wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2026 – 09:32 pm BST

PDB ID	:	8CFF / pdb_00008cff
Title	:	Crystal structure of arsenite oxidase from Alcaligenes faecalis (Af Aio) bound to arsenite
Authors	:	Engrola, F.; Correia, M.A.S.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2023-02-03
Resolution	:	1.57 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:

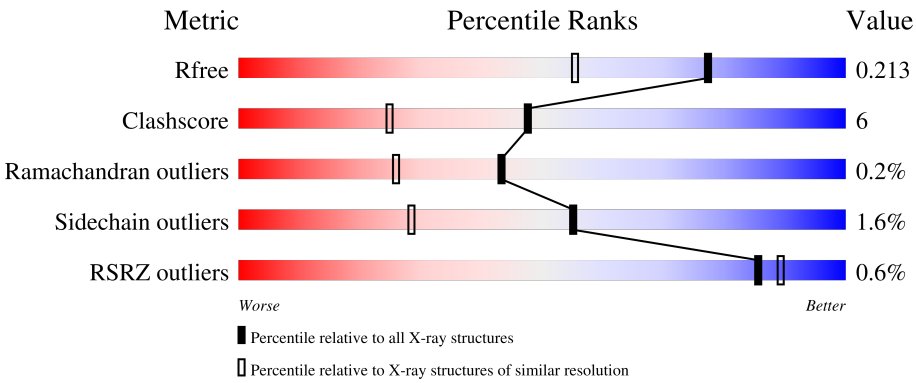
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.57 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}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	823	89% 10% •
1	C	823	88% 12% •
1	E	823	89% 10%
1	G	823	88% 11%
2	B	134	2% 90% 10% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	134	2% 93% 6%
2	F	134	3% 90% 9%
2	H	134	2% 87% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEG	B	2301	-	-	X	-
11	IPA	C	906	-	-	X	-
11	IPA	G	908	-	-	X	-
7	GOL	C	912	-	-	X	-
7	GOL	E	912	-	-	X	-
9	EDO	A	908[A]	-	-	X	-
9	EDO	A	908[B]	-	-	X	-
9	EDO	A	909	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34530 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 Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	823	6523	4106	1155	1220	42	0	7	0
1	C	822	6555	4124	1161	1226	44	5	10	0
1	E	822	6526	4108	1157	1218	43	0	7	0
1	G	822	6517	4101	1153	1221	42	1	8	0

- Molecule 2 is a protein called Arsenite oxidase subunit AioB.

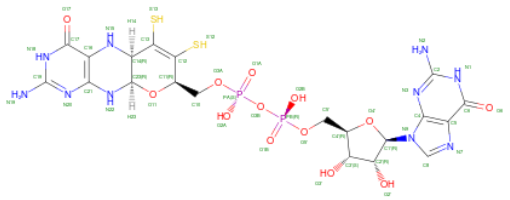
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	134	1018	637	170	202	9	0	3	0
2	D	134	1015	635	170	201	9	2	2	0
2	F	134	1009	632	169	199	9	1	2	0
2	H	134	1018	637	170	202	9	2	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q7SIF3
D	0	LEU	-	expression tag	UNP Q7SIF3
F	0	LEU	-	expression tag	UNP Q7SIF3
H	0	LEU	-	expression tag	UNP Q7SIF3

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).

MGD



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	47	20	10	13	2	2	0	0
3	A	1	47	20	10	13	2	2	0	0
3	C	1	47	20	10	13	2	2	0	0
3	C	1	47	20	10	13	2	2	0	0
3	E	1	47	20	10	13	2	2	0	0
3	E	1	47	20	10	13	2	2	0	0
3	G	1	47	20	10	13	2	2	0	0
3	G	1	47	20	10	13	2	2	0	0

- Molecule 4 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

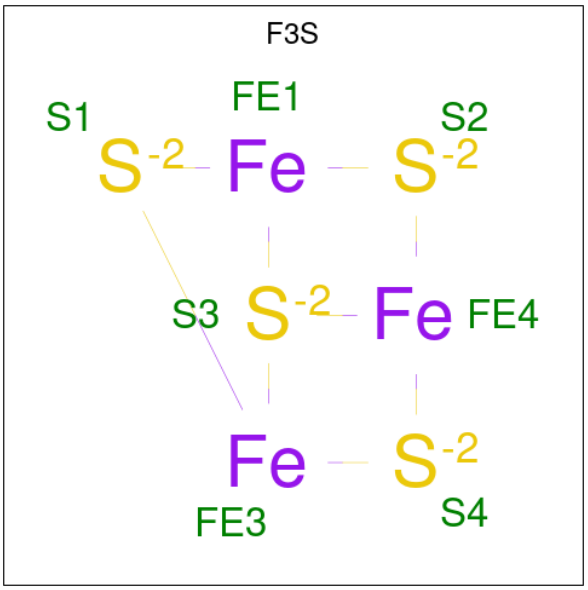
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
4	A	1	1	1	0	0
4	C	1	1	1	0	0
4	E	1	1	1	0	0

Continued on next page...

Continued from previous page...

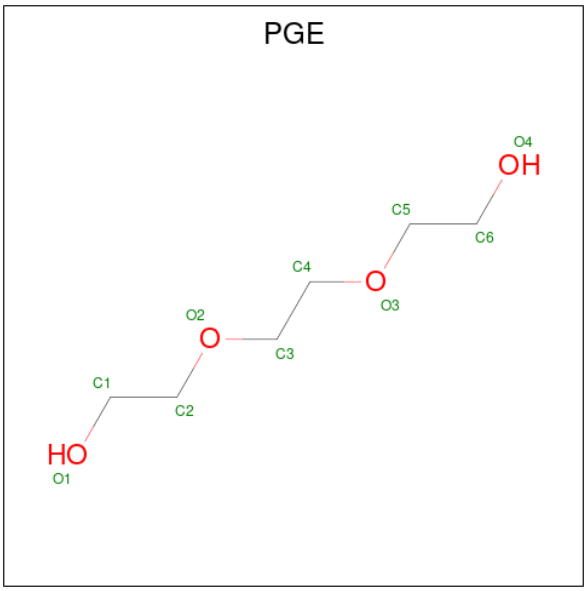
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
4	G	1	1	1	0	0

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



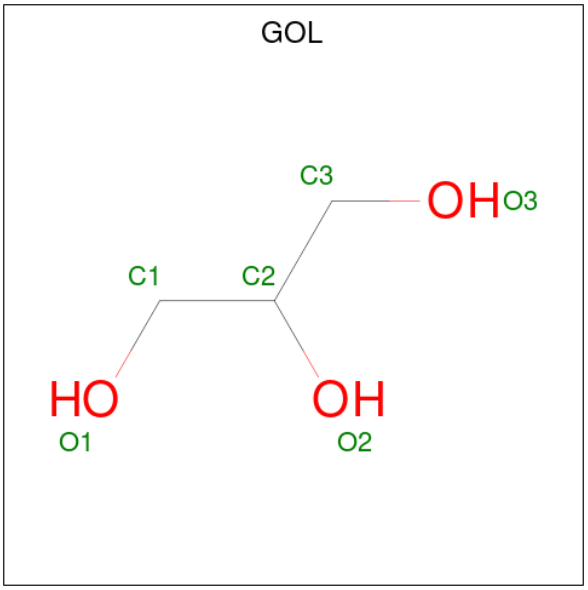
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	A	1	7	3	4	0	0
5	C	1	7	3	4	0	0
5	E	1	7	3	4	0	0
5	G	1	7	3	4	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	20	12	8	0	1
			Total	C	O		
6	G	1	10	6	4	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



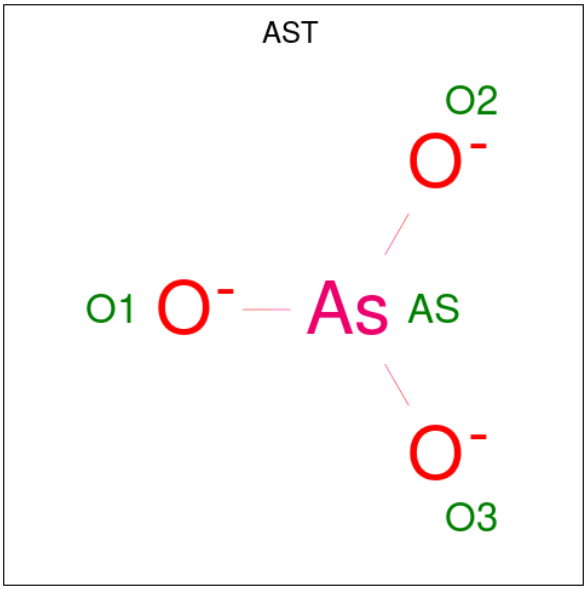
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	C	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

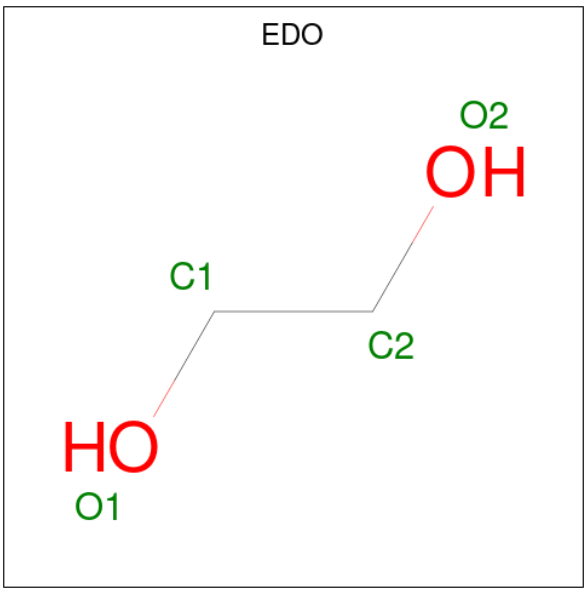
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	6	3	3	0	0
			Total	C	O		
7	C	1	6	3	3	0	0
			Total	C	O		
7	E	1	6	3	3	0	0
			Total	C	O		
7	E	1	6	3	3	0	0
			Total	C	O		
7	E	1	6	3	3	0	0
			Total	C	O		
7	G	1	6	3	3	0	0
			Total	C	O		
7	G	1	6	3	3	0	0

- Molecule 8 is ARSENITE (CCD ID: AST) (formula: AsO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	O		
8	A	1	4	1	3	0	0
			Total	As	O		
8	C	1	4	1	3	0	0
			Total	As	O		
8	E	1	4	1	3	0	0
			Total	As	O		
8	G	1	4	1	3	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



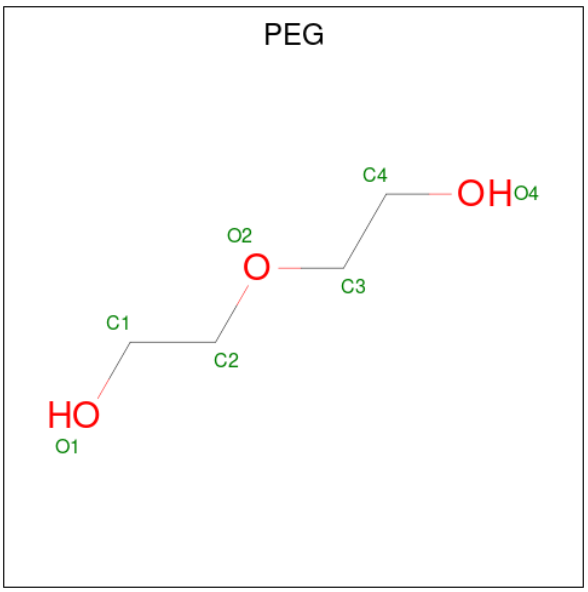
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 8	C 4	O 4	0	1
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 8	C 4	O 4	0	1
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

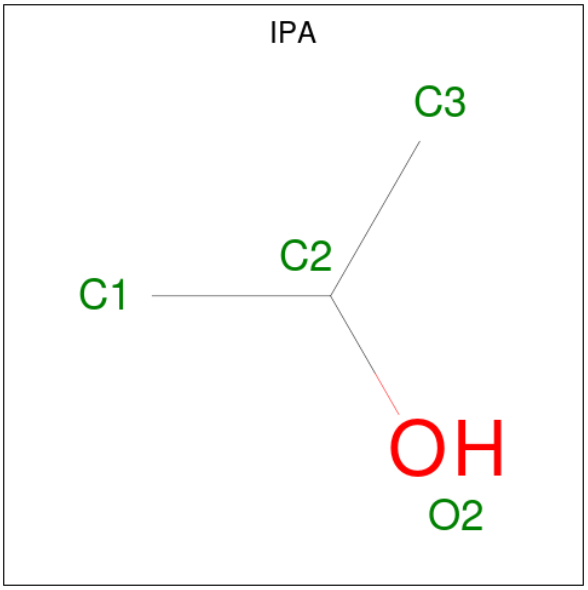
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	D	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	G	1	8	4	4	0	1
9	G	1	4	2	2	0	0
9	G	1	4	2	2	0	0
9	G	1	4	2	2	0	0
9	G	1	4	2	2	0	0
9	G	1	4	2	2	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



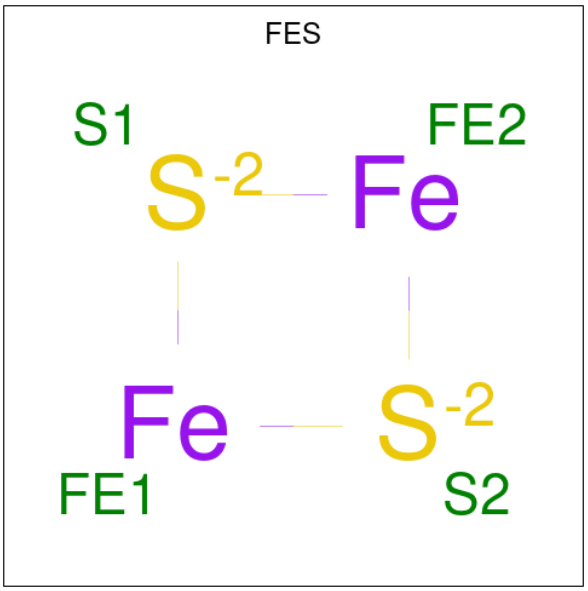
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	7	4	3	0	0
			Total	C	O		
10	B	1	7	4	3	0	0

- Molecule 11 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	4	3	1	0	0
			Total	C	O		
11	C	1	4	3	1	0	0
			Total	C	O		
11	E	1	4	3	1	0	0
			Total	C	O		
11	G	1	4	3	1	0	0

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
12	B	1	4	2	2	0	0
12	D	1	4	2	2	0	0
12	F	1	4	2	2	0	0
12	H	1	4	2	2	0	0

- Molecule 13 is water.

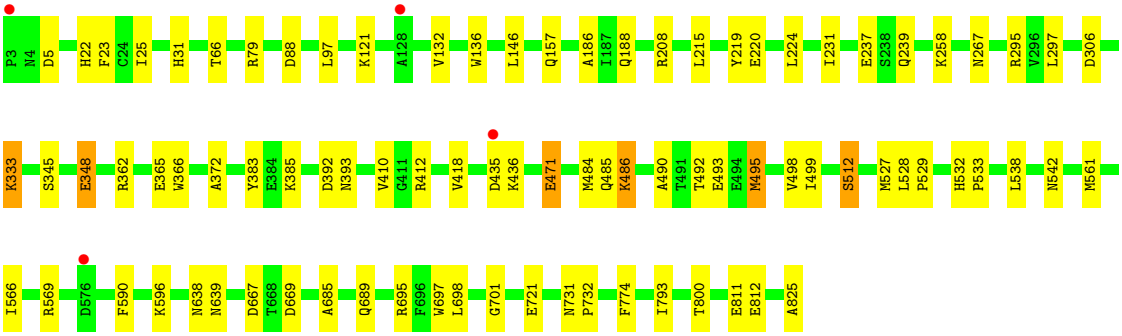
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	806	806	806	0	0
13	B	137	137	137	0	0
13	C	760	760	760	0	0
13	D	148	148	148	0	0
13	E	751	751	751	0	0
13	F	129	129	129	0	0
13	G	799	799	799	0	0
13	H	153	153	153	0	0

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.

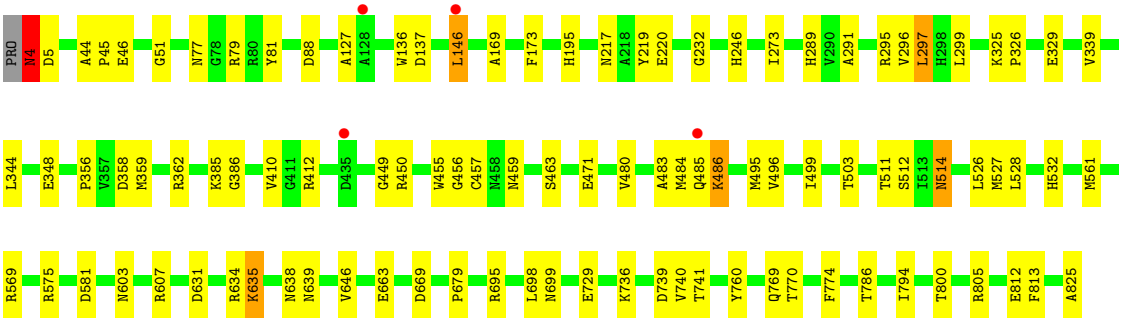
- Molecule 1: Arsenite oxidase subunit AioA

Chain A:



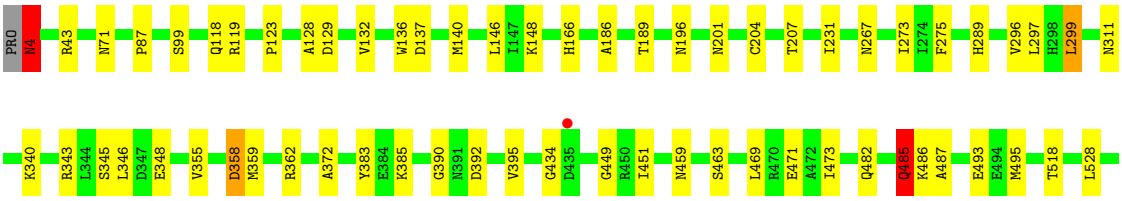
- Molecule 1: Arsenite oxidase subunit AioA

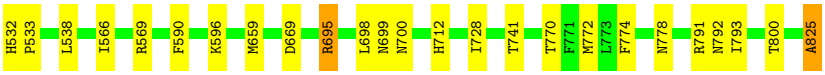
Chain C:



- Molecule 1: Arsenite oxidase subunit AioA

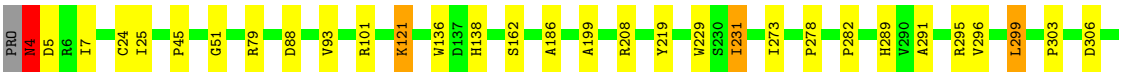
Chain E:

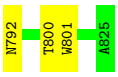




• Molecule 1: Arsenite oxidase subunit AioA

Chain G:



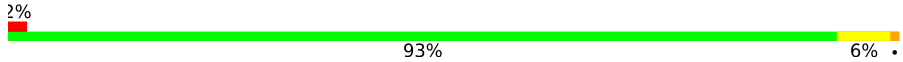


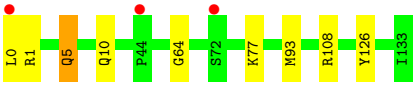
• Molecule 2: Arsenite oxidase subunit AioB

Chain B:

• Molecule 2: Arsenite oxidase subunit AioB

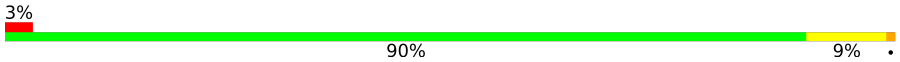
Chain D:





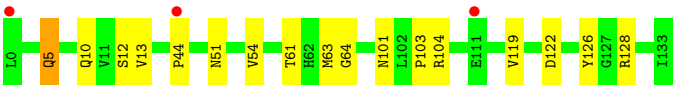
• Molecule 2: Arsenite oxidase subunit AioB

Chain F:



• Molecule 2: Arsenite oxidase subunit AioB

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.31Å 108.98Å 116.89Å 97.50° 90.21° 96.06°	Depositor
Resolution (Å)	65.62 – 1.57 65.62 – 1.57	Depositor EDS
% Data completeness (in resolution range)	73.2 (65.62-1.57) 73.7 (65.62-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.204 0.178 , 0.213	Depositor DCC
R_{free} test set	22459 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.8	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	34530	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.54% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, FES, EDO, IPA, GOL, AST, PEG, F3S, MO, MGD

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	1.19	10/6691 (0.1%)	1.30	12/9069 (0.1%)
1	C	1.17	14/6722 (0.2%)	1.32	12/9107 (0.1%)
1	E	1.19	16/6696 (0.2%)	1.31	13/9073 (0.1%)
1	G	1.21	15/6690 (0.2%)	1.31	9/9066 (0.1%)
2	B	1.17	2/1042 (0.2%)	1.26	0/1419
2	D	2.18	2/1036 (0.2%)	1.38	3/1412 (0.2%)
2	F	1.18	1/1033 (0.1%)	1.25	2/1407 (0.1%)
2	H	1.21	2/1042 (0.2%)	1.27	1/1419 (0.1%)
All	All	1.24	62/30952 (0.2%)	1.30	52/41972 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	GLN	CD-NE2	59.11	2.57	1.33
1	G	121	LYS	CE-NZ	-17.48	0.96	1.49
2	D	5	GLN	CD-OE1	-9.73	1.05	1.23
1	A	418	VAL	C-O	7.22	1.31	1.24
1	E	395	VAL	C-O	7.14	1.32	1.24

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLN	OE1-CD-NE2	15.05	137.65	122.60
1	G	121	LYS	CD-CE-NZ	13.48	155.03	111.90
2	D	5	GLN	CB-CG-CD	-12.10	92.03	112.60
1	C	4	ASN	CA-CB-CG	10.01	122.61	112.60
1	A	669	ASP	CA-CB-CG	8.23	120.83	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6523	0	6319	80	0
1	C	6555	0	6342	72	1
1	E	6526	0	6328	66	0
1	G	6517	0	6311	66	1
2	B	1018	0	999	14	0
2	D	1015	0	995	8	0
2	F	1009	0	994	7	0
2	H	1018	0	999	10	0
3	A	94	0	44	1	0
3	C	94	0	44	3	0
3	E	94	0	44	2	0
3	G	94	0	44	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	7	0	0	0	0
5	C	7	0	0	0	0
5	E	7	0	0	0	0
5	G	7	0	0	0	0
6	A	20	0	28	5	0
6	G	10	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	2	0
7	C	18	0	24	6	0
7	E	18	0	24	8	0
7	G	12	0	16	4	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
8	E	4	0	0	0	0
8	G	4	0	0	0	0
9	A	32	0	45	18	0
9	C	28	0	42	7	0
9	D	4	0	6	1	0
9	E	20	0	30	0	0
9	G	28	0	41	8	0
10	A	7	0	10	3	0
10	B	7	0	10	4	0
11	A	4	0	8	3	0
11	C	4	0	8	4	0
11	E	4	0	8	0	0
11	G	4	0	8	7	0
12	B	4	0	0	0	0
12	D	4	0	0	0	0
12	F	4	0	0	0	0
12	H	4	0	0	0	0
13	A	806	0	0	19	3
13	B	137	0	0	4	0
13	C	760	0	0	28	11
13	D	148	0	0	2	1
13	E	751	0	0	14	4
13	F	129	0	0	3	0
13	G	799	0	0	30	7
13	H	153	0	0	4	4
All	All	34530	0	29793	336	16

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 6.

