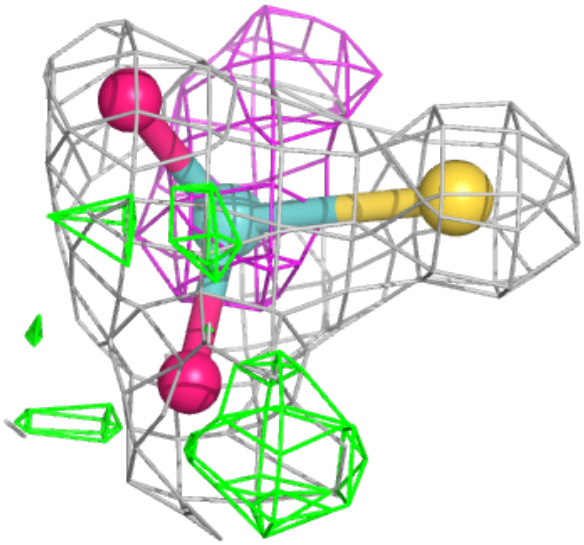


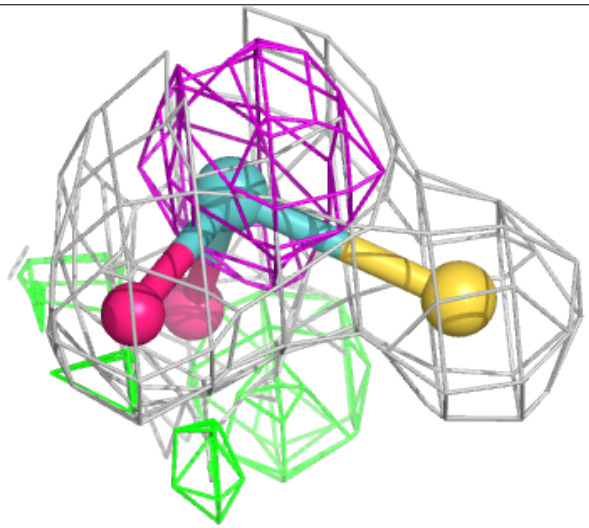


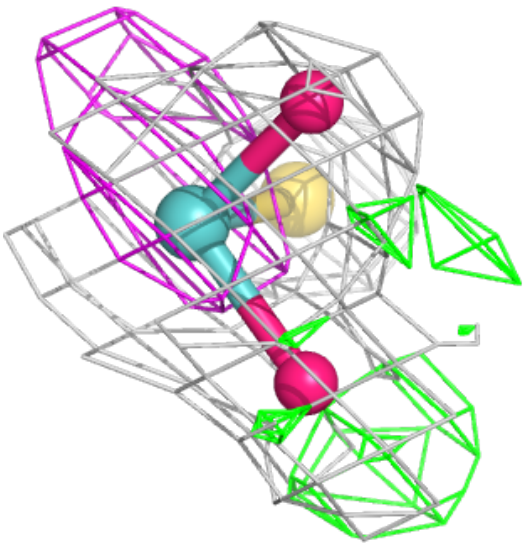


Electron density around MOS A 1304:

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

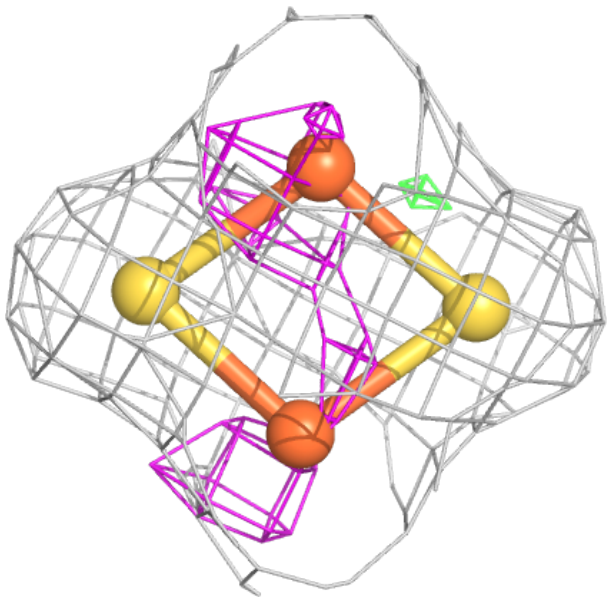


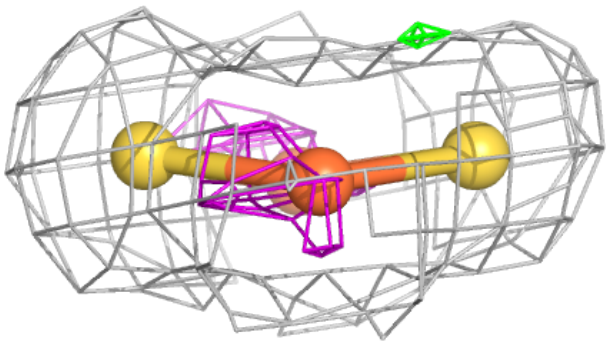


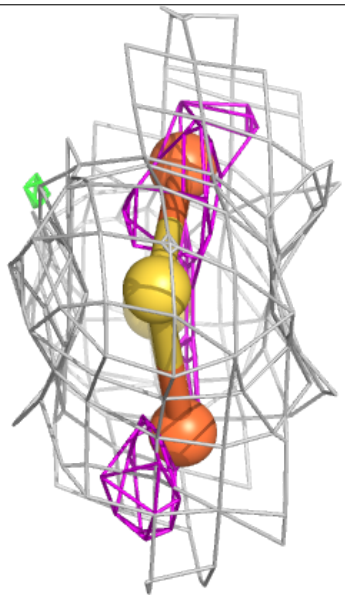


Electron density around FES D 1302:

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

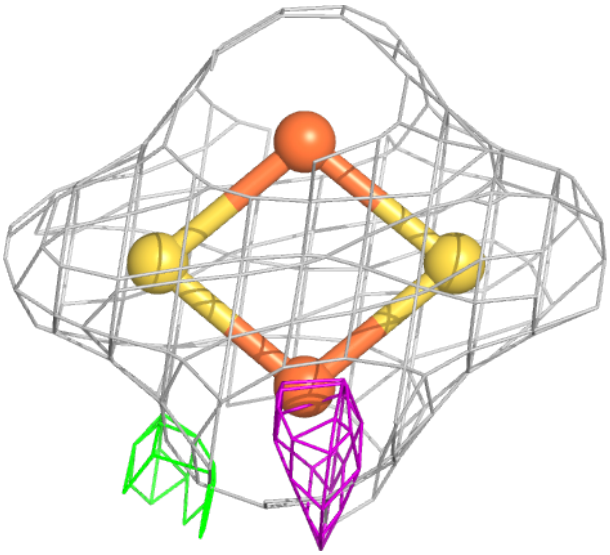


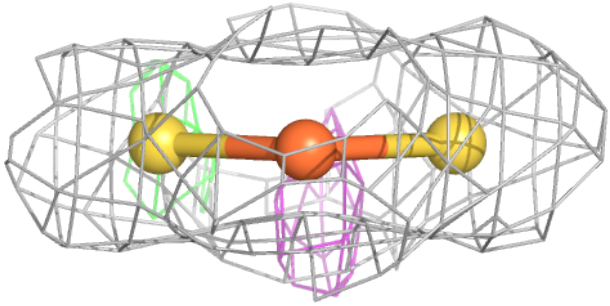


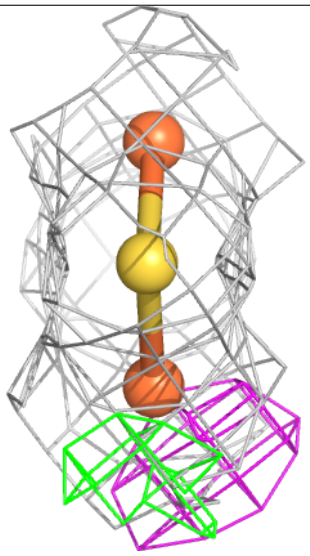


Electron density around FES D 1301:

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

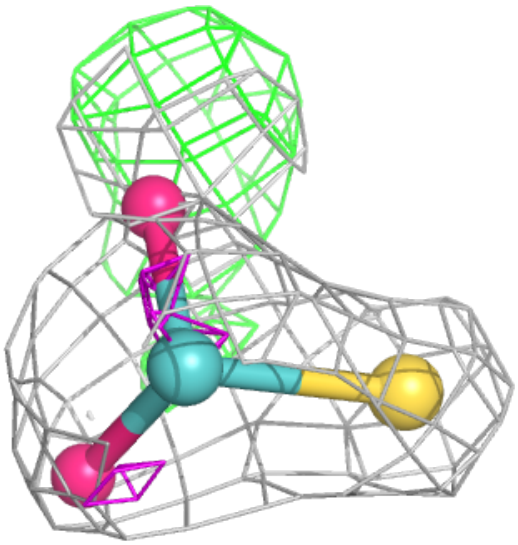


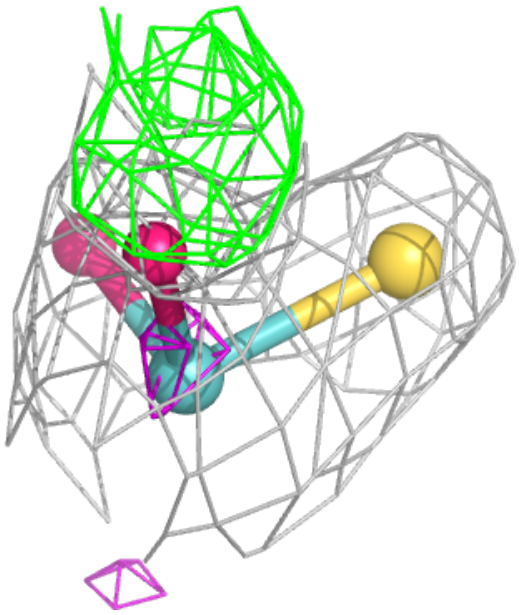


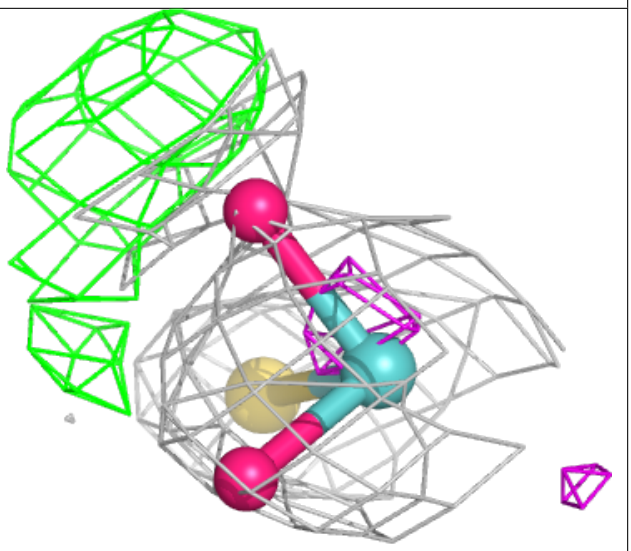


Electron density around MOS B 1304:

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

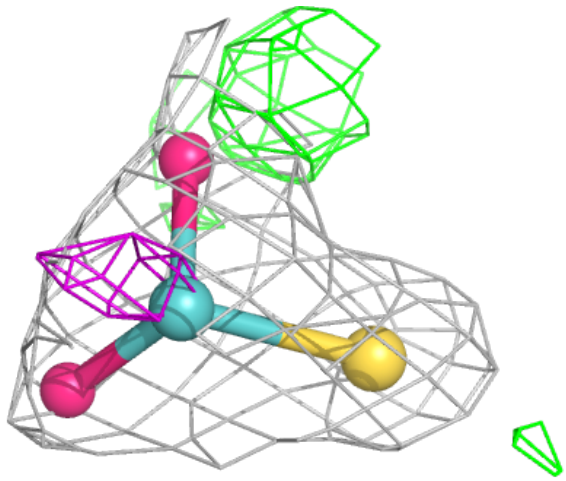


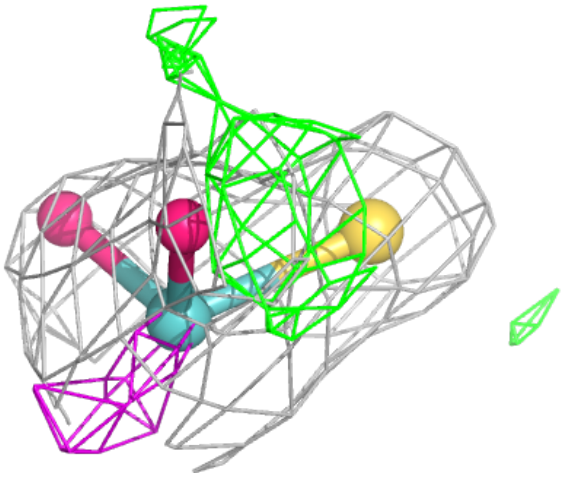


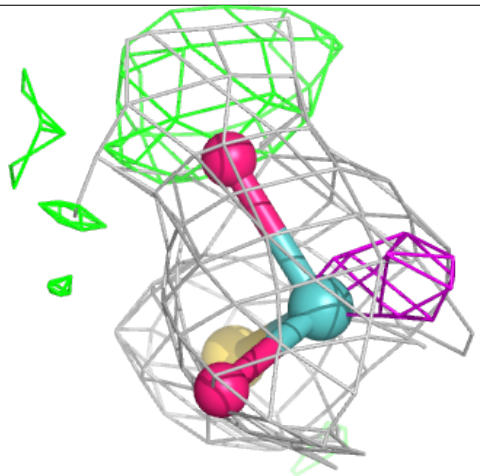


Electron density around MOS C 1304:

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

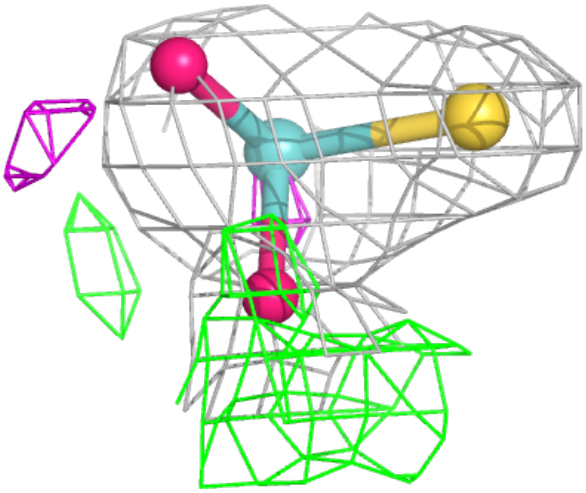


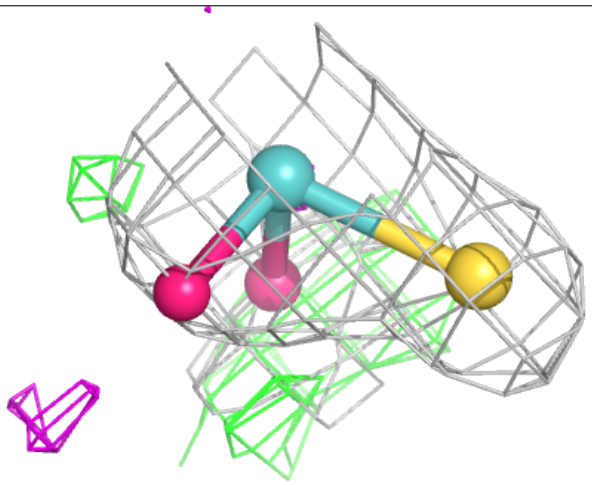


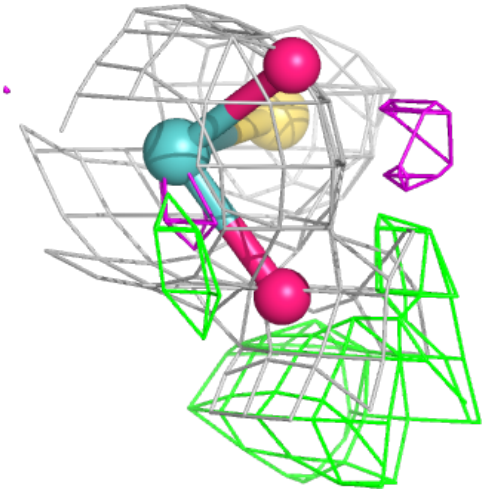


Electron density around MOS D 1304:

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

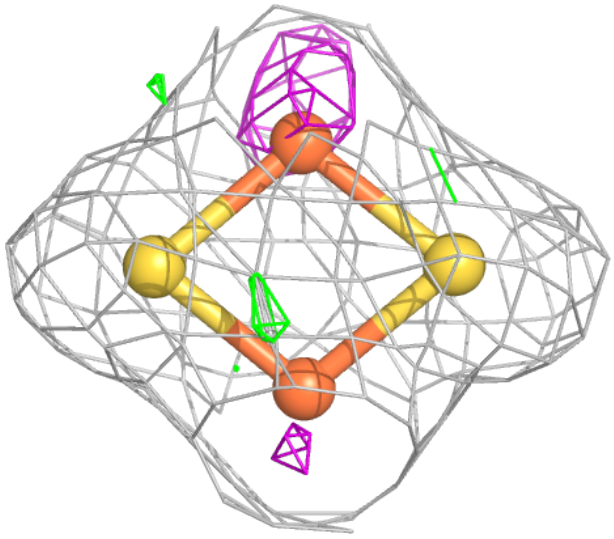


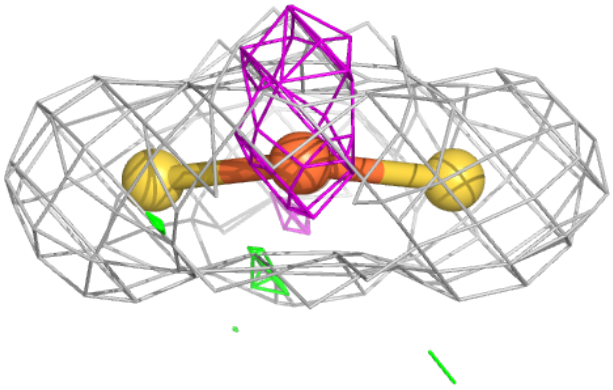


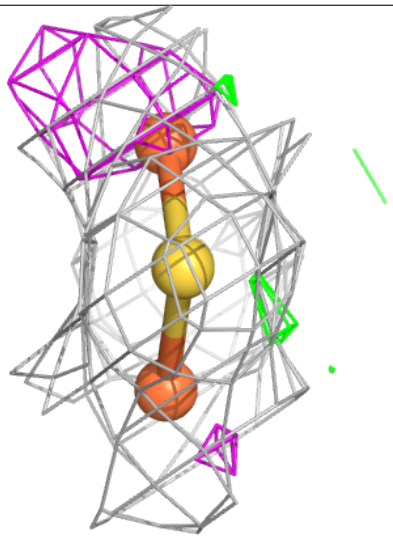


Electron density around FES A 1301:

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

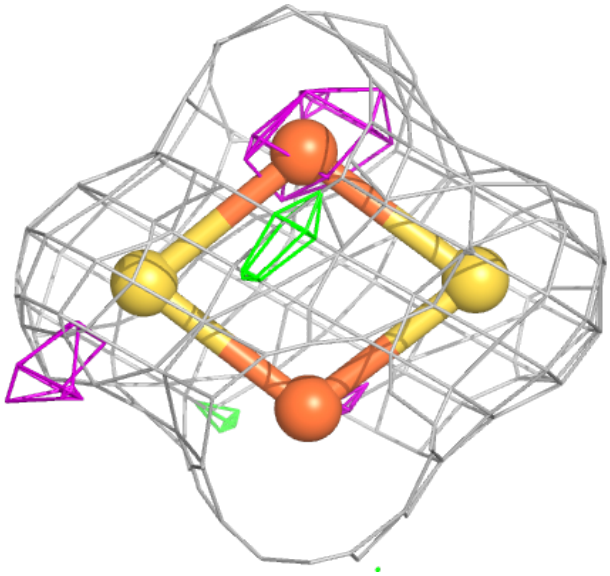


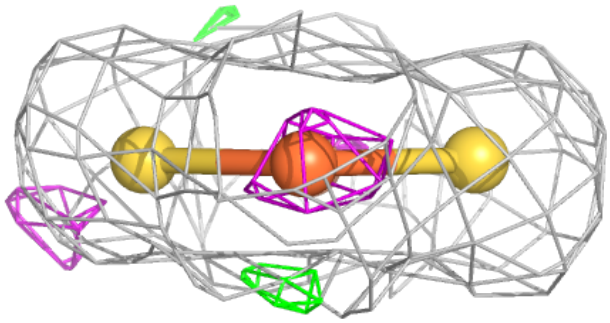


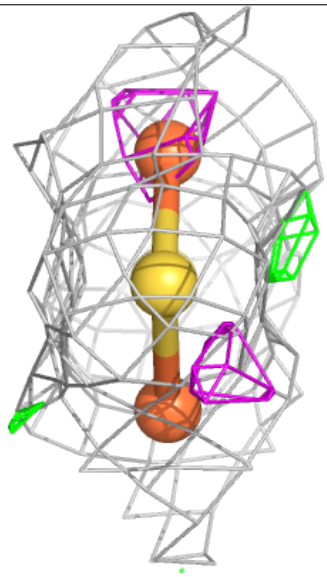


Electron density around FES A 1302:

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

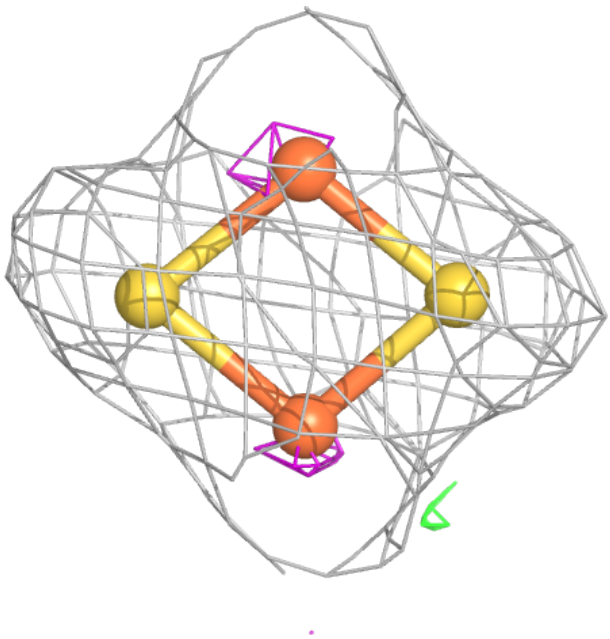


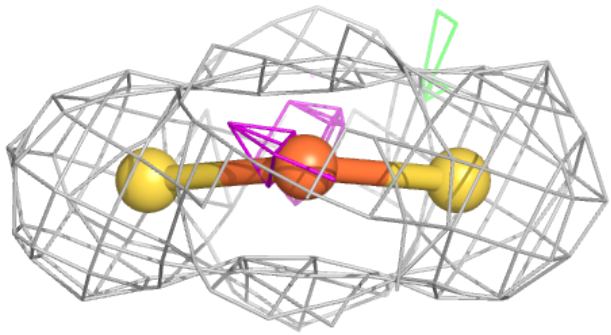


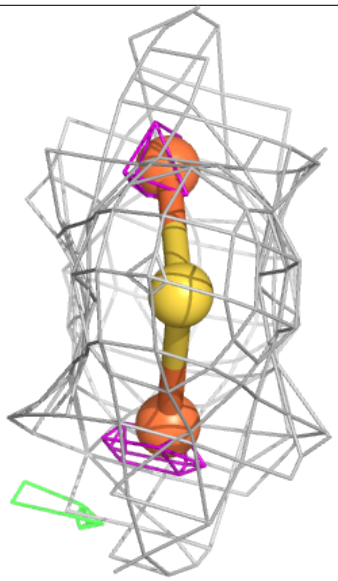


Electron density around FES B 1301:

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

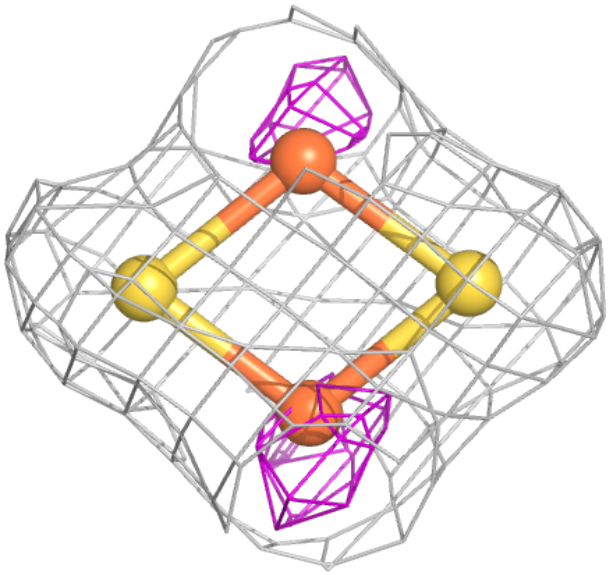


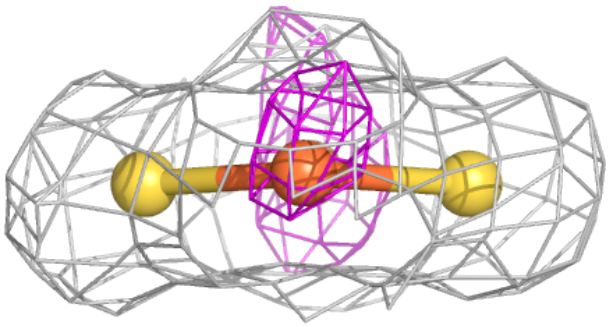


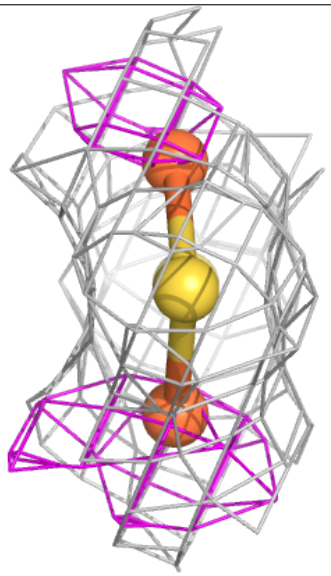


Electron density around FES B 1302:

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

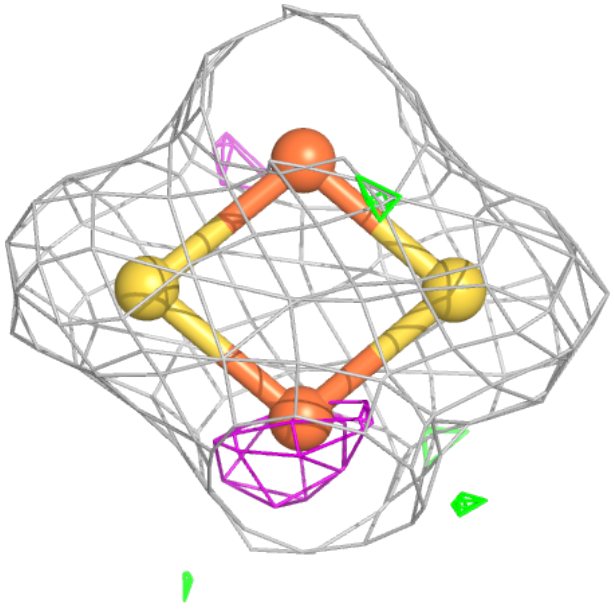


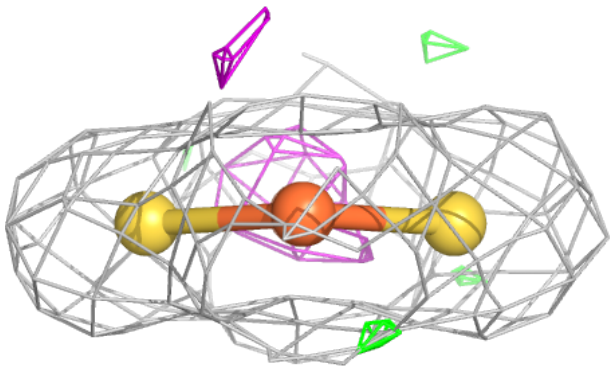


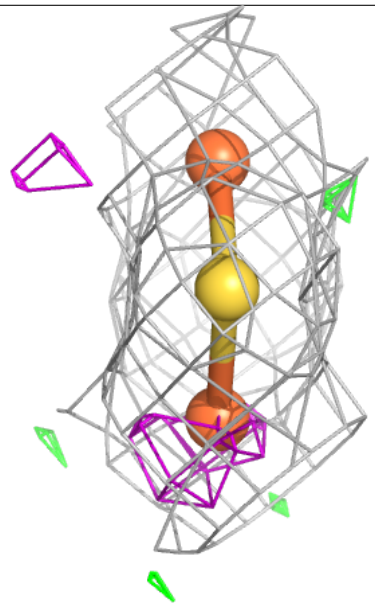


Electron density around FES C 1301:

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

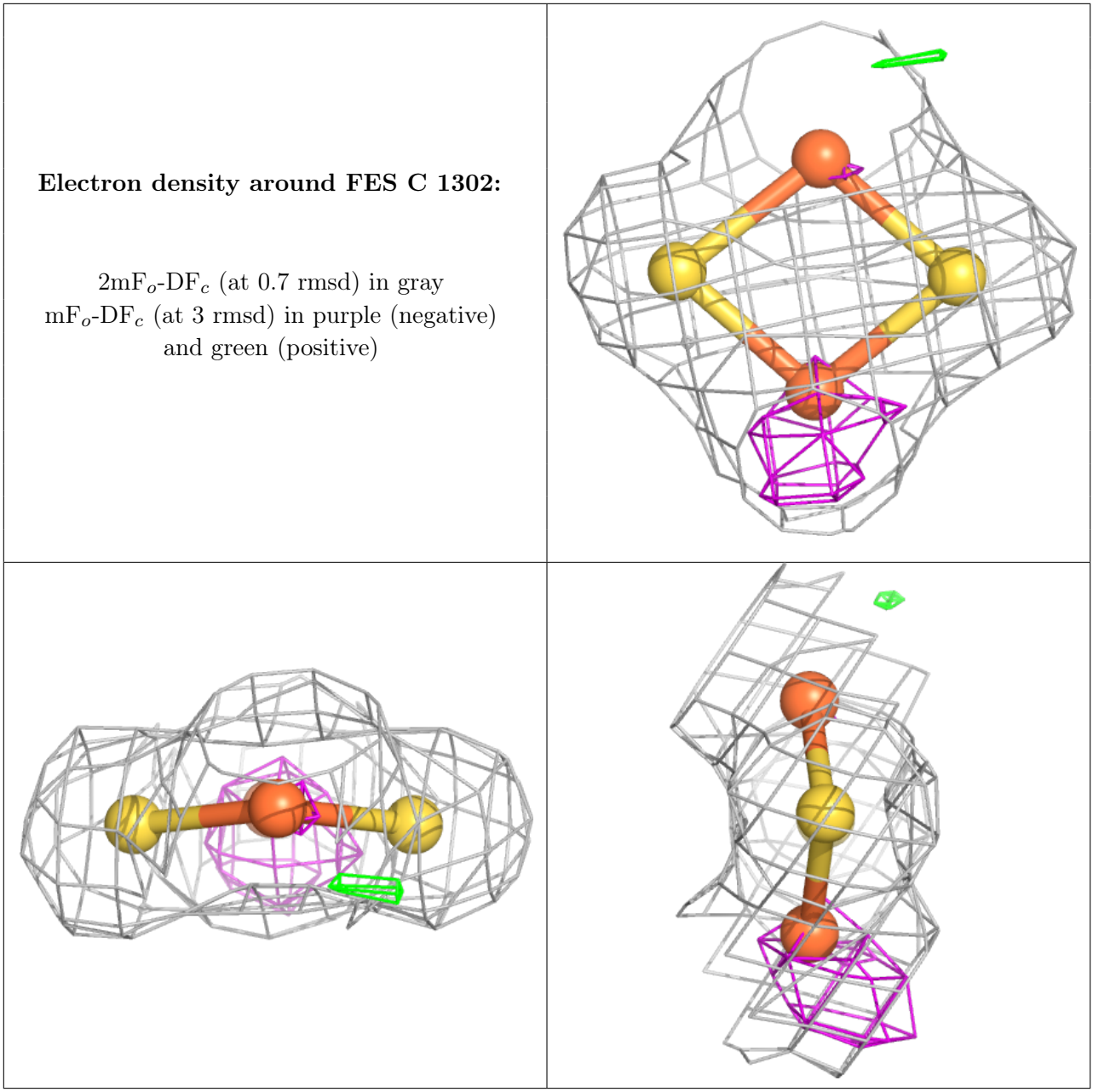






Electron density around FES C 1302:

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



6.5 Other polymers

There are no such residues in this entry.