The worst 5 of 336 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)
9:A:908[A]:EDO:O1	9:A:909:EDO:C1	1.91	1.19
9:A:908[A]:EDO:O1	9:A:909:EDO:H11	1.40	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:910:EDO:H21	13:C:1110:HOH:O	1.44	1.12
11:A:913:IPA:H33	13:A:1527:HOH:O	1.52	1.10
1:A:136:TRP:CH2	1:A:528[B]:LEU:HD21	1.88	1.09

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:GLN:NE2	1:G:471[A]:GLU:OE2[1_455]	1.51	0.69
13:C:1758:HOH:O	13:G:1797:HOH:O[1_455]	1.64	0.56
13:C:1642:HOH:O	13:G:1732:HOH:O[1_455]	1.68	0.52
13:A:1806:HOH:O	13:G:1799:HOH:O[1_465]	1.69	0.51
13:A:1788:HOH:O	13:E:1744:HOH:O[1_455]	1.70	0.50

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	828/823 (101%)	796 (96%)	30 (4%)	2 (0%)	43	26
1	C	831/823 (101%)	802 (96%)	29 (4%)	0	100	100
1	E	828/823 (101%)	797 (96%)	28 (3%)	3 (0%)	30	12
1	G	828/823 (101%)	801 (97%)	26 (3%)	1 (0%)	48	28
2	B	135/134 (101%)	130 (96%)	5 (4%)	0	100	100
2	D	134/134 (100%)	128 (96%)	6 (4%)	0	100	100
2	F	134/134 (100%)	128 (96%)	6 (4%)	0	100	100
2	H	135/134 (101%)	126 (93%)	9 (7%)	0	100	100
All	All	3853/3828 (101%)	3708 (96%)	139 (4%)	6 (0%)	43	26

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	392	ASP
1	A	392	ASP
1	G	392	ASP
1	E	518	THR
1	A	793	ILE

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	683/676 (101%)	673 (98%)	10 (2%)	57	31
1	C	686/676 (102%)	675 (98%)	11 (2%)	55	28
1	E	683/676 (101%)	672 (98%)	11 (2%)	55	28
1	G	683/676 (101%)	668 (98%)	15 (2%)	45	15
2	B	115/112 (103%)	114 (99%)	1 (1%)	70	52
2	D	114/112 (102%)	113 (99%)	1 (1%)	70	52
2	F	114/112 (102%)	111 (97%)	3 (3%)	40	11
2	H	115/112 (103%)	112 (97%)	3 (3%)	40	11
All	All	3193/3152 (101%)	3138 (98%)	55 (2%)	55	25

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	343	ARG
2	F	35	VAL
2	H	128	ARG
1	G	652	LYS
1	E	485	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	792	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	311	ASN
1	E	267	ASN
2	H	5	GLN
2	F	51	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 4 are monoatomic - leaving 66 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	$\#\|Z\| > 2$
3	MGD	C	902	4	45,52,52	0.78	1 (2%)	54,81,81	1.07	3 (5%)
6	PGE	G	907	-	9,9,9	0.83	0	8,8,8	0.33	0
7	GOL	A	906	-	5,5,5	0.47	0	5,5,5	0.94	0
9	EDO	E	911	-	3,3,3	0.52	0	2,2,2	0.51	0
5	F3S	E	904	1	0,9,9	-	-	-		
8	AST	C	905	4	0,3,3	-	-	0,3,3	-	-
9	EDO	C	915	-	3,3,3	0.16	0	2,2,2	0.41	0
12	FES	F	201	2	0,4,4	-	-	-		
3	MGD	E	903	4	45,52,52	0.83	1 (2%)	54,81,81	1.15	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FES	D	201	2	0,4,4	-	-	-		
7	GOL	C	908	-	5,5,5	0.20	0	5,5,5	0.30	0
9	EDO	A	908[A]	-	3,3,3	0.26	0	2,2,2	0.40	0
6	PGE	A	905[A]	-	9,9,9	0.61	0	8,8,8	0.58	0
9	EDO	E	910	-	3,3,3	0.94	0	2,2,2	0.83	0
9	EDO	G	914	-	3,3,3	0.71	0	2,2,2	0.37	0
7	GOL	E	913	-	5,5,5	0.21	0	5,5,5	0.62	0
8	AST	G	906	4	0,3,3	-	-	0,3,3	-	-
9	EDO	A	914	-	3,3,3	0.58	0	2,2,2	0.67	0
9	EDO	G	911	-	3,3,3	0.19	0	2,2,2	0.53	0
10	PEG	B	2301	-	6,6,6	0.30	0	5,5,5	0.25	0
9	EDO	E	907	-	3,3,3	0.94	0	2,2,2	0.57	0
12	FES	B	2302	2	0,4,4	-	-	-		
7	GOL	G	905	-	5,5,5	0.49	0	5,5,5	0.86	0
9	EDO	C	907	-	3,3,3	0.70	0	2,2,2	1.19	0
12	FES	H	201	2	0,4,4	-	-	-		
9	EDO	C	911[B]	-	3,3,3	0.30	0	2,2,2	0.39	0
9	EDO	A	915	-	3,3,3	0.69	0	2,2,2	0.64	0
11	IPA	E	905	-	3,3,3	0.46	0	3,3,3	0.58	0
9	EDO	A	911	-	3,3,3	0.19	0	2,2,2	0.73	0
3	MGD	A	902	4	45,52,52	0.74	0	54,81,81	1.23	5 (9%)
9	EDO	C	914	-	3,3,3	1.01	0	2,2,2	0.91	0
7	GOL	C	912	-	5,5,5	0.38	0	5,5,5	0.97	0
9	EDO	E	908	-	3,3,3	0.74	0	2,2,2	1.13	0
9	EDO	D	202	-	3,3,3	0.73	0	2,2,2	0.49	0
7	GOL	C	909	-	5,5,5	0.24	0	5,5,5	0.82	0
9	EDO	G	909[B]	-	3,3,3	0.36	0	2,2,2	0.59	0
10	PEG	A	910	-	6,6,6	0.32	0	5,5,5	0.24	0
5	F3S	C	904	1	0,9,9	-	-	-		
9	EDO	C	913	-	3,3,3	0.29	0	2,2,2	0.37	0
3	MGD	C	903	4	45,52,52	0.86	1 (2%)	54,81,81	1.12	3 (5%)
3	MGD	E	901	4	45,52,52	0.89	1 (2%)	54,81,81	1.07	3 (5%)
8	AST	E	906	4	0,3,3	-	-	0,3,3	-	-
7	GOL	E	914	-	5,5,5	0.20	0	5,5,5	0.23	0
11	IPA	A	913	-	3,3,3	0.42	0	3,3,3	0.40	0
9	EDO	A	916	-	3,3,3	1.05	0	2,2,2	0.89	0
5	F3S	G	904	1	0,9,9	-	-	-		
9	EDO	A	909	-	3,3,3	0.71	0	2,2,2	0.94	0
6	PGE	A	905[B]	-	9,9,9	0.19	0	8,8,8	0.25	0
9	EDO	C	910	-	3,3,3	0.57	0	2,2,2	0.63	0
9	EDO	G	915	-	3,3,3	0.28	0	2,2,2	0.21	0
5	F3S	A	904	1	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MGD	G	902	4	45,52,52	0.70	0	54,81,81	1.09	6 (11%)
9	EDO	A	908[B]	-	3,3,3	1.05	0	2,2,2	0.82	0
9	EDO	G	910	-	3,3,3	0.15	0	2,2,2	0.36	0
8	AST	A	907	4	0,3,3	-	-	0,3,3	-	-
9	EDO	C	911[A]	-	3,3,3	0.37	0	2,2,2	0.81	0
3	MGD	G	903	4	45,52,52	0.80	2 (4%)	54,81,81	0.95	4 (7%)
11	IPA	C	906	-	3,3,3	0.98	0	3,3,3	0.63	0
9	EDO	E	909	-	3,3,3	0.78	0	2,2,2	0.53	0
9	EDO	G	909[A]	-	3,3,3	0.23	0	2,2,2	0.61	0
9	EDO	G	912	-	3,3,3	0.76	0	2,2,2	0.44	0
7	GOL	G	913	-	5,5,5	0.27	0	5,5,5	1.07	0
3	MGD	A	901	4	45,52,52	0.78	1 (2%)	54,81,81	1.26	2 (3%)
7	GOL	E	912	-	5,5,5	0.14	0	5,5,5	0.55	0
11	IPA	G	908	-	3,3,3	0.87	0	3,3,3	1.18	0
9	EDO	A	912	-	3,3,3	0.42	0	2,2,2	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGD	C	902	4	-	4/22/66/66	0/6/6/6
6	PGE	G	907	-	-	5/7/7/7	-
7	GOL	A	906	-	-	2/4/4/4	-
9	EDO	E	911	-	-	1/1/1/1	-
5	F3S	E	904	1	-	-	0/3/3/3
9	EDO	C	915	-	-	0/1/1/1	-
12	FES	F	201	2	-	-	0/1/1/1
3	MGD	E	903	4	-	4/22/66/66	0/6/6/6
12	FES	D	201	2	-	-	0/1/1/1
7	GOL	C	908	-	-	4/4/4/4	-
9	EDO	A	908[A]	-	-	1/1/1/1	-
6	PGE	A	905[A]	-	-	3/7/7/7	-
9	EDO	E	910	-	-	1/1/1/1	-
9	EDO	G	914	-	-	0/1/1/1	-
7	GOL	E	913	-	-	0/4/4/4	-
9	EDO	A	914	-	-	0/1/1/1	-
9	EDO	G	911	-	-	0/1/1/1	-
10	PEG	B	2301	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	E	907	-	-	1/1/1/1	-
12	FES	B	2302	2	-	-	0/1/1/1
7	GOL	G	905	-	-	4/4/4/4	-
9	EDO	C	907	-	-	0/1/1/1	-
12	FES	H	201	2	-	-	0/1/1/1
9	EDO	C	911[B]	-	-	1/1/1/1	-
9	EDO	A	915	-	-	0/1/1/1	-
9	EDO	A	911	-	-	0/1/1/1	-
3	MGD	A	902	4	-	4/22/66/66	0/6/6/6
9	EDO	C	914	-	-	1/1/1/1	-
7	GOL	C	912	-	-	4/4/4/4	-
9	EDO	E	908	-	-	1/1/1/1	-
9	EDO	D	202	-	-	0/1/1/1	-
7	GOL	C	909	-	-	4/4/4/4	-
9	EDO	G	909[B]	-	-	1/1/1/1	-
10	PEG	A	910	-	-	2/4/4/4	-
5	F3S	C	904	1	-	-	0/3/3/3
9	EDO	C	913	-	-	1/1/1/1	-
3	MGD	C	903	4	-	5/22/66/66	0/6/6/6
3	MGD	E	901	4	-	4/22/66/66	0/6/6/6
7	GOL	E	914	-	-	0/4/4/4	-
9	EDO	A	916	-	-	0/1/1/1	-
9	EDO	A	909	-	-	1/1/1/1	-
5	F3S	G	904	1	-	-	0/3/3/3
6	PGE	A	905[B]	-	-	5/7/7/7	-
9	EDO	C	910	-	-	1/1/1/1	-
9	EDO	G	915	-	-	1/1/1/1	-
9	EDO	A	908[B]	-	-	0/1/1/1	-
3	MGD	G	902	4	-	4/22/66/66	0/6/6/6
9	EDO	G	910	-	-	1/1/1/1	-
5	F3S	A	904	1	-	-	0/3/3/3
9	EDO	C	911[A]	-	-	0/1/1/1	-
3	MGD	G	903	4	-	5/22/66/66	0/6/6/6
9	EDO	E	909	-	-	0/1/1/1	-
9	EDO	G	909[A]	-	-	1/1/1/1	-
9	EDO	G	912	-	-	1/1/1/1	-
7	GOL	G	913	-	-	4/4/4/4	-
3	MGD	A	901	4	-	4/22/66/66	0/6/6/6
7	GOL	E	912	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	912	-	-	0/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	MGD	C23-C14	4.02	1.56	1.53
3	C	903	MGD	C23-C14	3.40	1.56	1.53
3	C	902	MGD	C23-C14	-2.82	1.51	1.53
3	E	903	MGD	C10-C11	-2.62	1.48	1.52
3	G	903	MGD	C10-C11	-2.40	1.48	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	MGD	O11-C23-C14	6.18	113.08	108.96
3	C	903	MGD	O11-C23-C14	5.35	112.53	108.96
3	A	902	MGD	O11-C23-C14	4.19	111.76	108.96
3	E	901	MGD	C19-N20-C21	3.66	120.04	113.43
3	A	902	MGD	C19-N20-C21	3.34	119.47	113.43

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	MGD	C5'-O5'-PB-O1B
3	A	902	MGD	C5'-O5'-PB-O1B
3	A	902	MGD	C5'-O5'-PB-O3B
3	C	902	MGD	C5'-O5'-PB-O1B
3	C	902	MGD	C5'-O5'-PB-O3B

There are no ring outliers.

33 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	907	PGE	1	0
7	A	906	GOL	2	0
9	A	908[A]	EDO	7	0
6	A	905[A]	PGE	5	0
9	G	914	EDO	2	0
9	A	914	EDO	2	0
10	B	2301	PEG	4	0

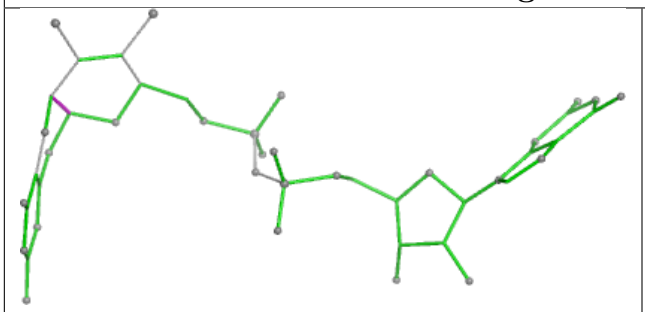
Continued on next page...

Continued from previous page...

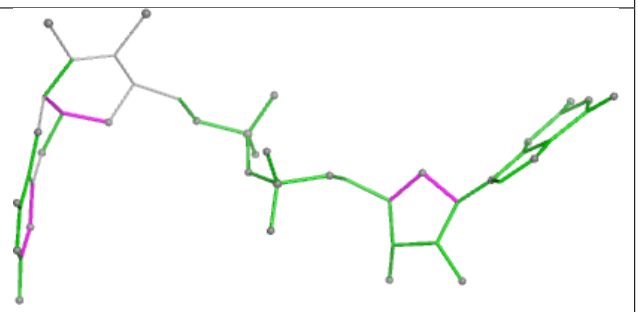
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	905	GOL	1	0
9	C	907	EDO	2	0
9	C	911[B]	EDO	1	0
7	C	912	GOL	4	0
9	D	202	EDO	1	0
7	C	909	GOL	2	0
9	G	909[B]	EDO	2	0
10	A	910	PEG	3	0
3	C	903	MGD	3	0
3	E	901	MGD	2	0
7	E	914	GOL	1	0
11	A	913	IPA	3	0
9	A	916	EDO	1	0
9	A	909	EDO	8	0
9	C	910	EDO	1	0
9	G	915	EDO	3	0
9	A	908[B]	EDO	5	0
9	C	911[A]	EDO	3	0
3	G	903	MGD	1	0
11	C	906	IPA	4	0
9	G	912	EDO	1	0
7	G	913	GOL	3	0
3	A	901	MGD	1	0
7	E	912	GOL	7	0
11	G	908	IPA	7	0
9	A	912	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

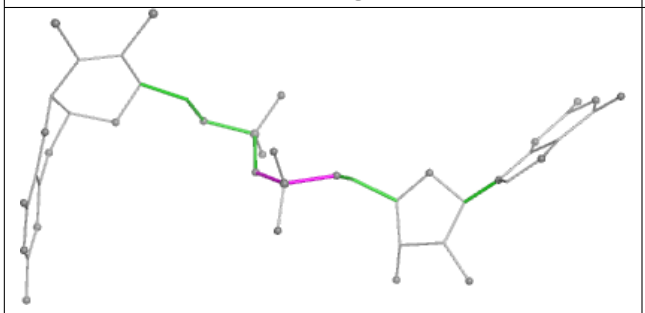
Ligand MGD C 902



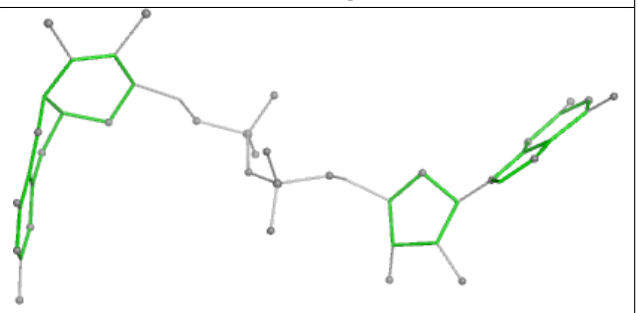
Bond lengths



Bond angles

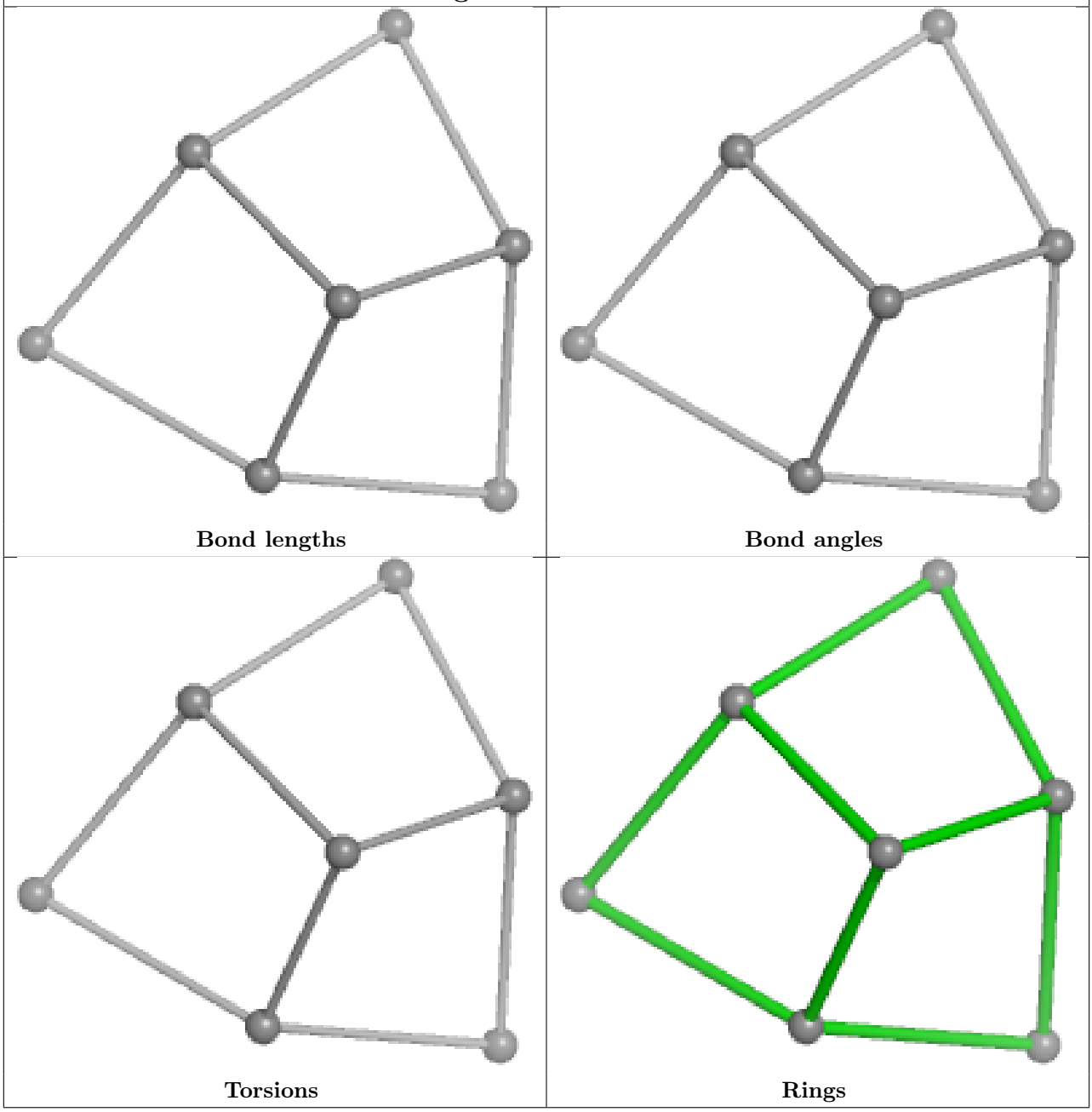


Torsions

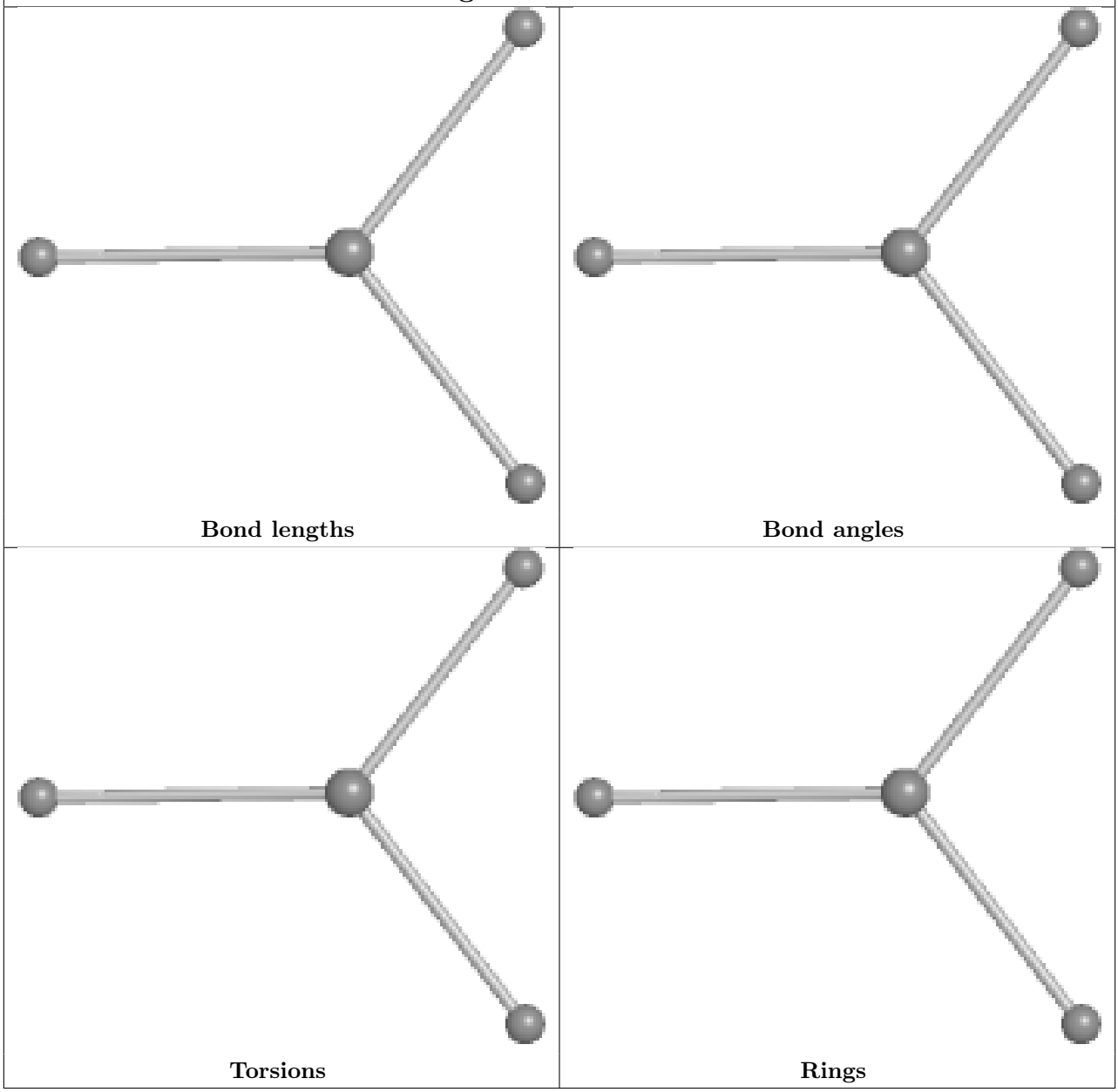


Rings

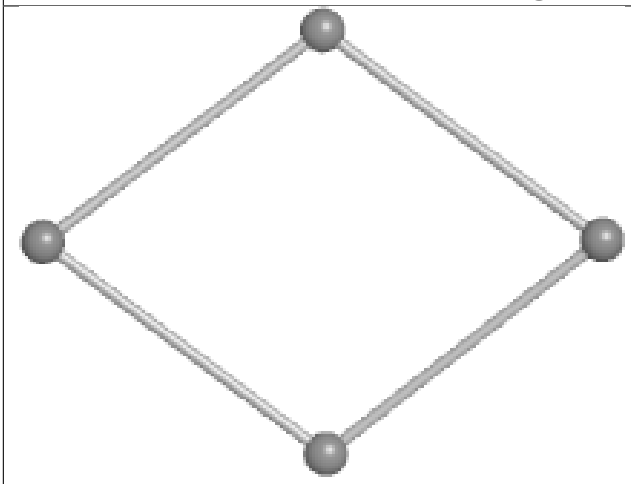
Ligand F3S E 904



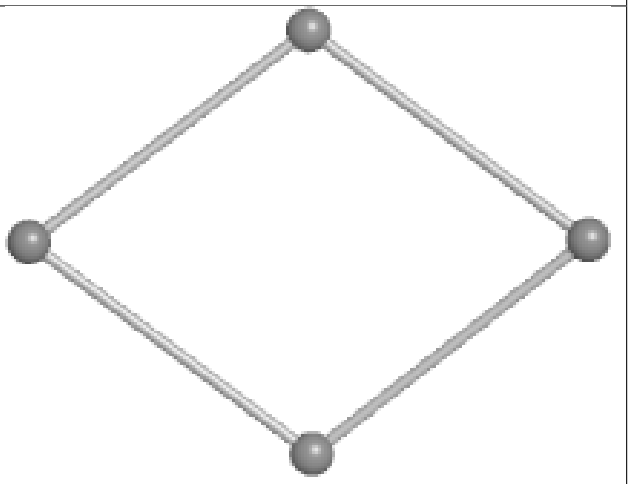
Ligand AST C 905



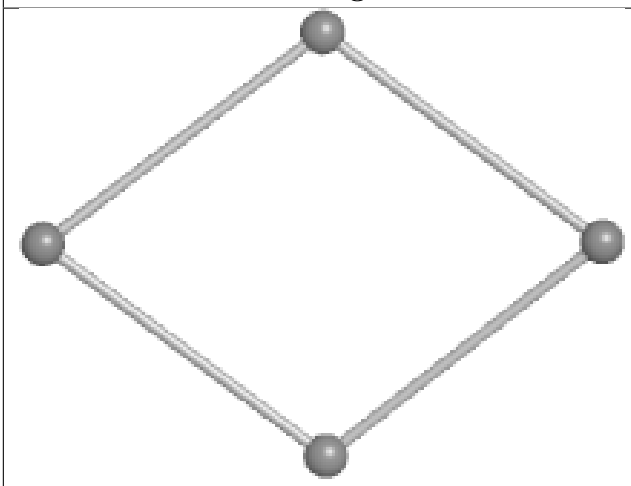
Ligand FES F 201



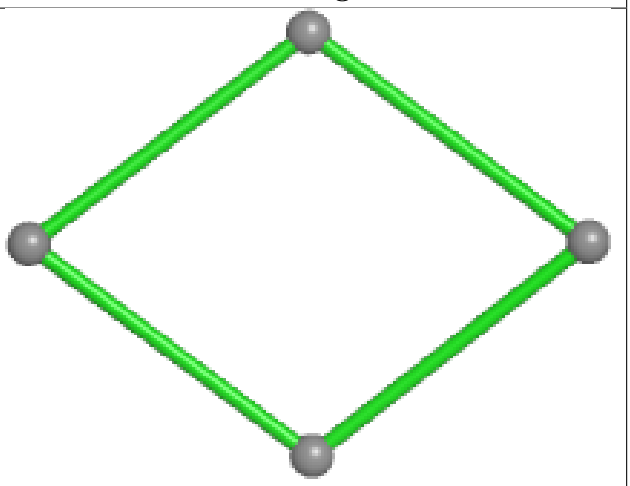
Bond lengths



Bond angles

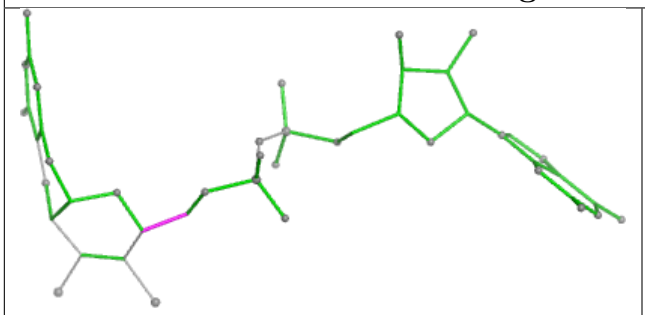


Torsions

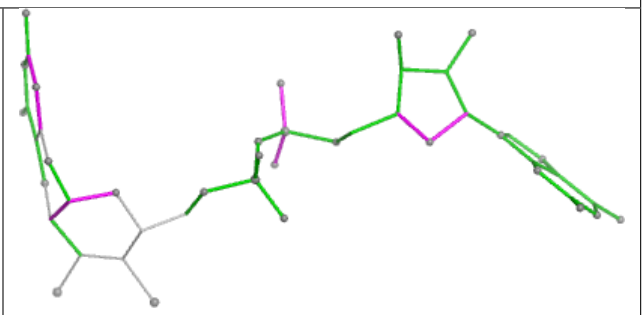


Rings

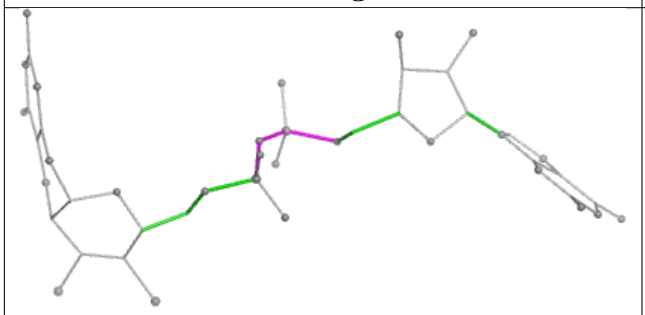
Ligand MGD E 903



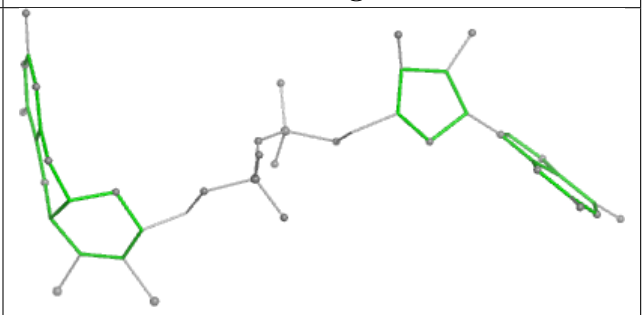
Bond lengths



Bond angles

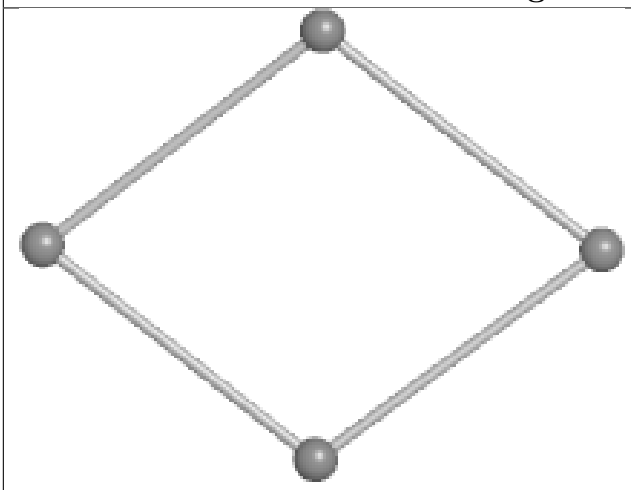


Torsions

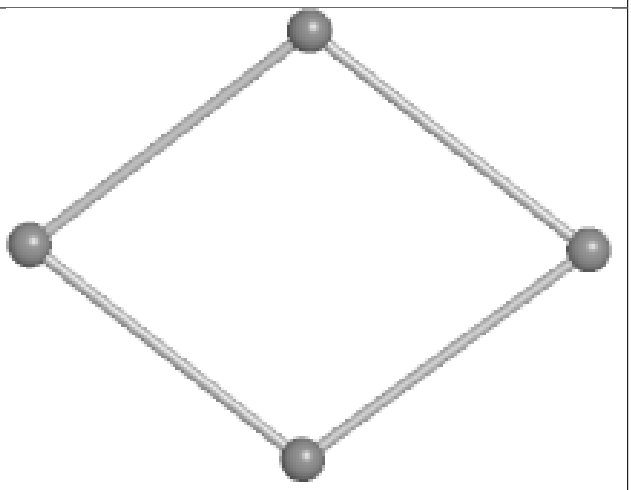


Rings

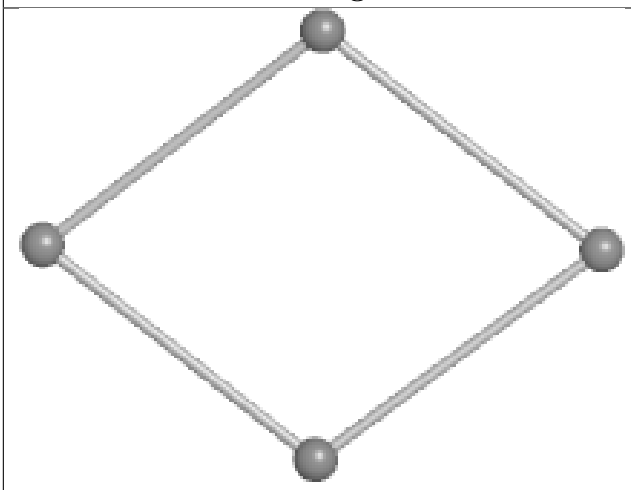
Ligand FES D 201



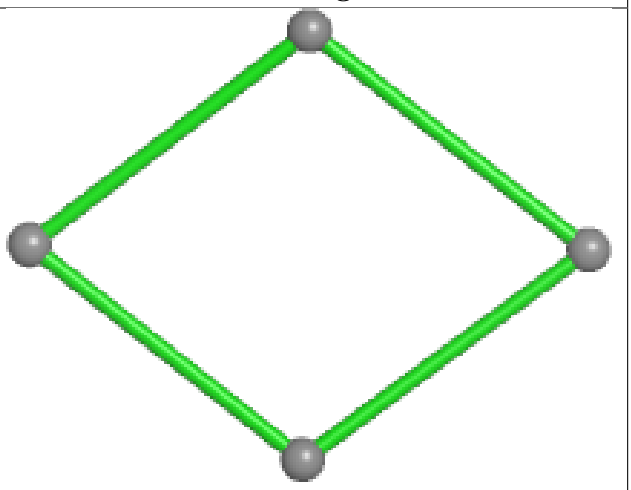
Bond lengths



Bond angles

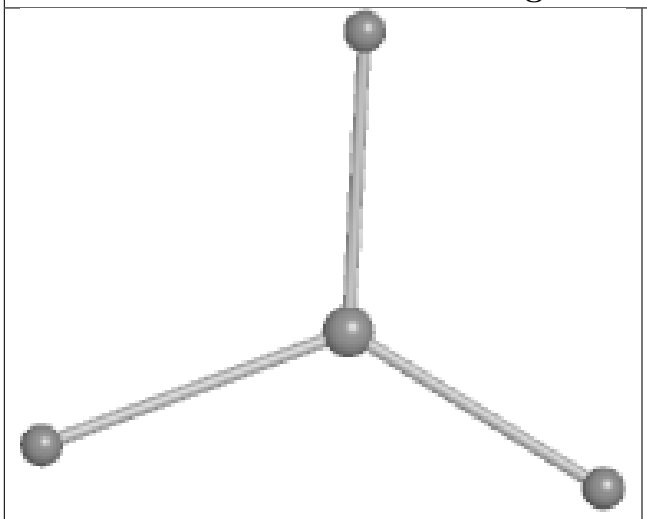


Torsions

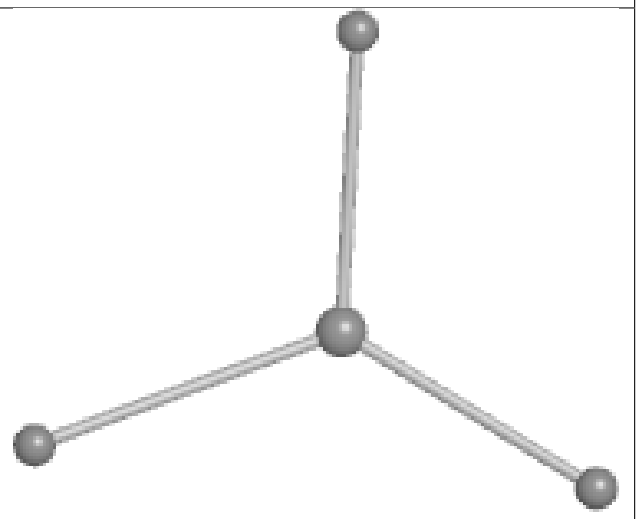


Rings

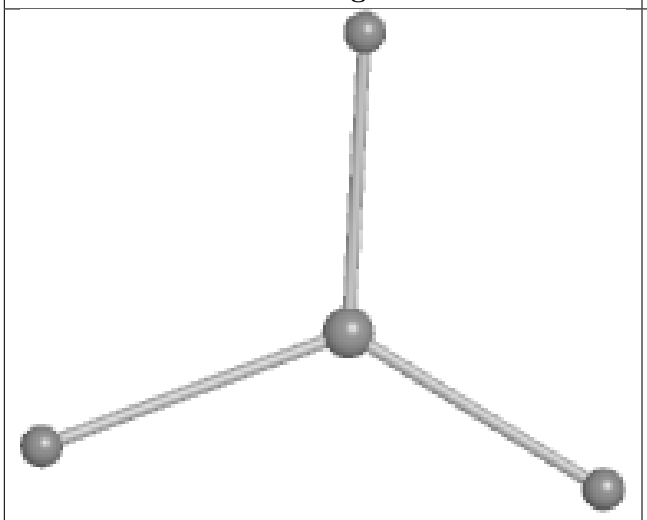
Ligand AST G 906



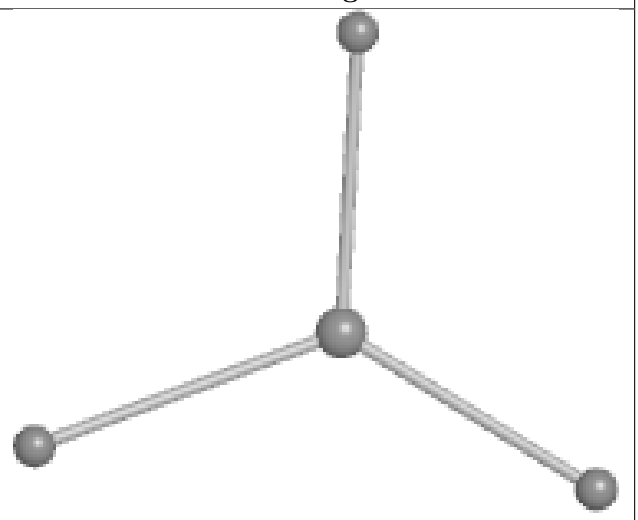
Bond lengths



Bond angles

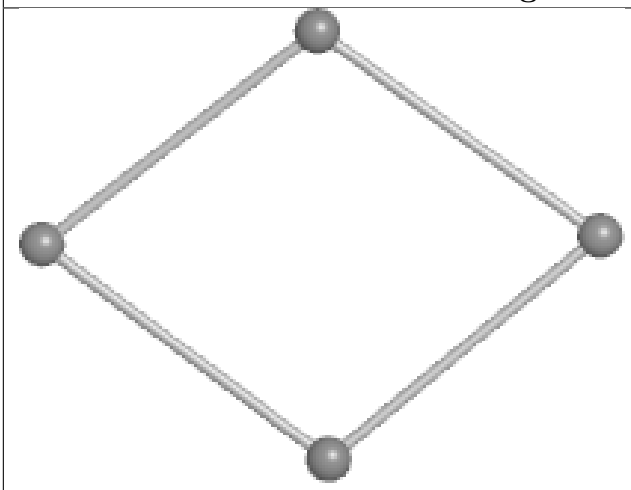


Torsions

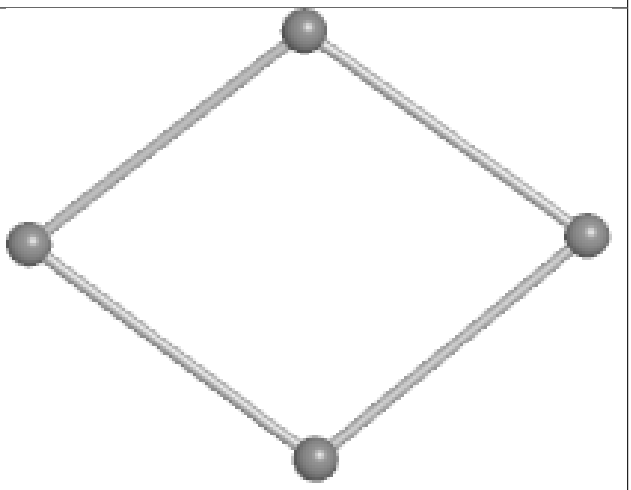


Rings

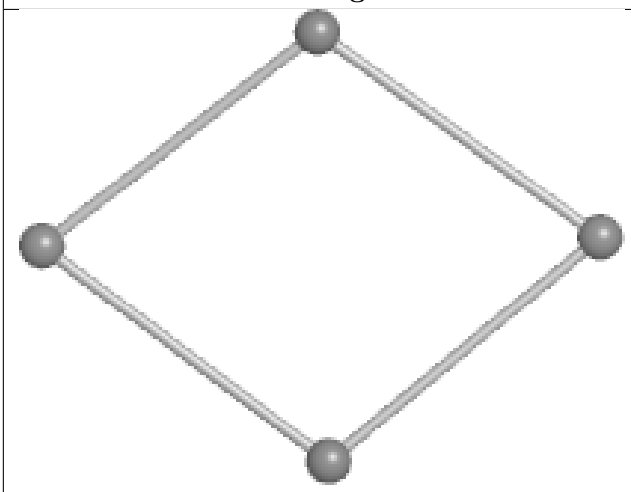
Ligand FES B 2302



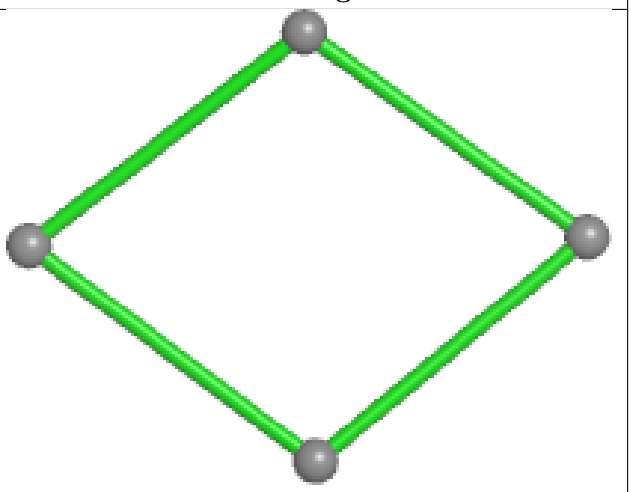
Bond lengths



Bond angles

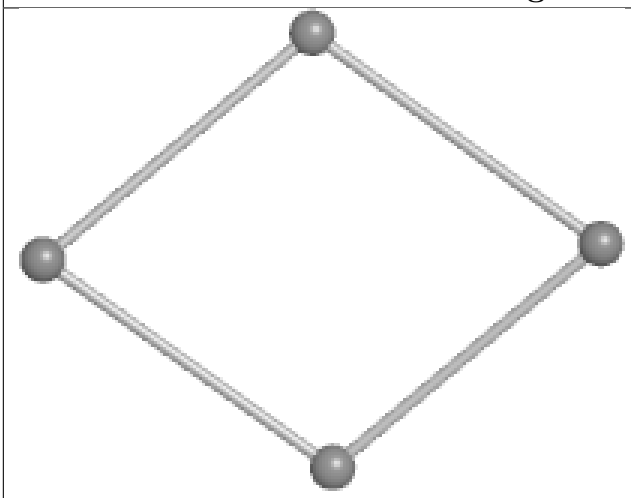


Torsions

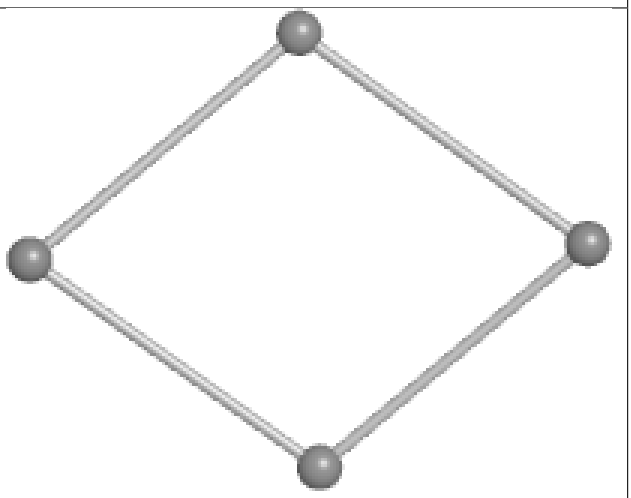


Rings

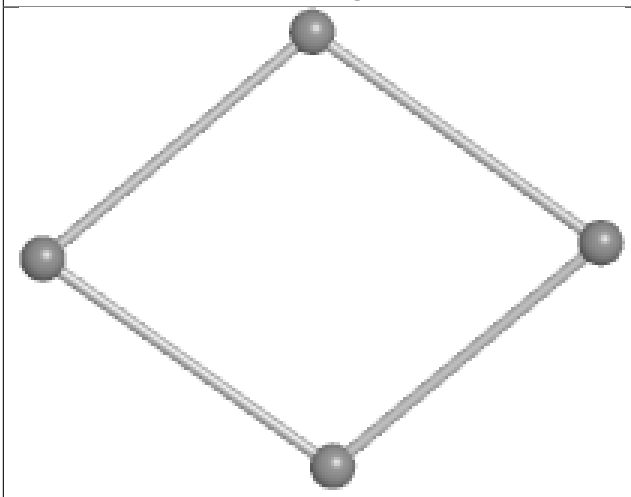
Ligand FES H 201



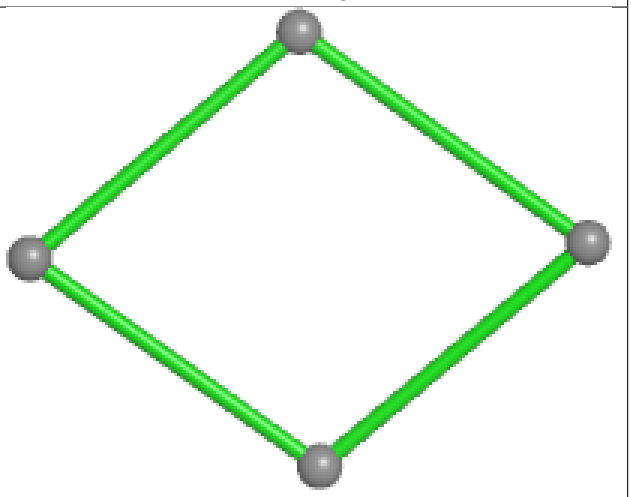
Bond lengths



Bond angles

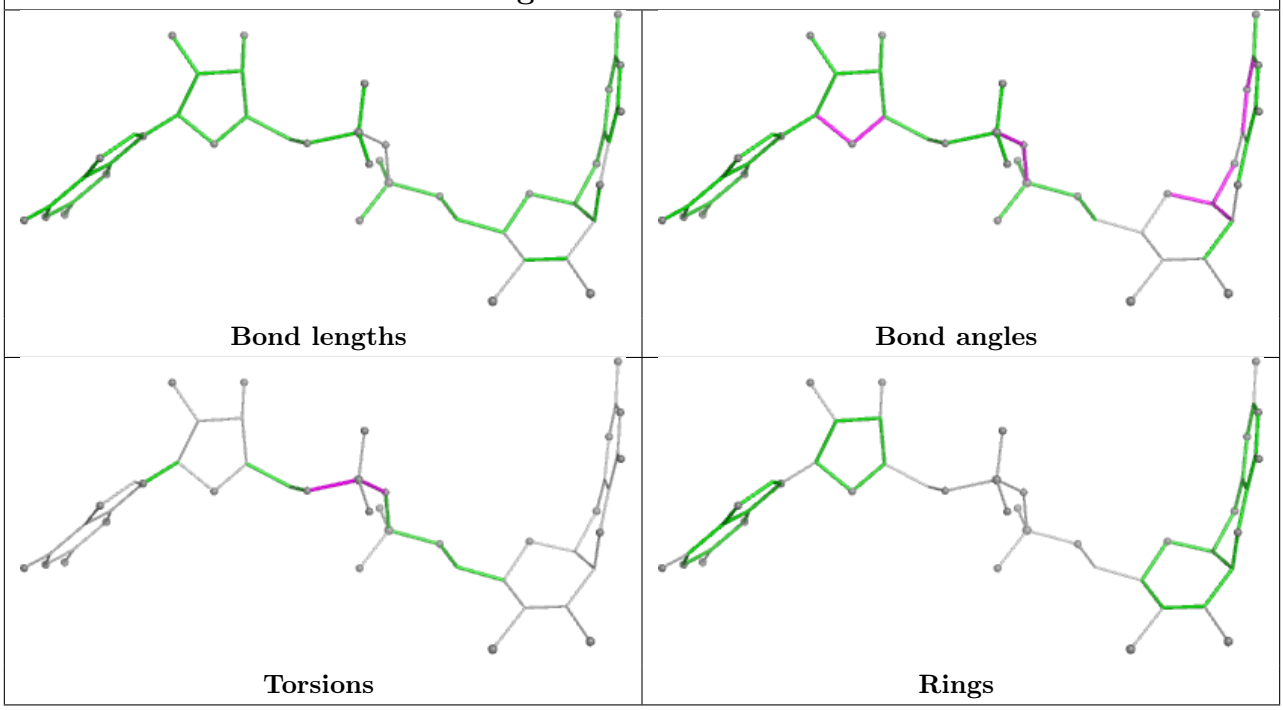


Torsions

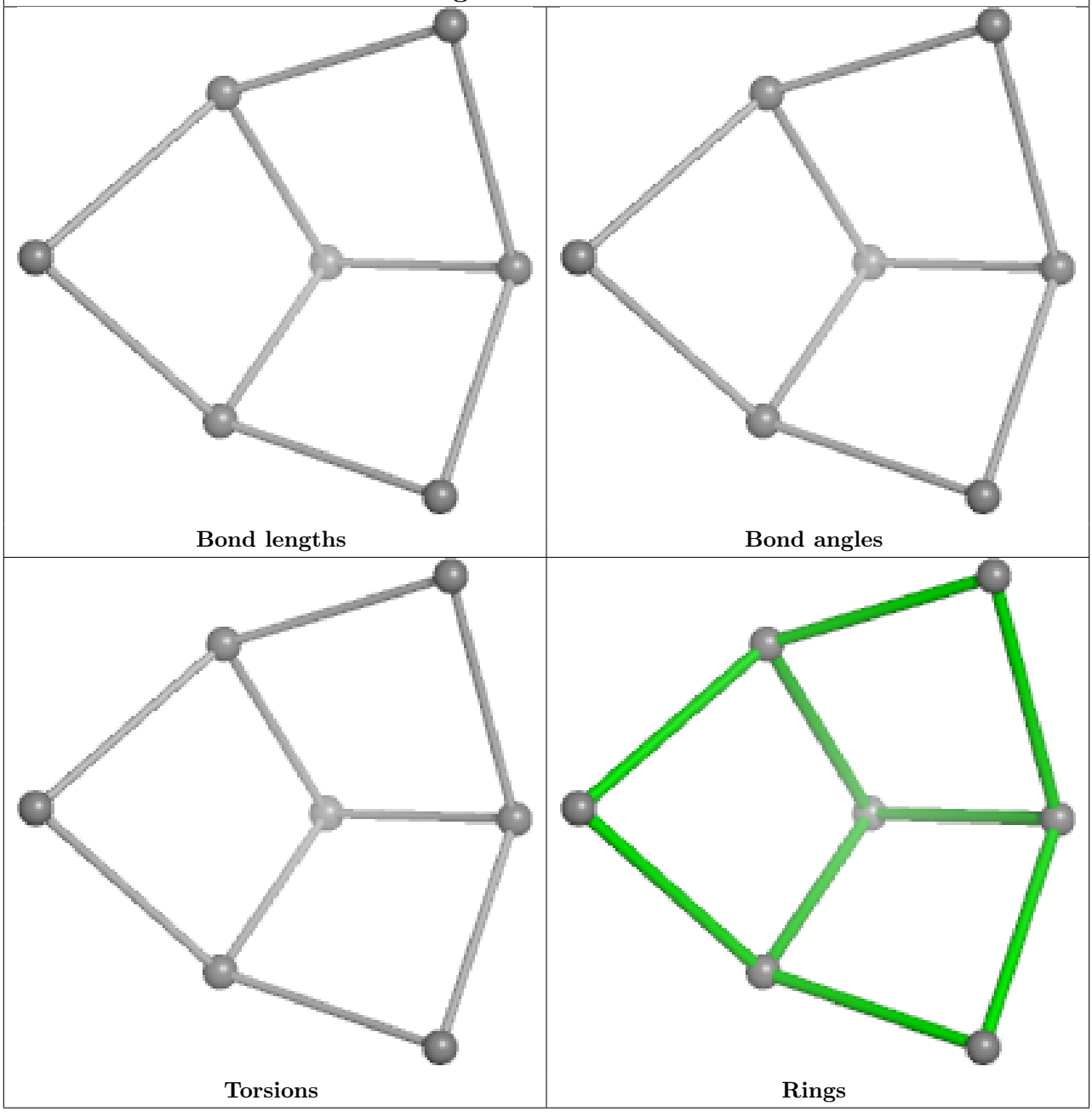


Rings

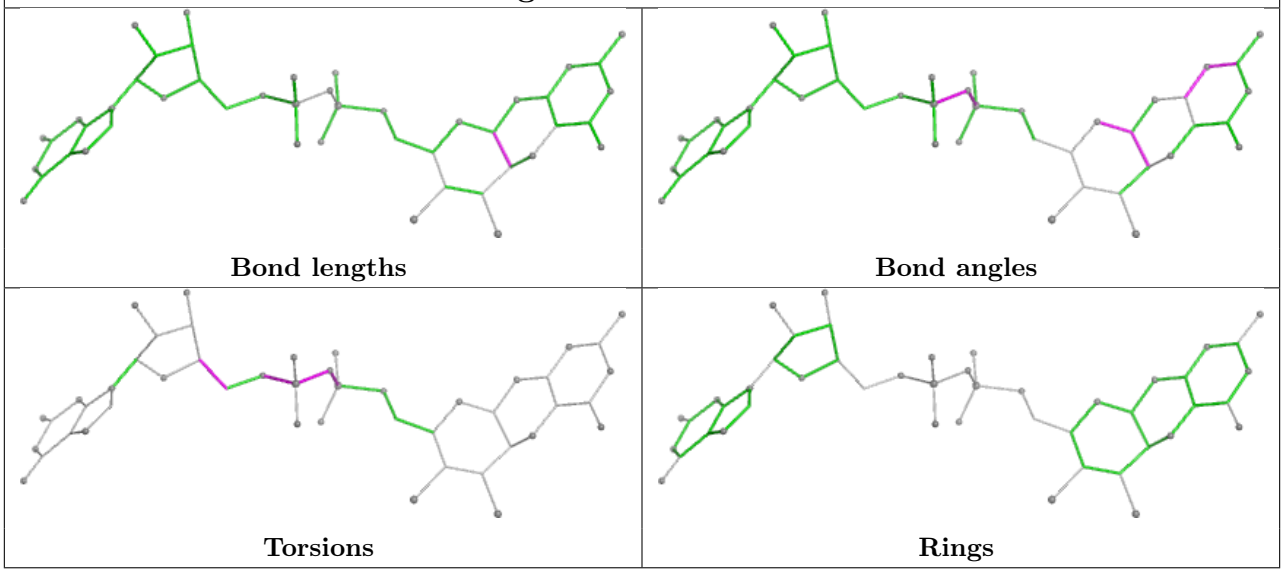
Ligand MGD A 902



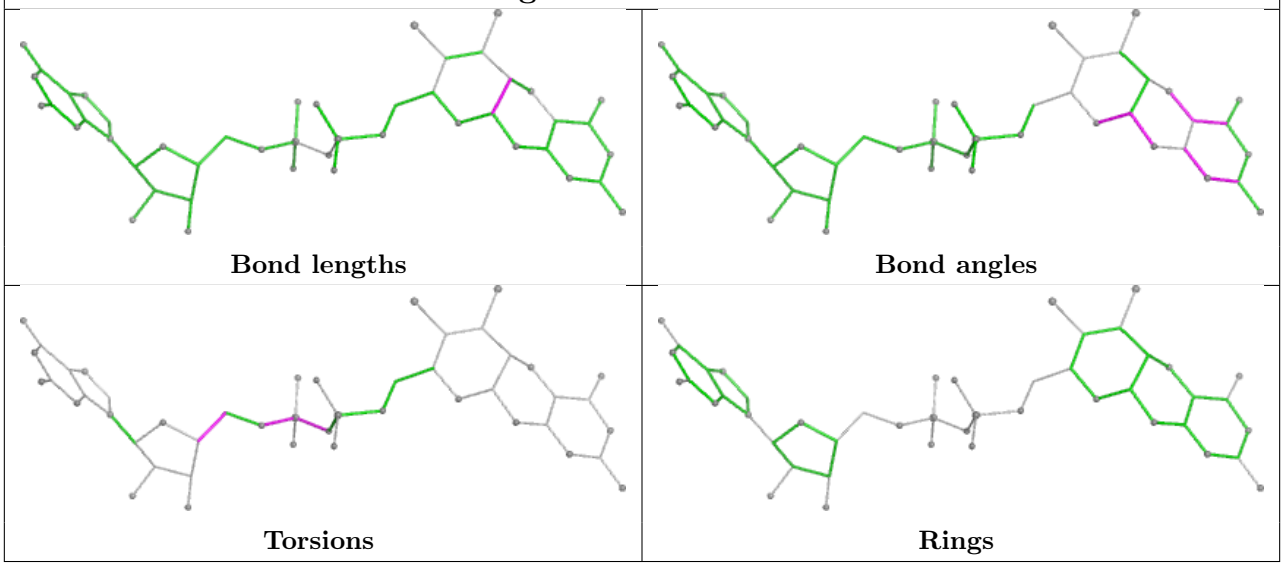
Ligand F3S C 904



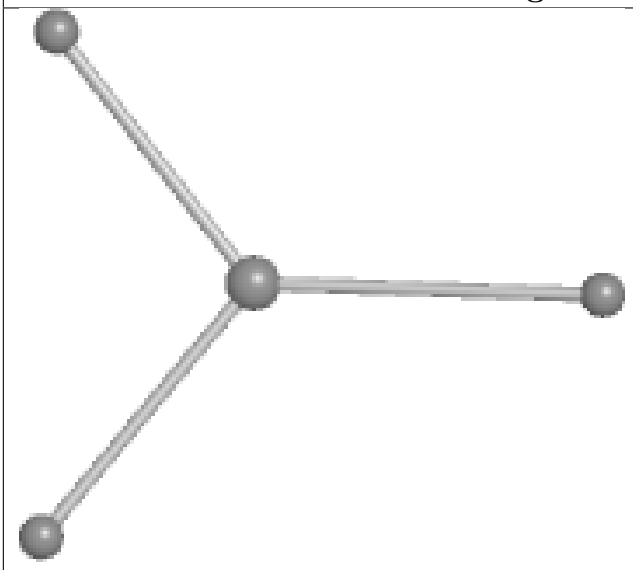
Ligand MGD C 903



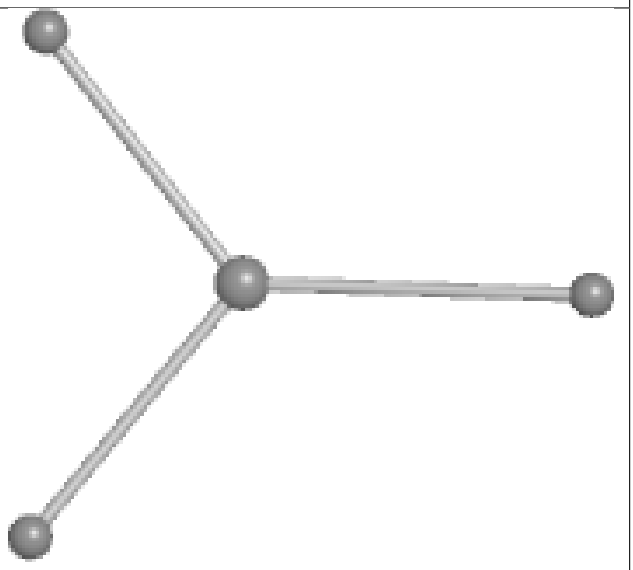
Ligand MGD E 901



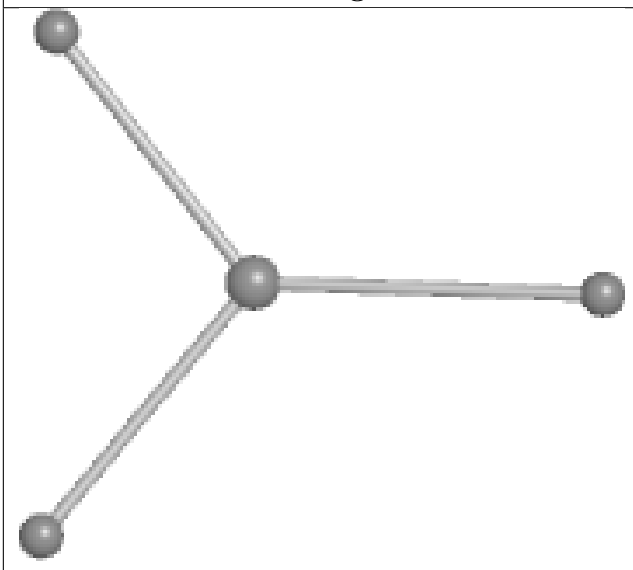
Ligand AST E 906



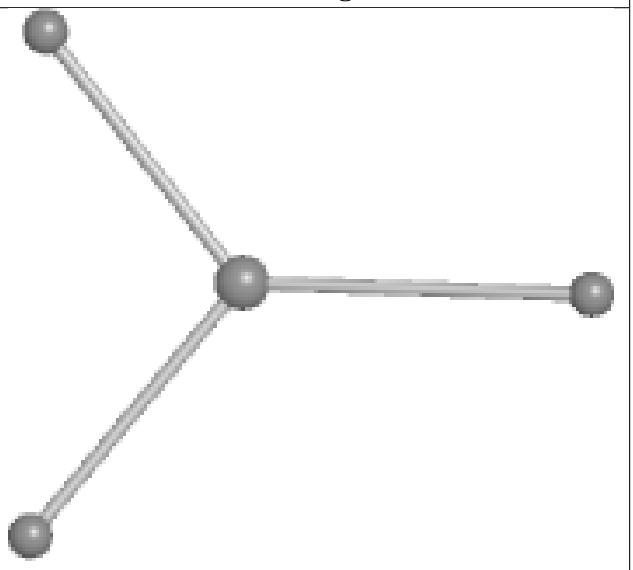
Bond lengths



Bond angles

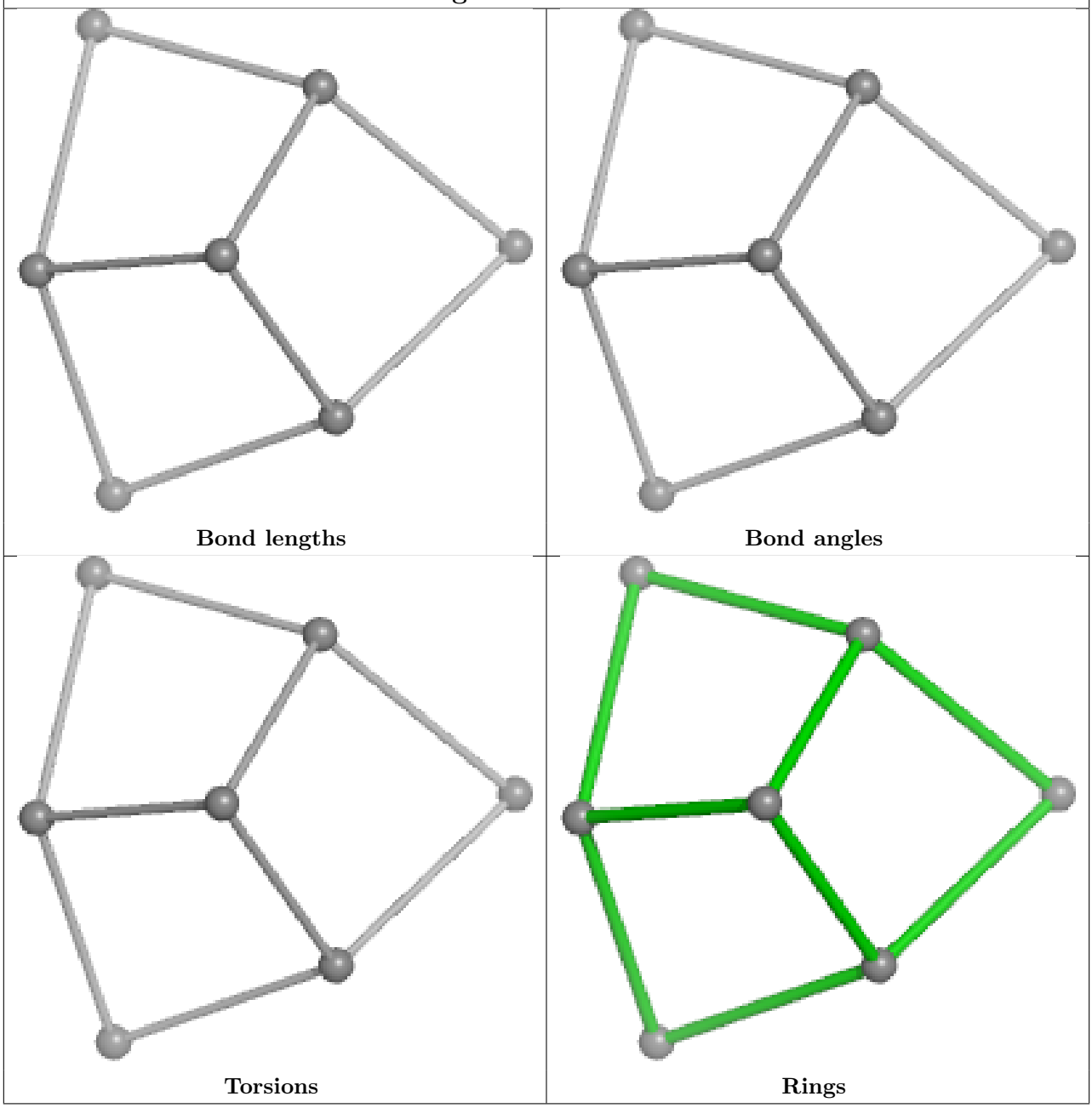


Torsions

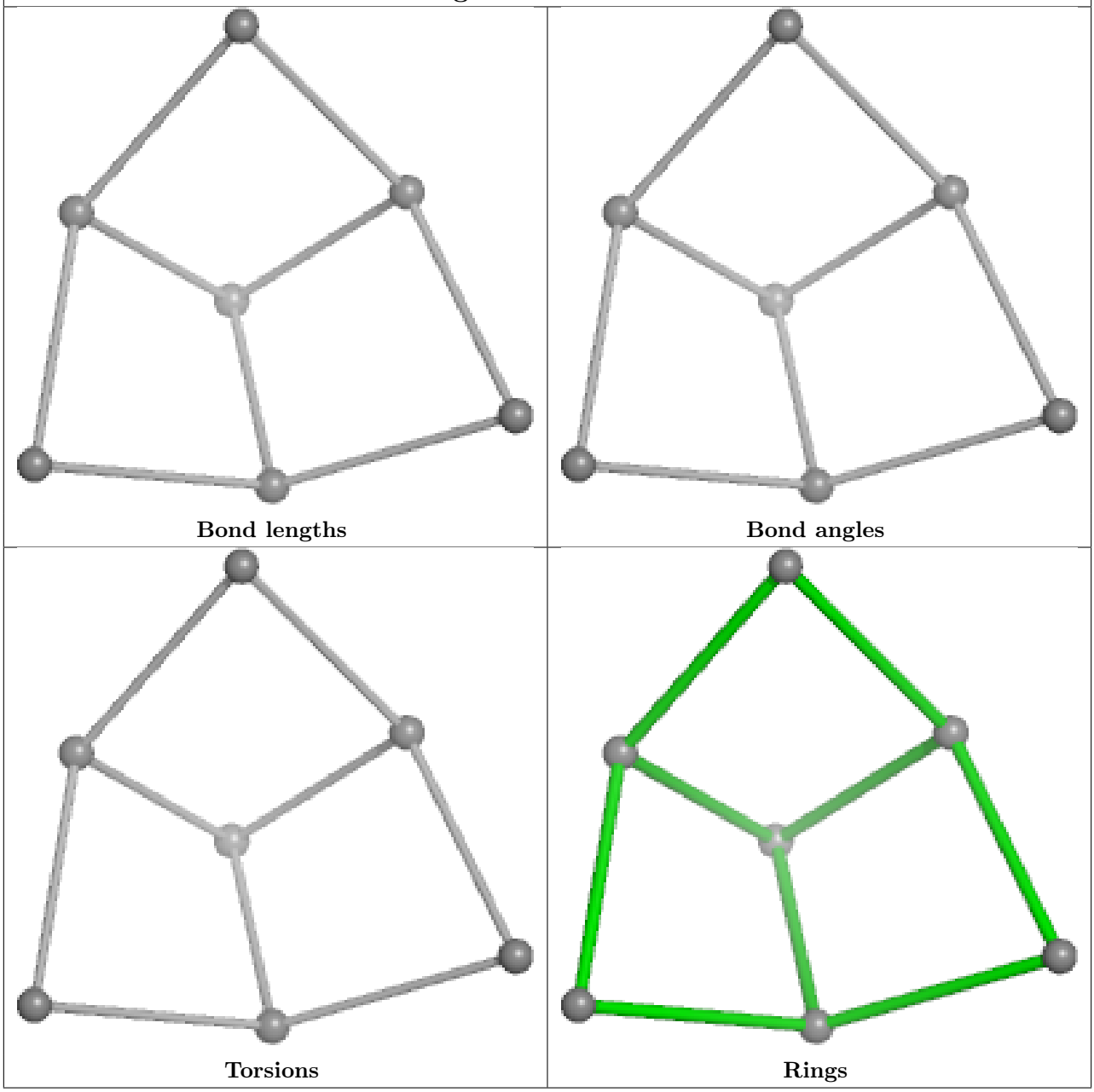


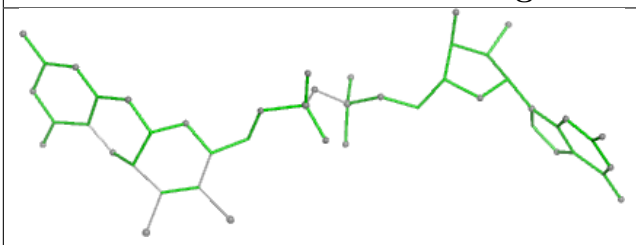
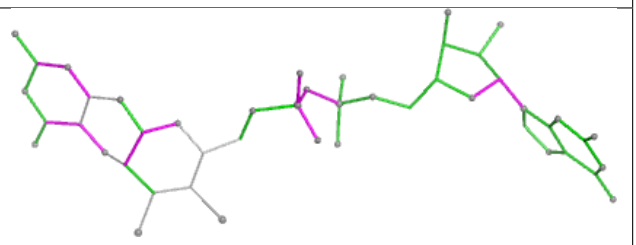
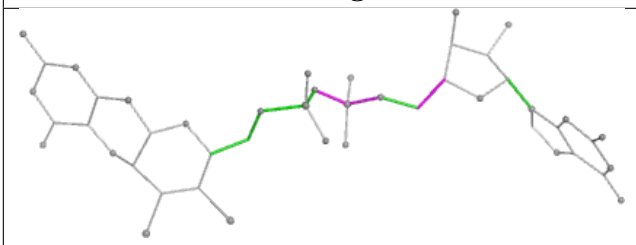
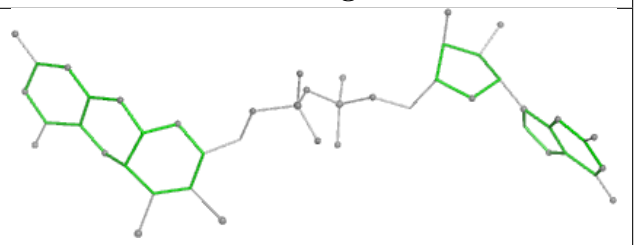
Rings

Ligand F3S G 904

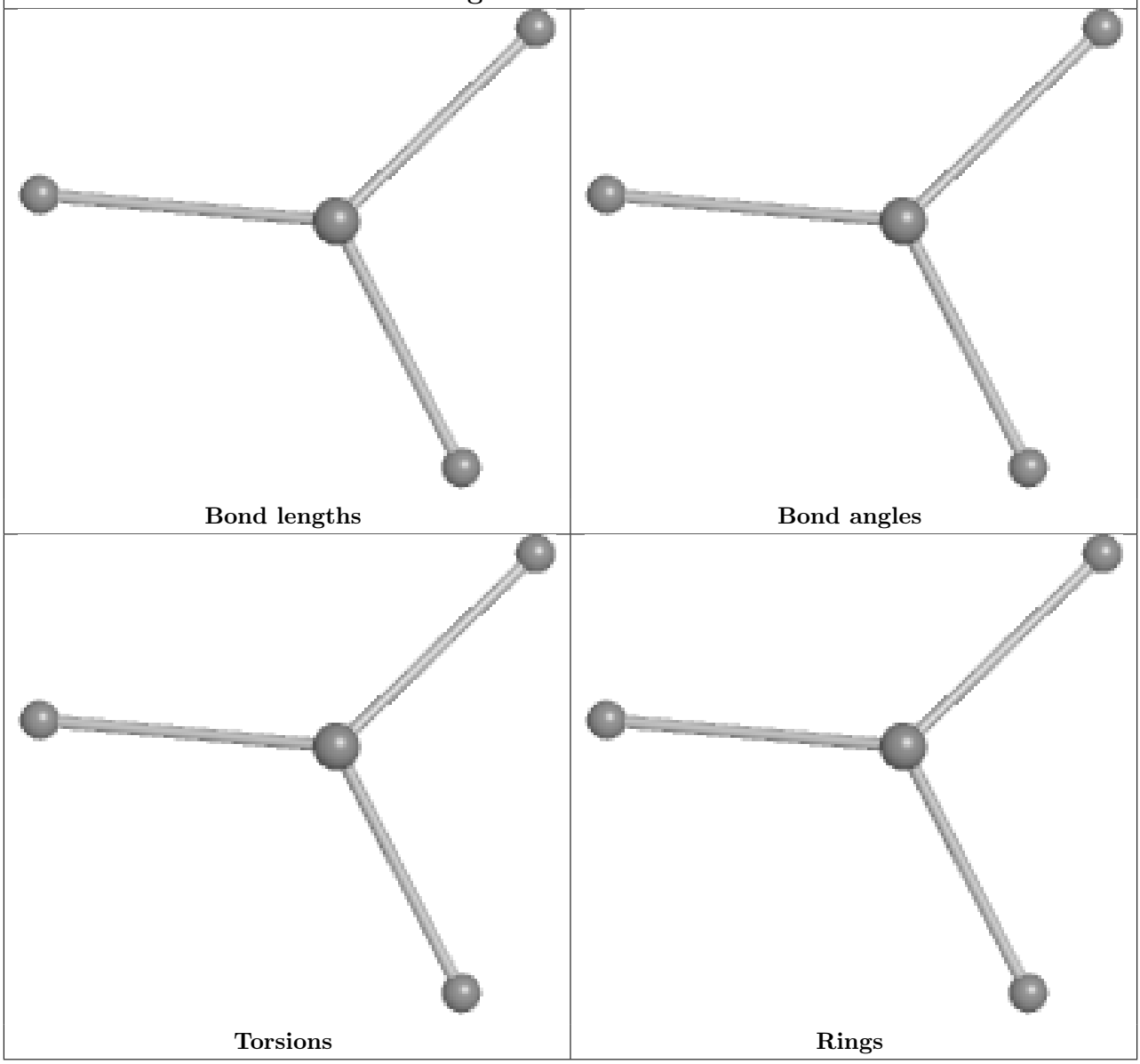


Ligand F3S A 904

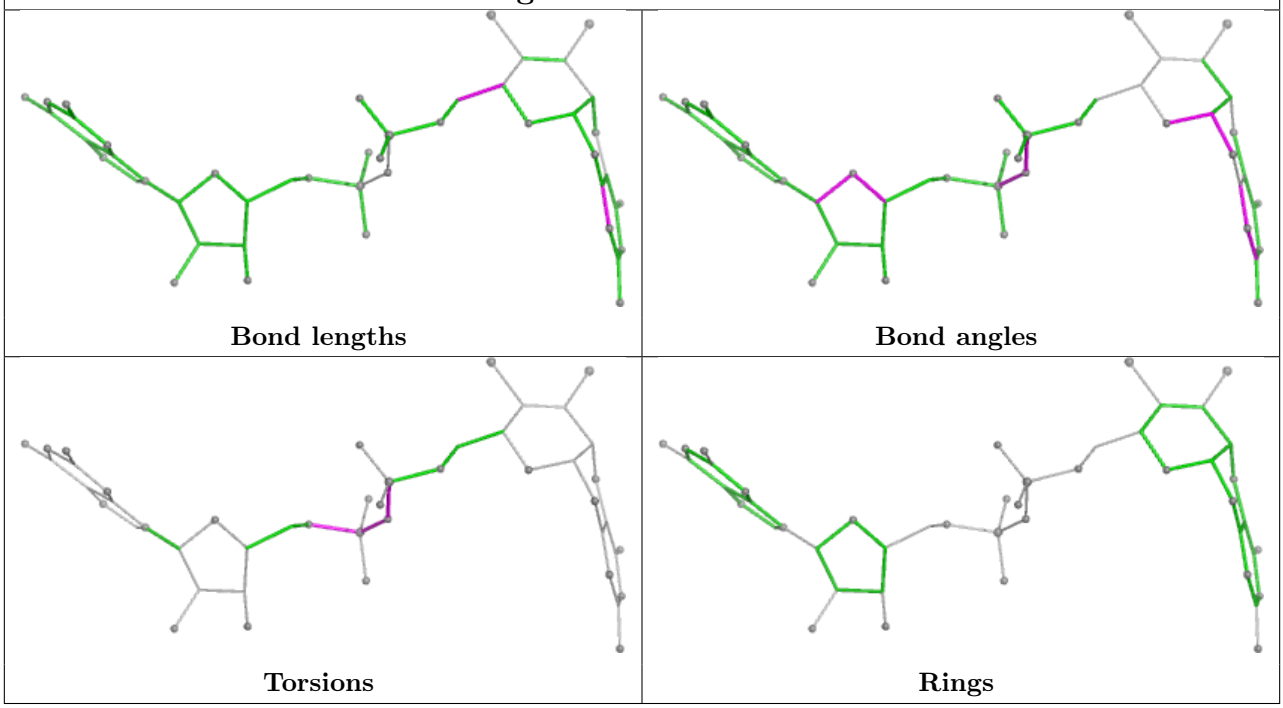


Ligand MGD G 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

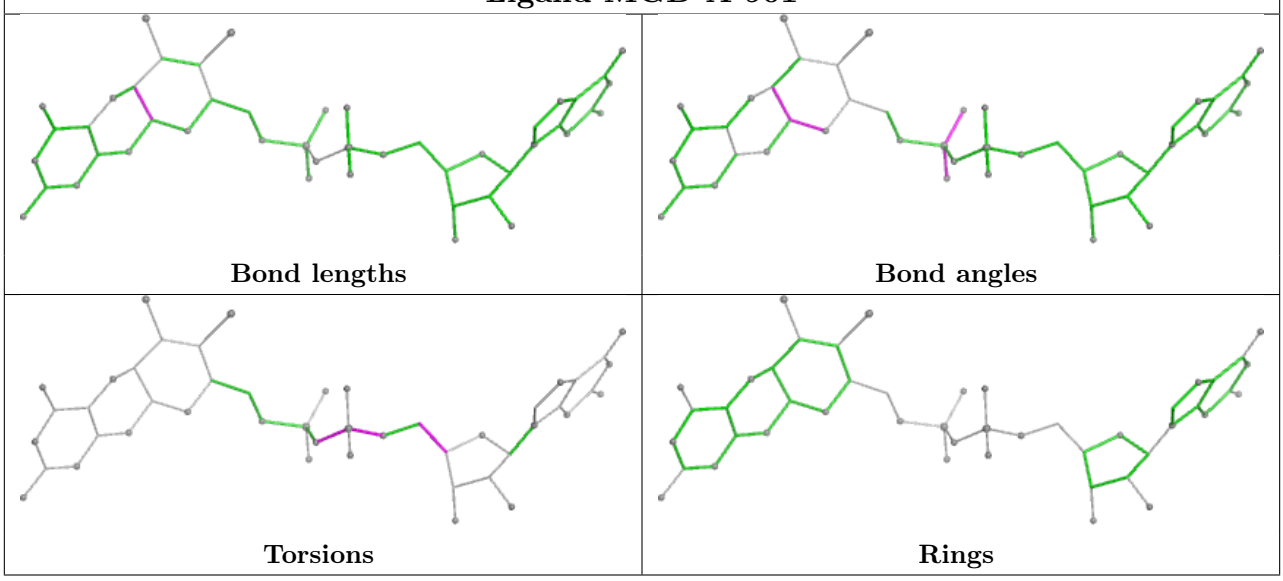
Ligand AST A 907



Ligand MGD G 903



Ligand MGD A 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	823/823 (100%)	-0.18	4 (0%)	87	90	5, 13, 22, 33	8 (0%)
1	C	822/823 (99%)	-0.15	4 (0%)	87	90	6, 13, 22, 36	13 (1%)
1	E	822/823 (99%)	-0.18	1 (0%)	92	92	4, 13, 22, 33	8 (0%)
1	G	822/823 (99%)	-0.16	2 (0%)	91	92	5, 13, 22, 34	10 (1%)
2	B	134/134 (100%)	-0.02	3 (2%)	62	73	5, 13, 22, 35	3 (2%)
2	D	134/134 (100%)	-0.04	3 (2%)	62	73	5, 14, 20, 34	4 (2%)
2	F	134/134 (100%)	0.01	4 (2%)	52	65	6, 14, 22, 32	3 (2%)
2	H	134/134 (100%)	0.01	3 (2%)	62	73	6, 13, 23, 39	5 (3%)
All	All	3825/3828 (99%)	-0.14	24 (0%)	85	89	4, 13, 22, 39	54 (1%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	0	LEU	6.1
1	A	3	PRO	4.4
2	B	0	LEU	4.2
2	D	0	LEU	3.9
2	F	0	LEU	3.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	IPA	G	908	4/4	0.64	0.21	15,16,19,23	0
6	PGE	G	907	10/10	0.65	0.21	29,32,36,36	0
11	IPA	C	906	4/4	0.67	0.19	16,16,18,21	0
9	EDO	C	911[A]	4/4	0.72	0.20	28,28,28,29	4
9	EDO	C	911[B]	4/4	0.72	0.20	23,24,25,25	4
9	EDO	A	908[A]	4/4	0.73	0.29	24,25,26,26	4
9	EDO	A	908[B]	4/4	0.73	0.29	20,21,23,24	4
11	IPA	A	913	4/4	0.74	0.17	23,24,24,26	0
9	EDO	G	911	4/4	0.77	0.18	31,32,32,33	0
7	GOL	E	912	6/6	0.78	0.20	16,17,18,18	0
11	IPA	E	905	4/4	0.80	0.17	27,28,28,29	0
9	EDO	C	913	4/4	0.83	0.12	32,32,33,35	0
9	EDO	G	912	4/4	0.84	0.15	34,35,35,36	0
10	PEG	A	910	7/7	0.84	0.15	28,28,29,32	0
9	EDO	G	915	4/4	0.85	0.16	25,25,26,26	0
9	EDO	C	910	4/4	0.85	0.14	25,28,29,32	0
9	EDO	E	910	4/4	0.85	0.12	26,26,26,27	0
9	EDO	G	910	4/4	0.85	0.13	30,30,30,31	0
7	GOL	C	908	6/6	0.85	0.13	32,33,34,34	0
9	EDO	A	914	4/4	0.85	0.14	20,24,24,26	0
6	PGE	A	905[B]	10/10	0.86	0.13	14,14,15,15	10
6	PGE	A	905[A]	10/10	0.86	0.13	16,19,22,22	10
9	EDO	A	911	4/4	0.86	0.12	30,32,33,34	0
9	EDO	A	912	4/4	0.86	0.14	26,26,28,28	0
9	EDO	D	202	4/4	0.86	0.20	22,22,24,24	0
7	GOL	E	913	6/6	0.86	0.11	23,24,25,25	0
9	EDO	E	911	4/4	0.86	0.15	24,25,27,28	0
9	EDO	C	907	4/4	0.86	0.14	25,26,27,28	0
9	EDO	E	909	4/4	0.87	0.13	23,26,27,27	0
7	GOL	E	914	6/6	0.87	0.11	21,23,25,26	0
9	EDO	A	916	4/4	0.88	0.18	22,22,23,25	0
9	EDO	C	914	4/4	0.89	0.10	19,20,21,22	0
7	GOL	C	909	6/6	0.89	0.11	28,29,31,32	0
7	GOL	G	913	6/6	0.90	0.11	21,25,27,27	0
7	GOL	G	905	6/6	0.90	0.14	14,16,18,22	0
9	EDO	E	907	4/4	0.90	0.10	24,27,27,28	0
9	EDO	G	909[B]	4/4	0.91	0.09	15,15,15,16	4

Continued on next page...

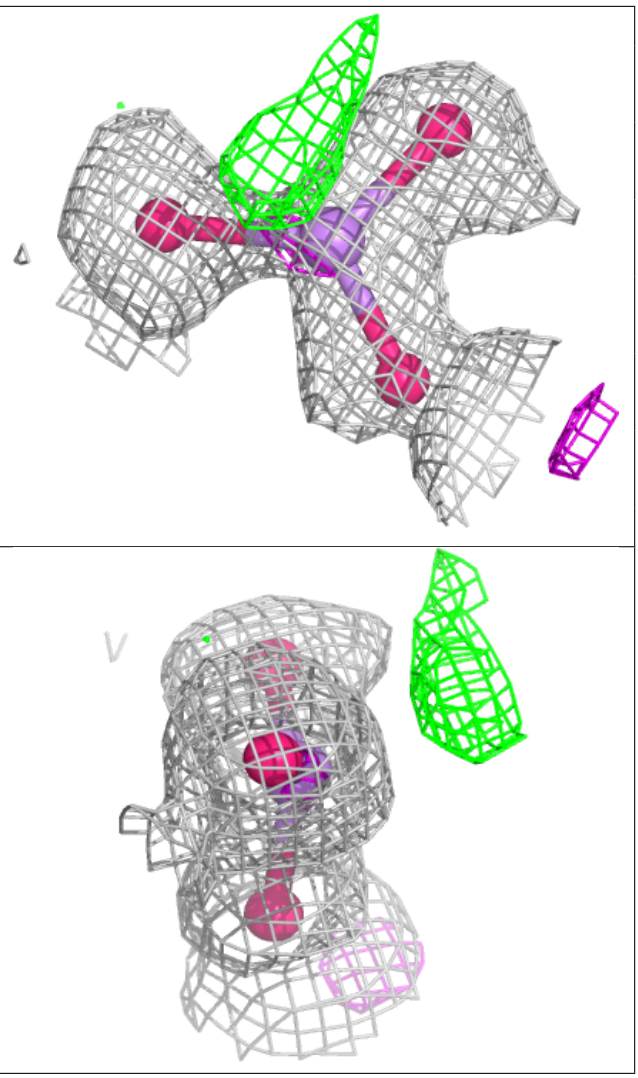
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	PEG	B	2301	7/7	0.91	0.11	23,24,24,25	0
9	EDO	A	909	4/4	0.91	0.11	14,15,17,17	0
7	GOL	A	906	6/6	0.91	0.15	13,16,19,25	0
9	EDO	A	915	4/4	0.91	0.11	15,17,17,18	0
9	EDO	G	909[A]	4/4	0.91	0.09	15,16,16,17	4
9	EDO	G	914	4/4	0.92	0.09	21,22,22,24	0
7	GOL	C	912	6/6	0.93	0.14	15,18,19,23	0
9	EDO	C	915	4/4	0.93	0.10	20,20,21,21	0
9	EDO	E	908	4/4	0.95	0.07	14,15,16,16	0
8	AST	A	907	4/4	0.96	0.08	13,14,14,15	1
8	AST	G	906	4/4	0.96	0.07	12,12,12,13	1
8	AST	C	905	4/4	0.97	0.07	11,12,13,13	1
3	MGD	C	902	47/47	0.98	0.04	8,9,10,12	0
3	MGD	C	903	47/47	0.98	0.04	9,9,10,10	0
3	MGD	E	901	47/47	0.98	0.04	9,9,10,10	0
3	MGD	G	902	47/47	0.98	0.04	8,9,10,11	0
3	MGD	A	901	47/47	0.98	0.04	8,9,10,11	0
3	MGD	A	902	47/47	0.98	0.04	7,9,10,10	0
8	AST	E	906	4/4	0.98	0.07	12,13,14,14	1
3	MGD	E	903	47/47	0.99	0.04	8,9,10,10	0
3	MGD	G	903	47/47	0.99	0.04	7,9,10,10	0
12	FES	B	2302	4/4	0.99	0.03	10,11,11,12	0
12	FES	H	201	4/4	0.99	0.03	10,11,11,11	0
5	F3S	A	904	7/7	1.00	0.02	8,9,9,9	0
5	F3S	C	904	7/7	1.00	0.02	9,9,9,9	0
5	F3S	E	904	7/7	1.00	0.02	8,9,9,10	0
5	F3S	G	904	7/7	1.00	0.02	8,8,8,8	0
4	MO	A	903	1/1	1.00	0.02	9,9,9,9	0
4	MO	C	901	1/1	1.00	0.02	10,10,10,10	0
4	MO	E	902	1/1	1.00	0.02	10,10,10,10	0
12	FES	D	201	4/4	1.00	0.03	11,11,11,12	0
12	FES	F	201	4/4	1.00	0.03	11,12,12,12	0
4	MO	G	901	1/1	1.00	0.01	9,9,9,9	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.

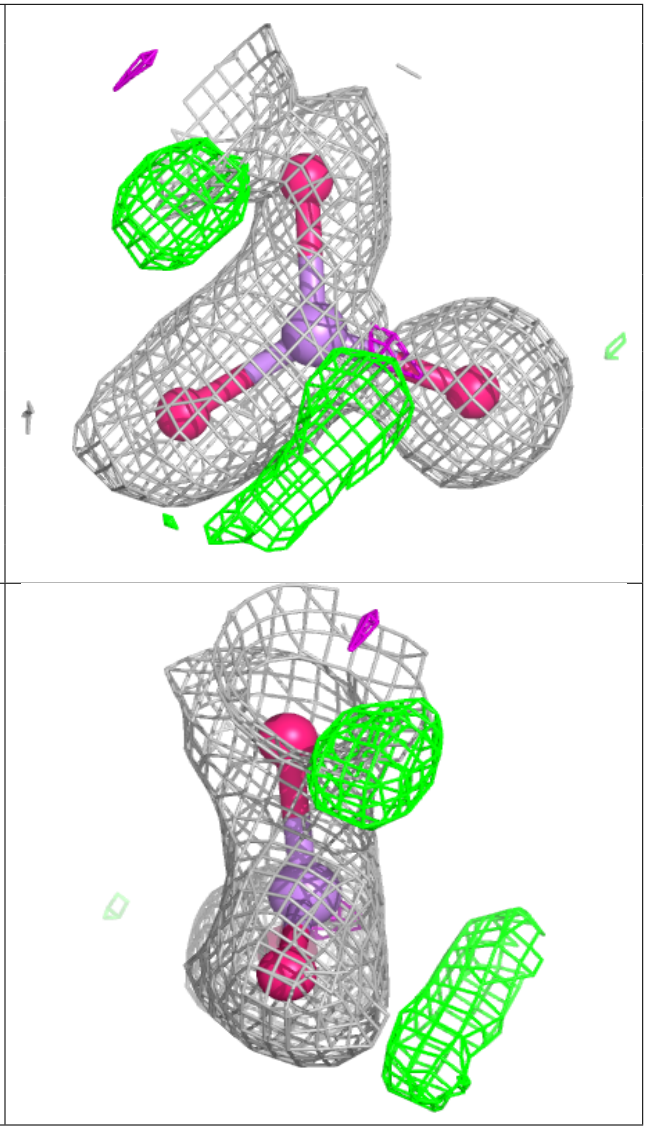
Electron density around AST A 907:

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



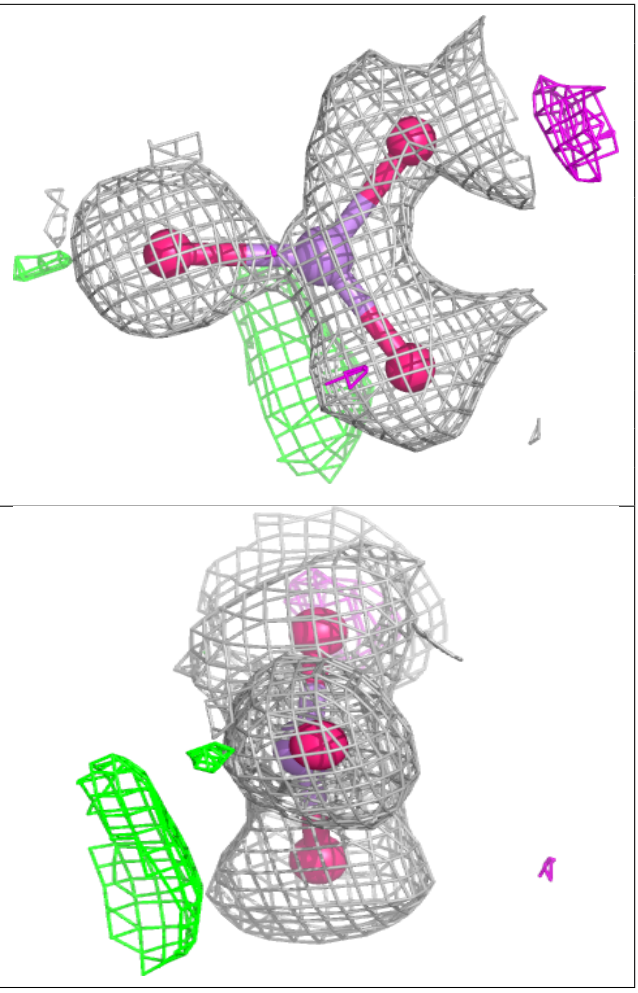
Electron density around AST G 906:

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



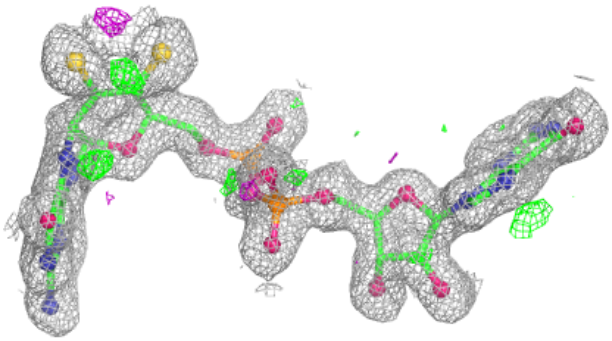
Electron density around AST C 905:

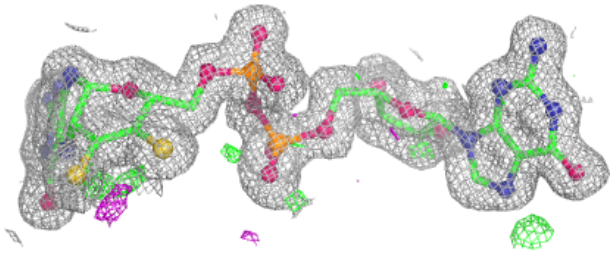
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

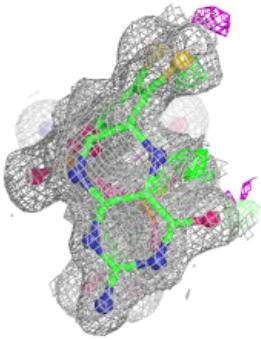


Electron density around MGD C 902:

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

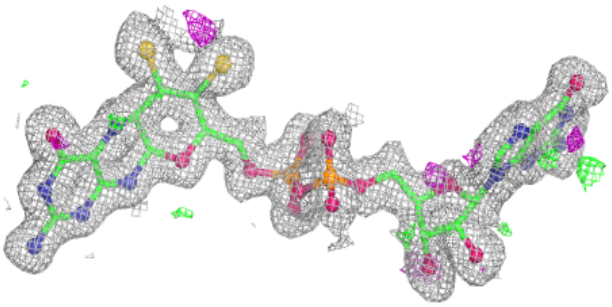


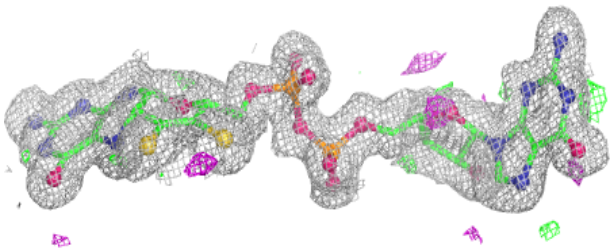


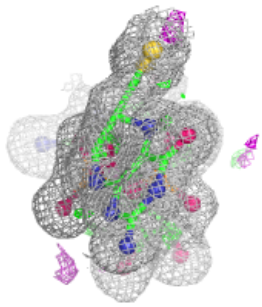


Electron density around MGD C 903:

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

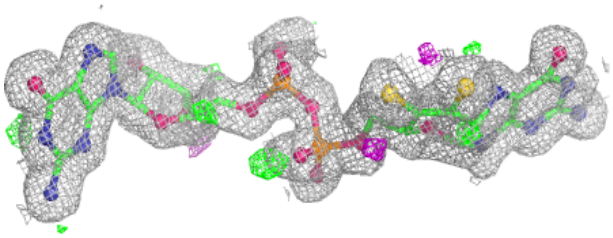


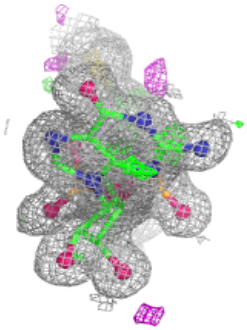




Electron density around MGD E 901:

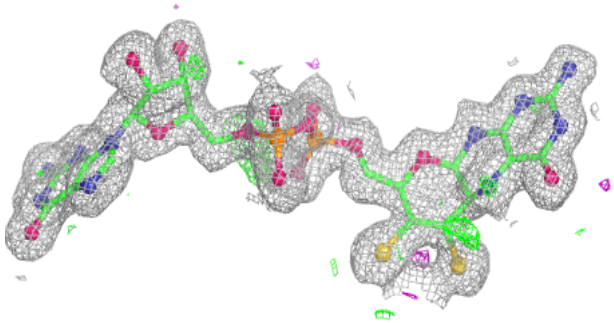
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

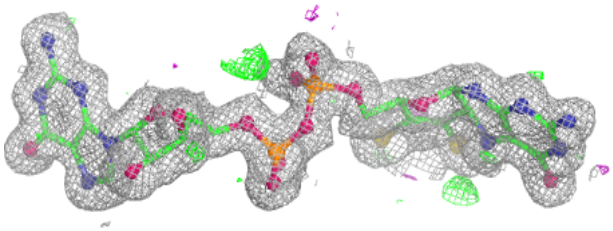


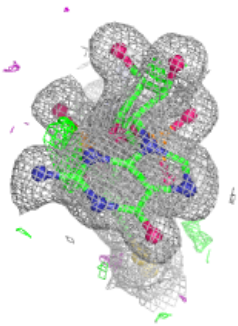


Electron density around MGD G 902:

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

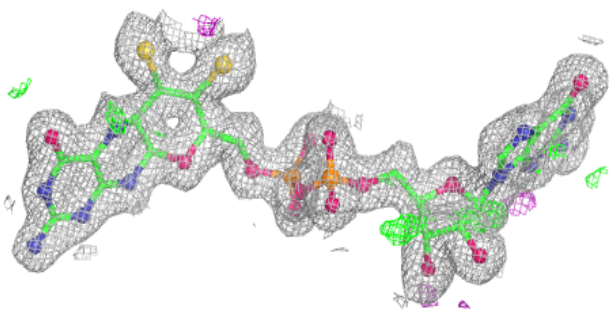


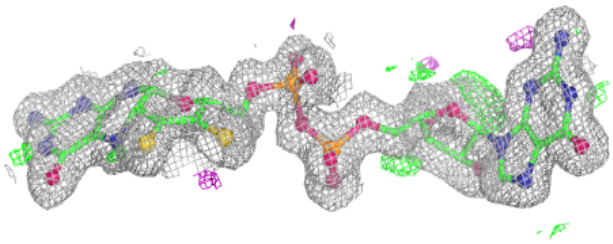


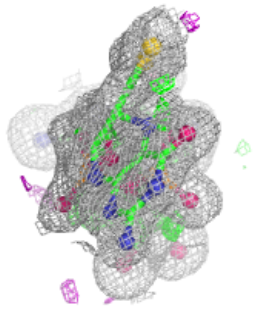


Electron density around MGD A 901:

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

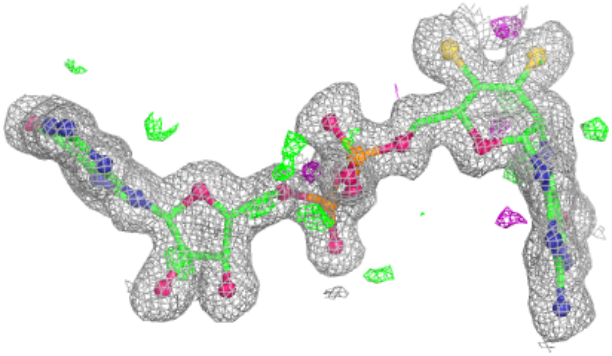


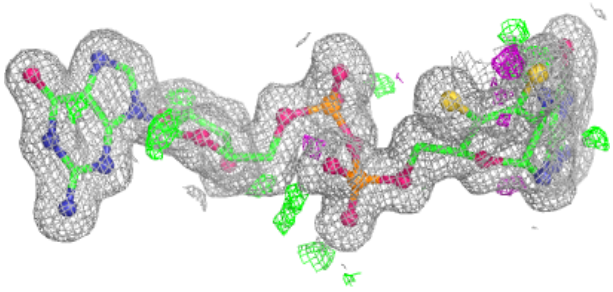


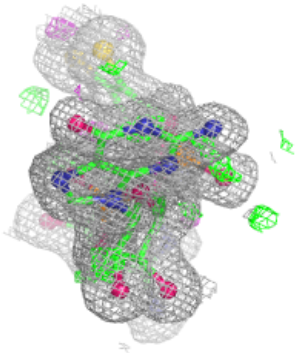


Electron density around MGD A 902:

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

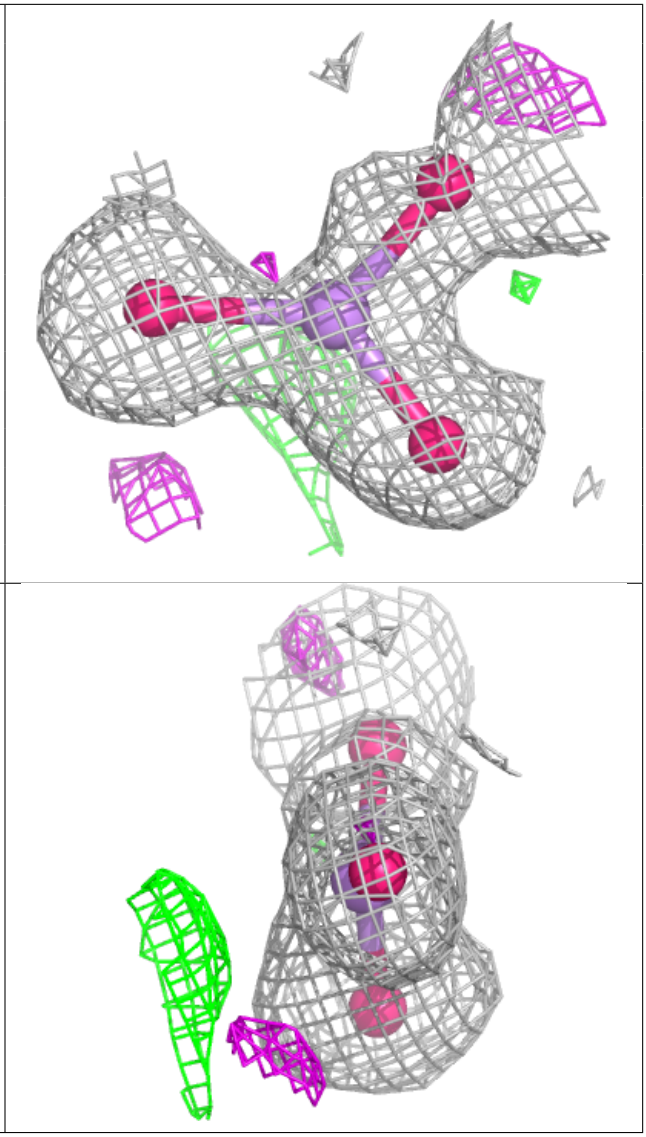






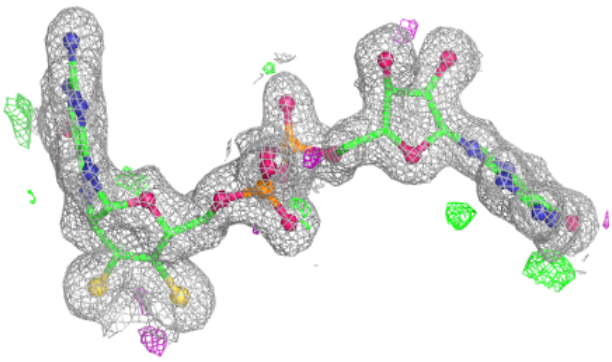
Electron density around AST E 906:

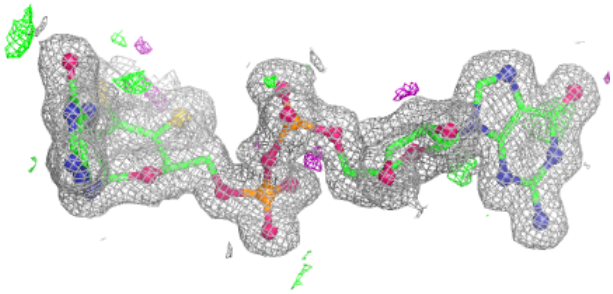
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

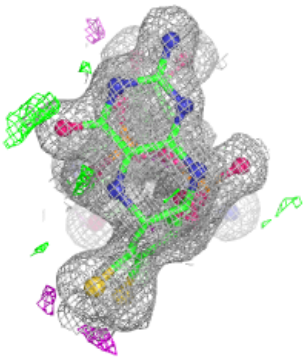


Electron density around MGD E 903:

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

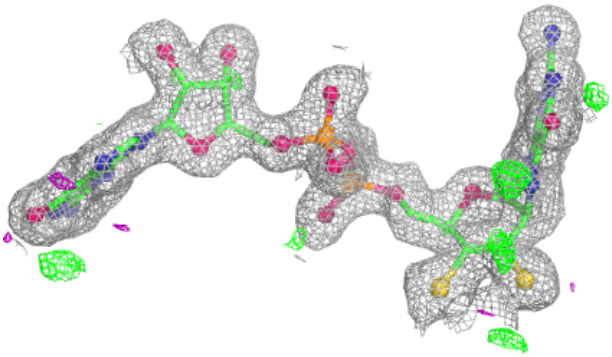


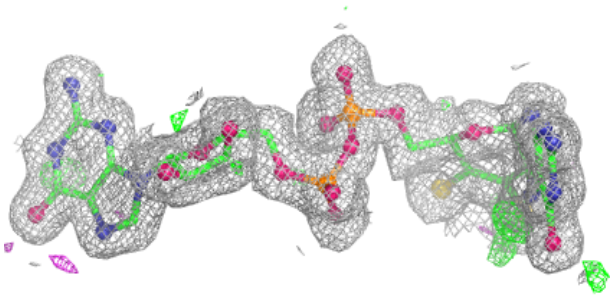


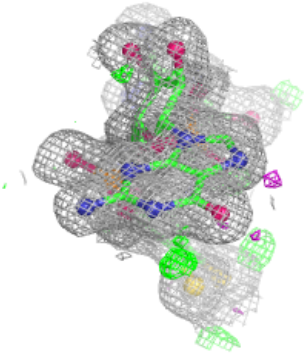


Electron density around MGD G 903:

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

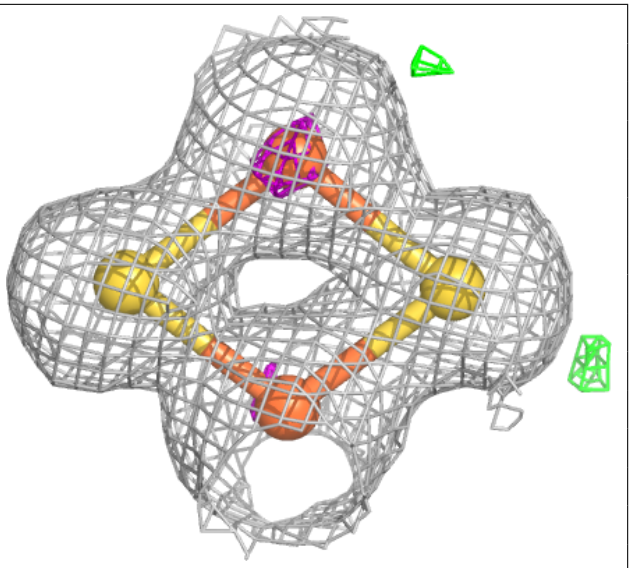


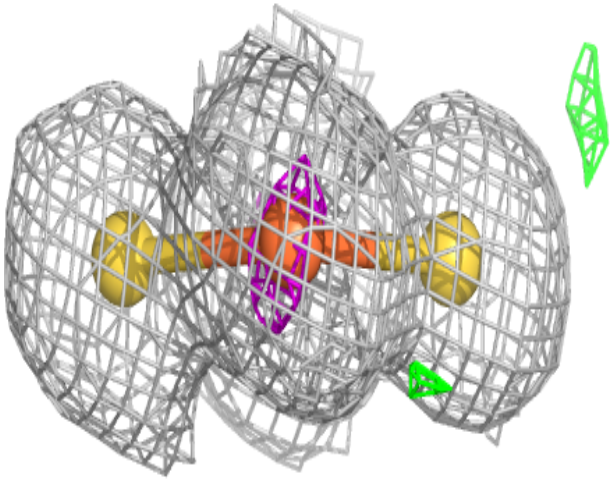


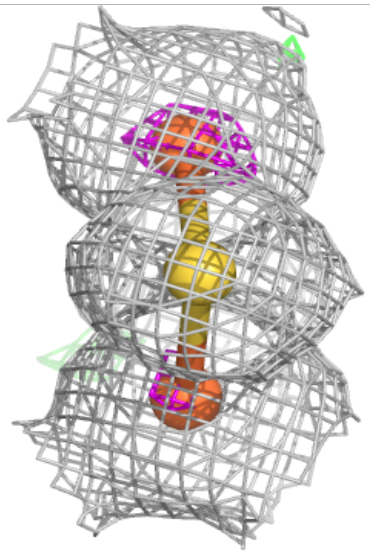


Electron density around FES B 2302:

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

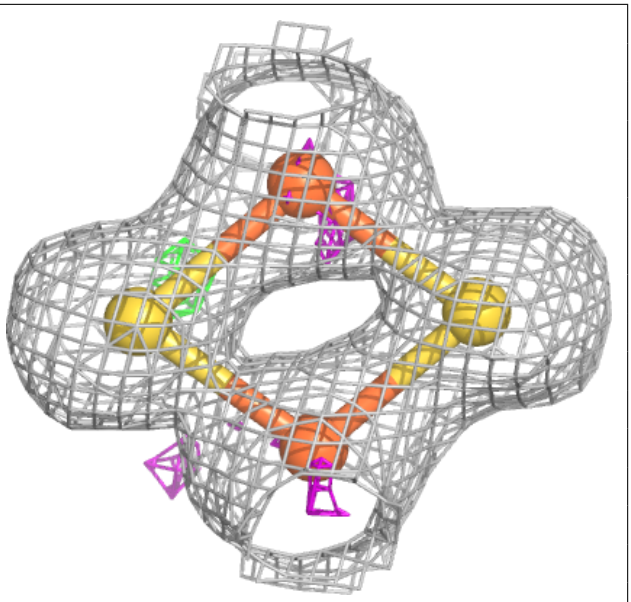


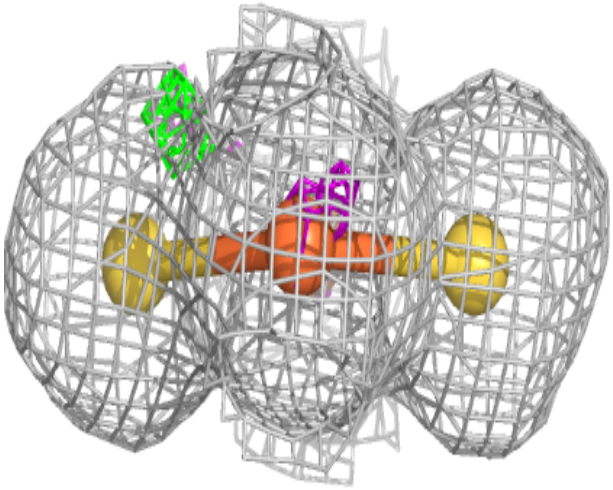


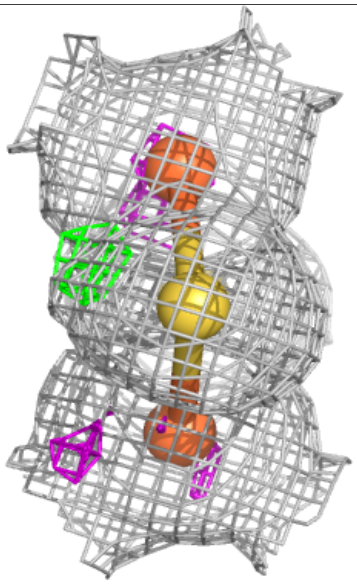


Electron density around FES H 201:

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

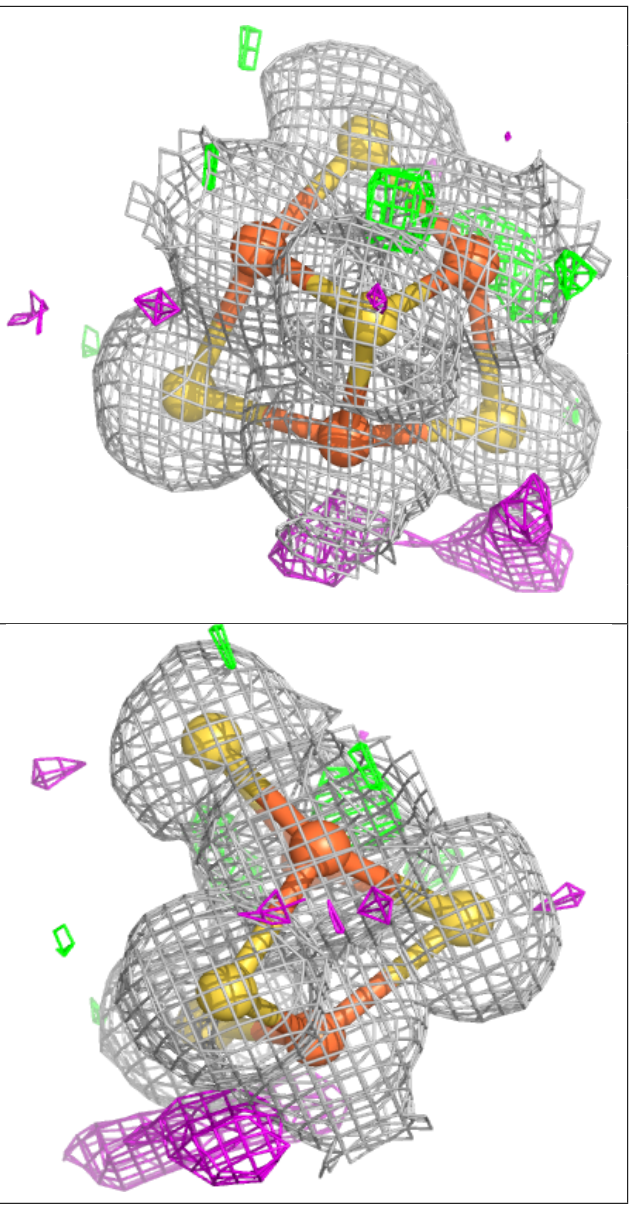






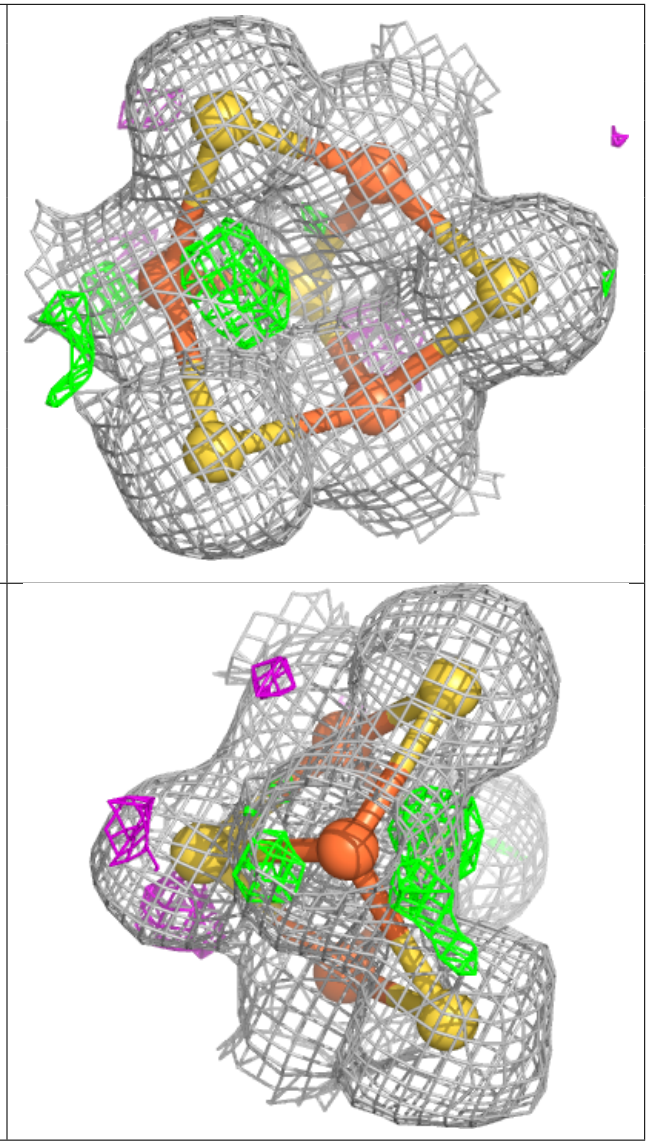
Electron density around F3S A 904:

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



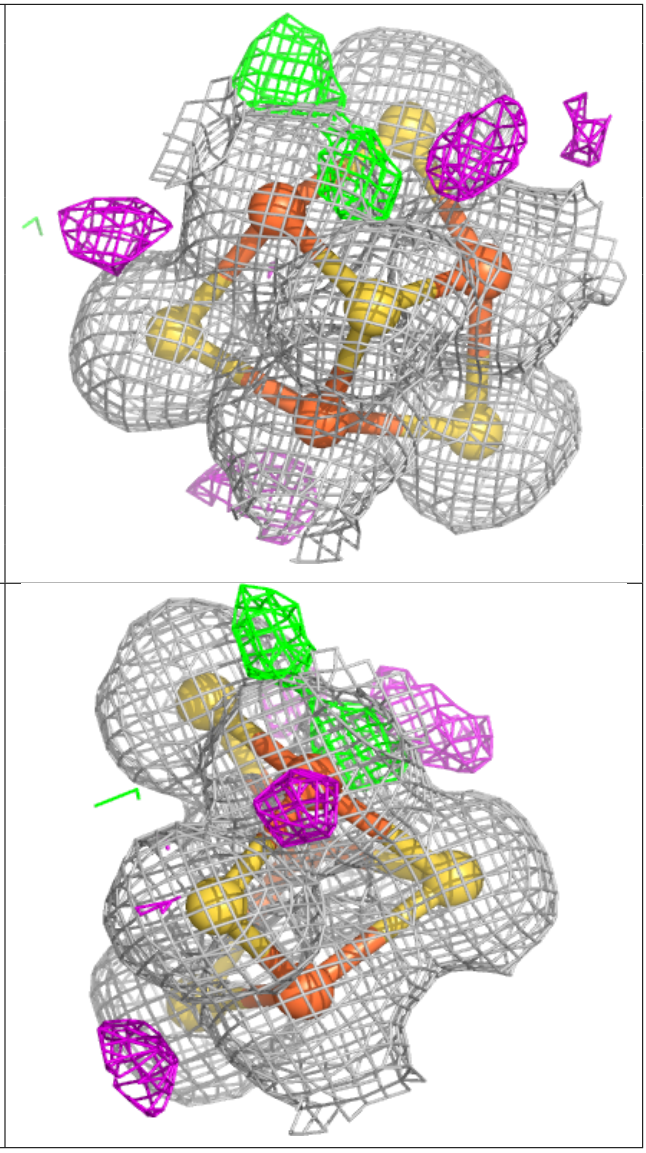
Electron density around F3S C 904:

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



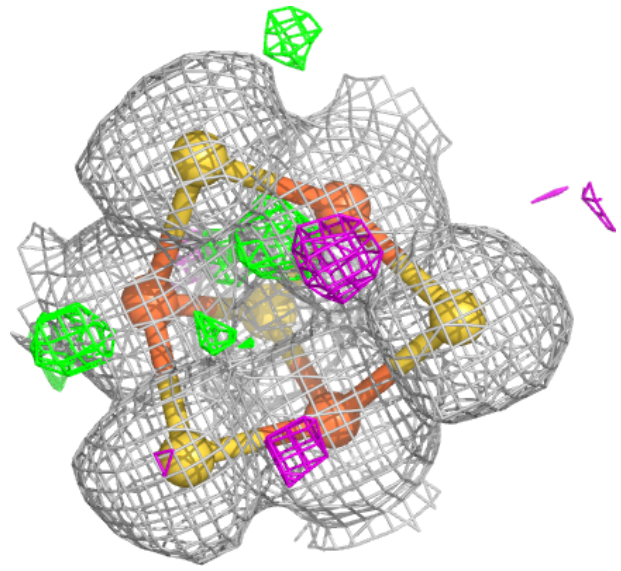
Electron density around F3S E 904:

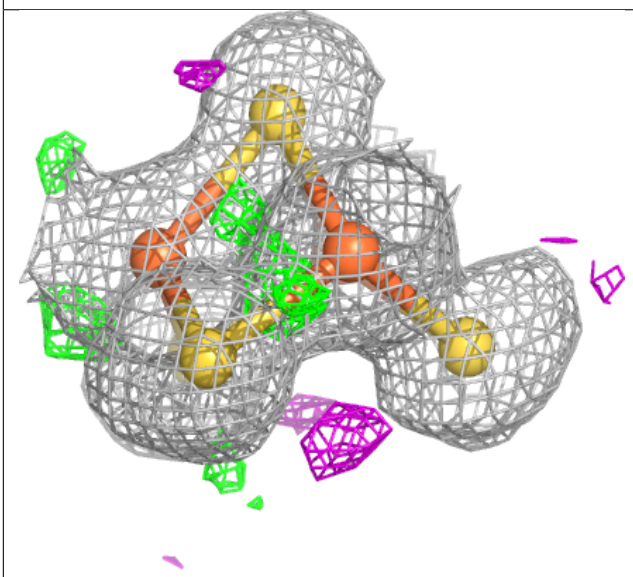
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

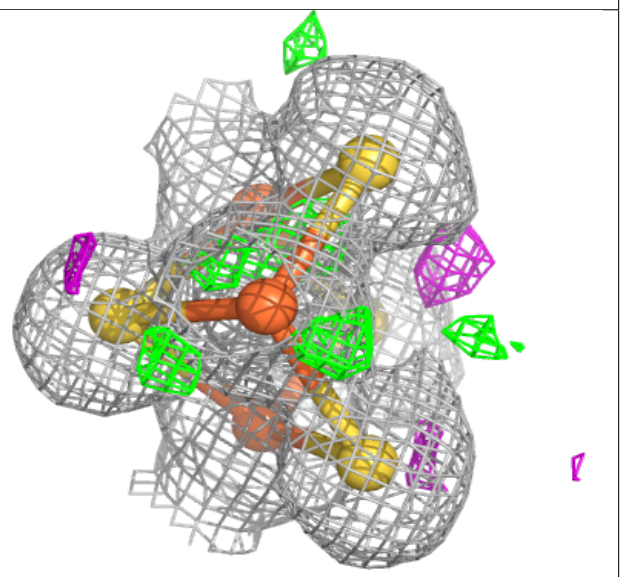


Electron density around F3S G 904:

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

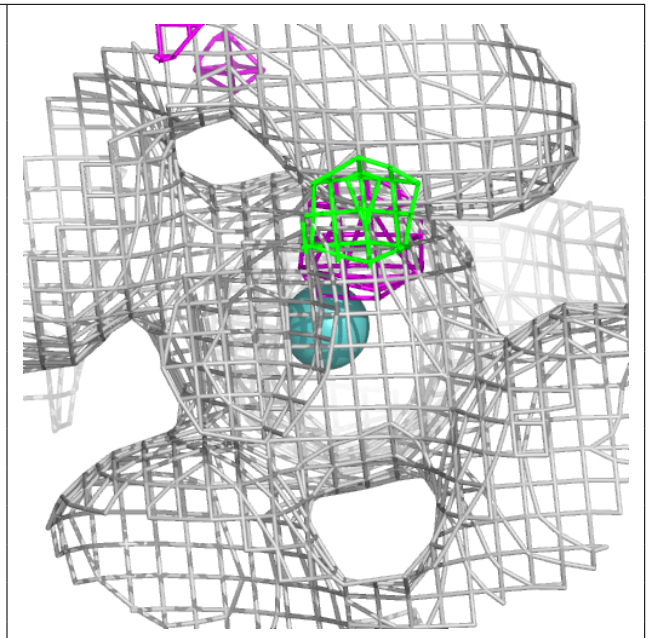


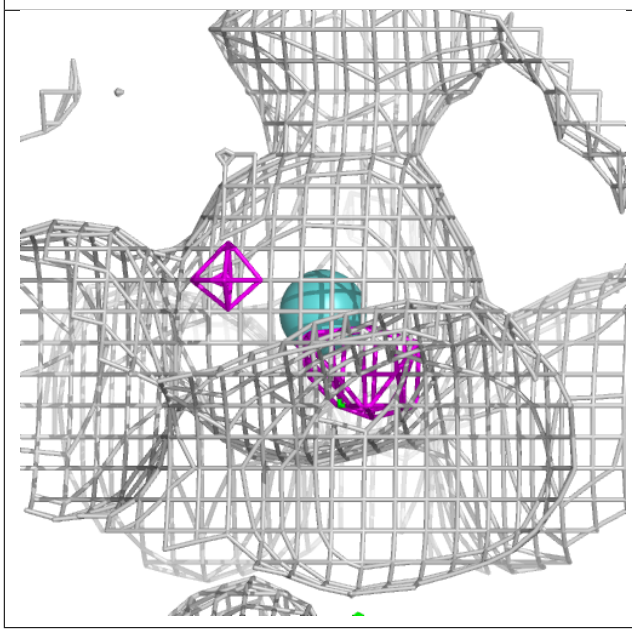


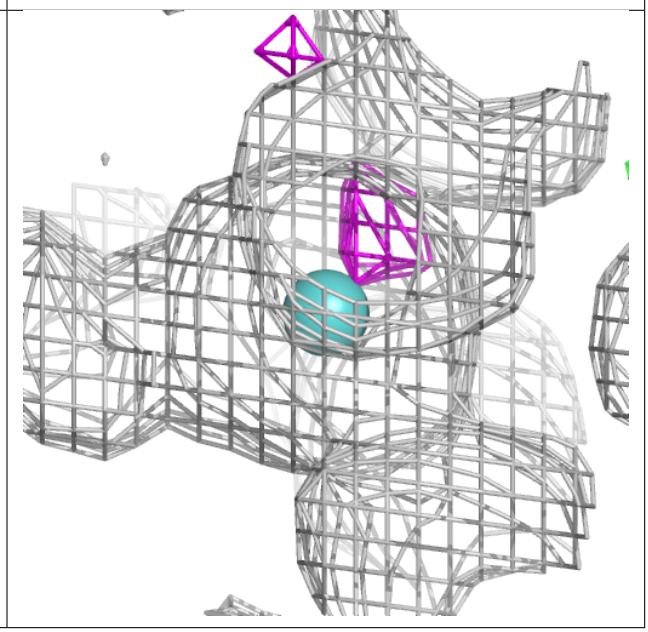


Electron density around MO A 903:

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

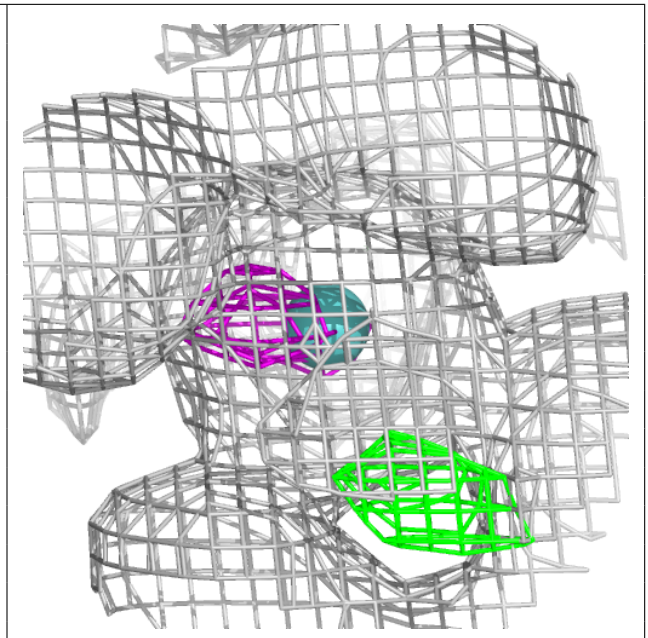


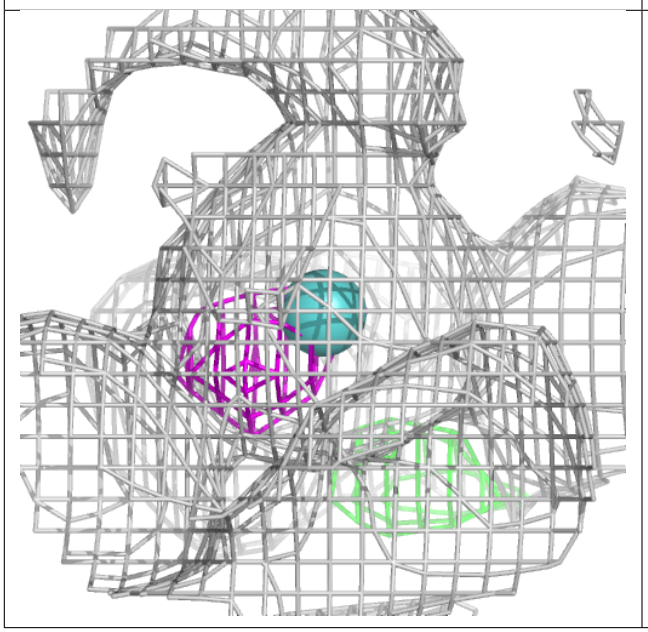


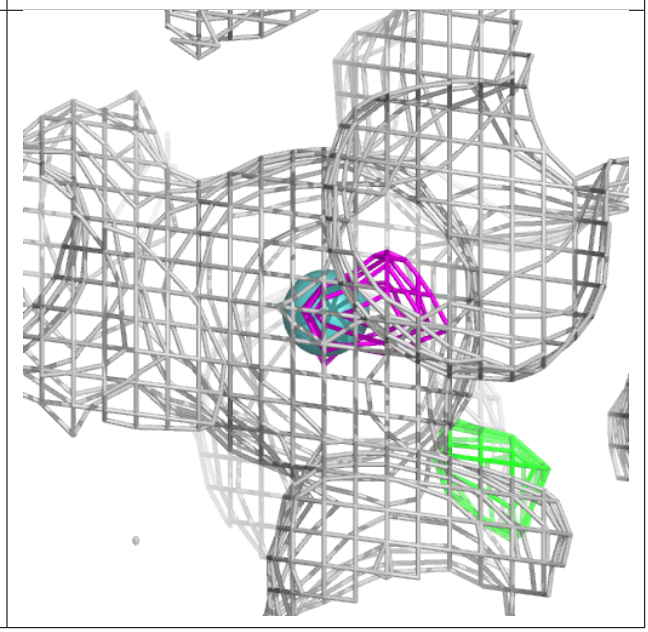


Electron density around MO C 901:

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

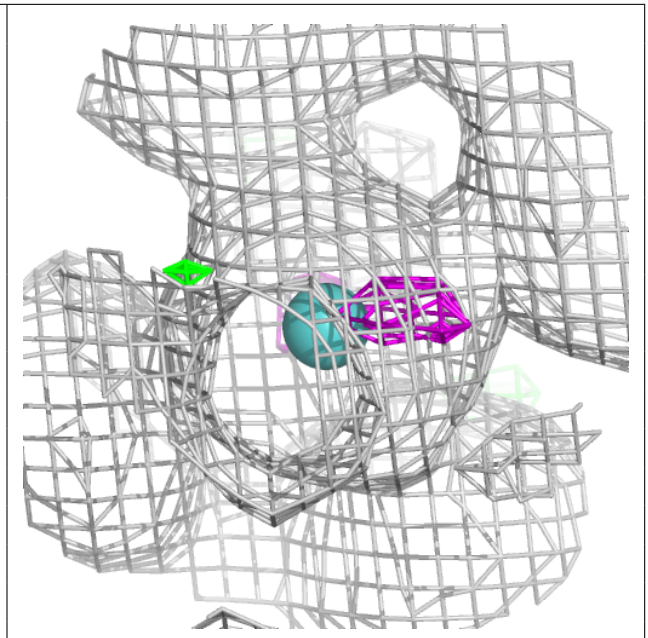


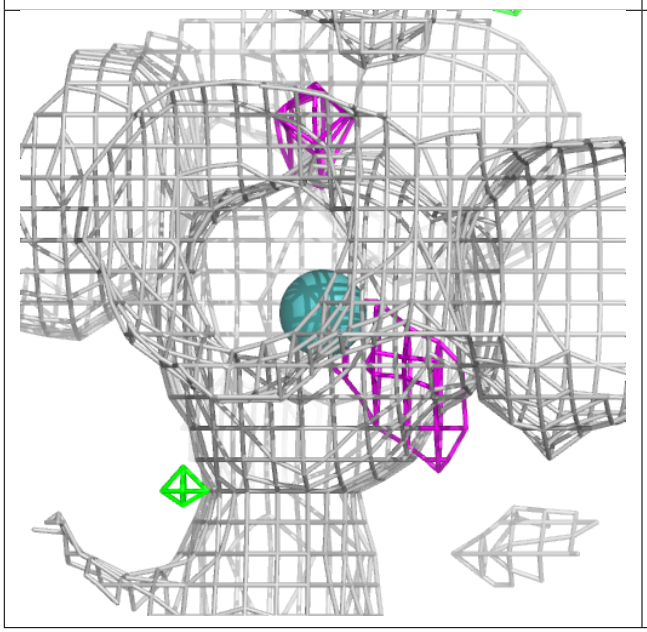


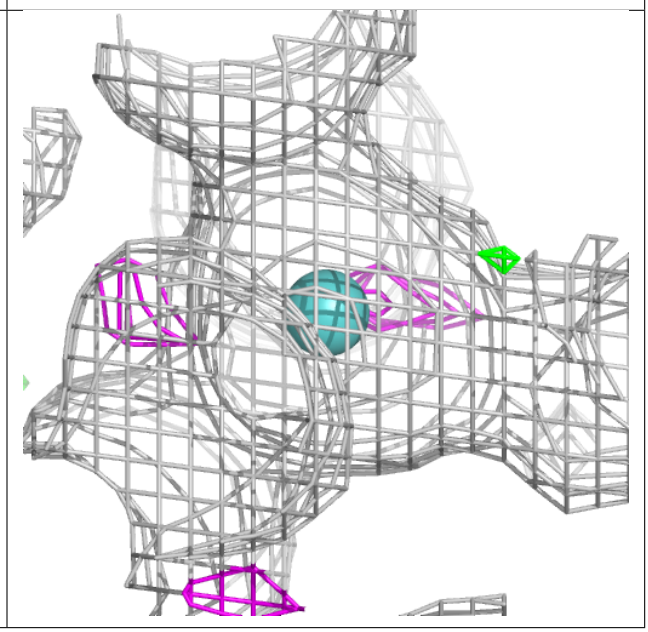


Electron density around MO E 902:

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

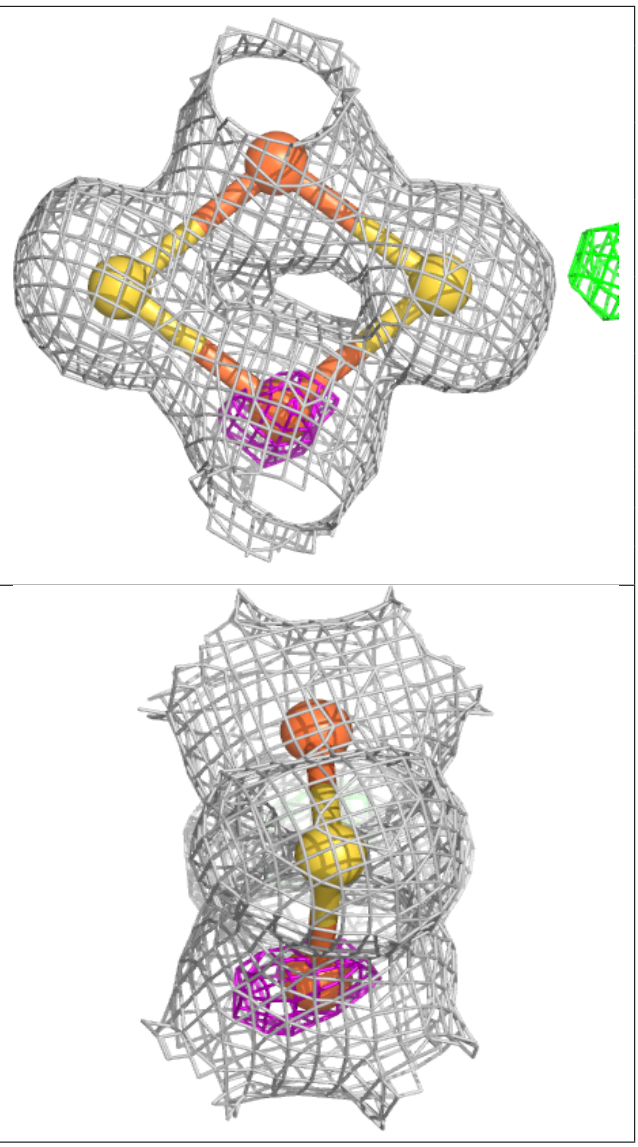






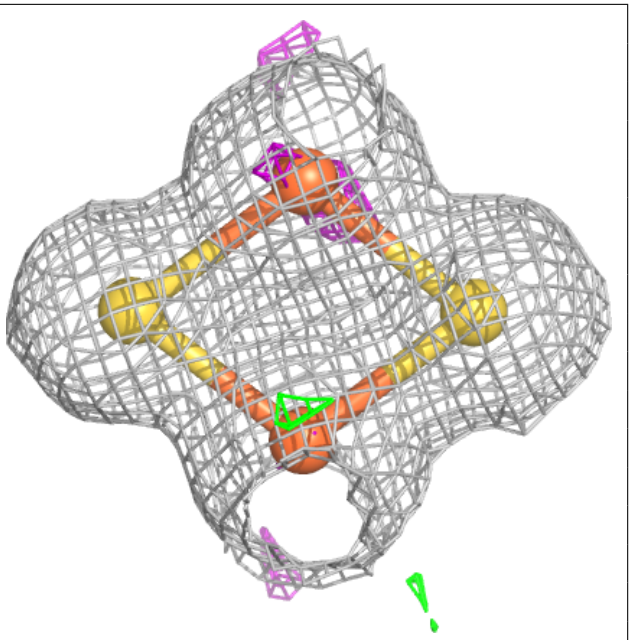
Electron density around FES D 201:

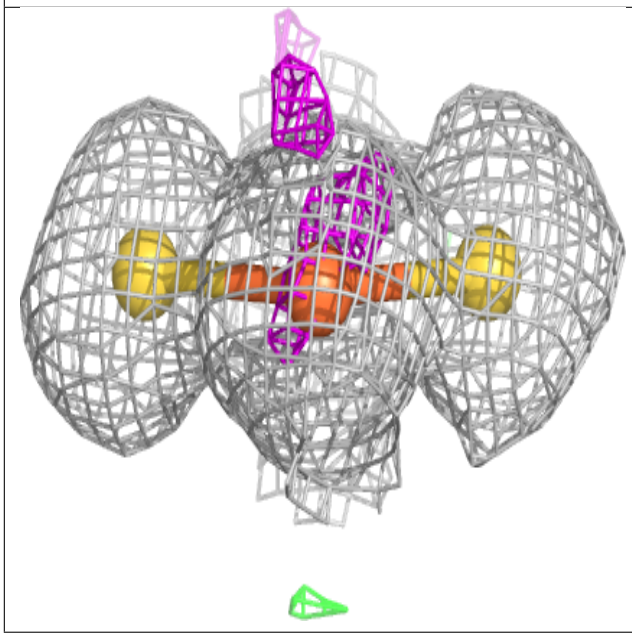
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

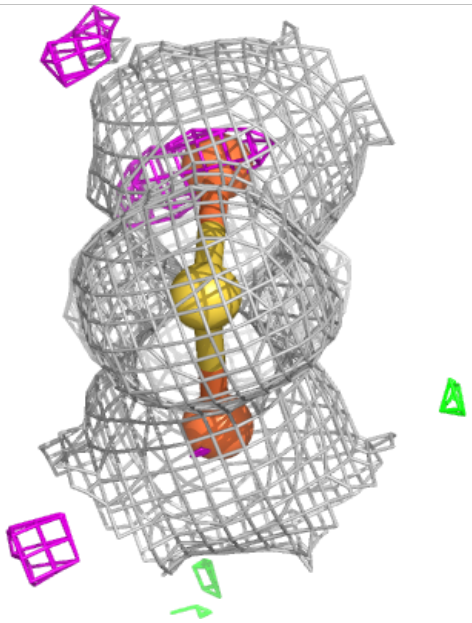


Electron density around FES F 201:

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

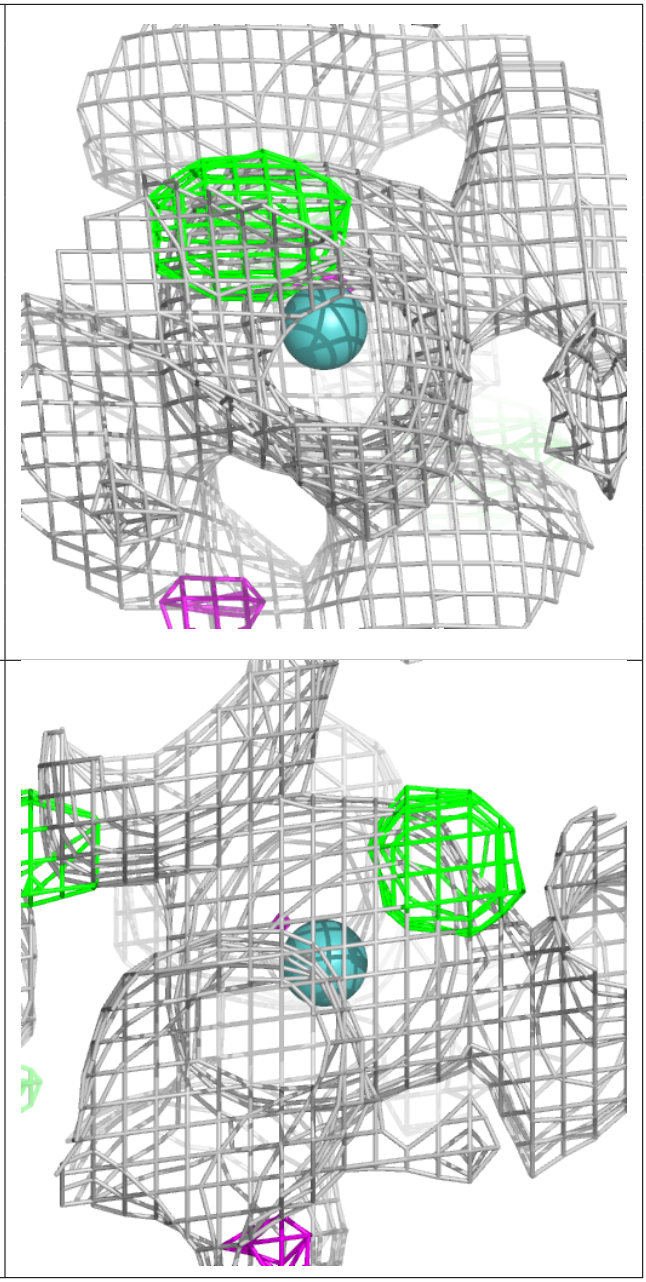






Electron density around MO G 901:

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



6.5 Other polymers (i)

There are no such residues in this entry.