wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 12:32 am BST

PDB ID	:	8RTM / pdb_00008rtm
Title	:	Af Aio C65F-C80G bound to Sb oxyanion
Authors	:	Engrola, F.; Romao, M.J.; Correia, M.; Santos-Silva, T.
Deposited on	:	2024-01-26
Resolution	:	1.87 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:

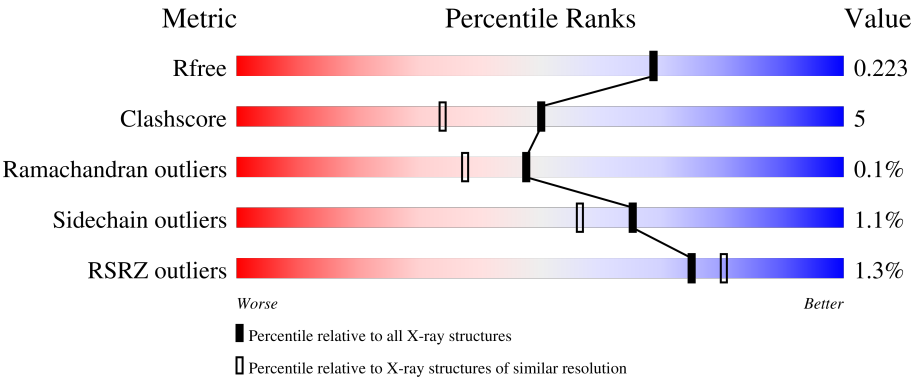
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.87 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.



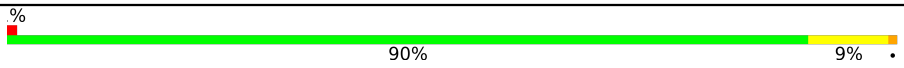
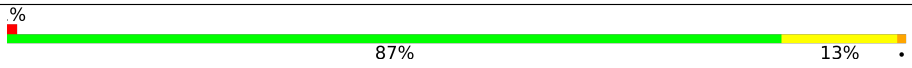
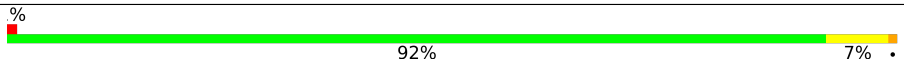
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	824	2% 89% 10%
1	C	824	1% 91% 8%
1	E	824	2% 89% 10%
1	G	824	1% 90% 9%
2	B	135	1% 90% 10%

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Mol	Chain	Length	Quality of chain
2	D	135	
2	F	135	
2	H	135	

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	PGE	A	918	-	-	X	-
10	PGE	G	913	-	-	X	-
16	P4G	C	911	-	-	X	-
17	1PE	C	912	-	-	X	-
17	1PE	G	910	-	-	X	-
7	PEG	A	909	-	-	X	-
7	PEG	A	914	-	-	X	-
7	PEG	A	915	-	-	X	-
7	PEG	A	917	-	-	X	-
7	PEG	B	2906	-	X	X	-
7	PEG	C	914	-	-	X	-
7	PEG	E	907	-	-	X	-
7	PEG	E	909	-	-	X	-
7	PEG	G	908	-	-	X	-
7	PEG	G	912	-	-	X	-
7	PEG	H	2201	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 33119 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
1	A	824	Total	C	N	O	S	0	3	0
			6500	4091	1149	1219	41			
1	C	824	Total	C	N	O	S	0	3	0
			6500	4091	1149	1219	41			
1	E	824	Total	C	N	O	S	0	2	0
			6492	4085	1148	1218	41			
1	G	824	Total	C	N	O	S	0	2	0
			6492	4085	1148	1218	41			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q7SIF4
A	77	ASP	ASN	conflict	UNP Q7SIF4
A	82	ASP	ASN	conflict	UNP Q7SIF4
C	2	ALA	-	expression tag	UNP Q7SIF4
C	77	ASP	ASN	conflict	UNP Q7SIF4
C	82	ASP	ASN	conflict	UNP Q7SIF4
E	2	ALA	-	expression tag	UNP Q7SIF4
E	77	ASP	ASN	conflict	UNP Q7SIF4
E	82	ASP	ASN	conflict	UNP Q7SIF4
G	2	ALA	-	expression tag	UNP Q7SIF4
G	77	ASP	ASN	conflict	UNP Q7SIF4
G	82	ASP	ASN	conflict	UNP Q7SIF4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			
2	D	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			
2	H	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			

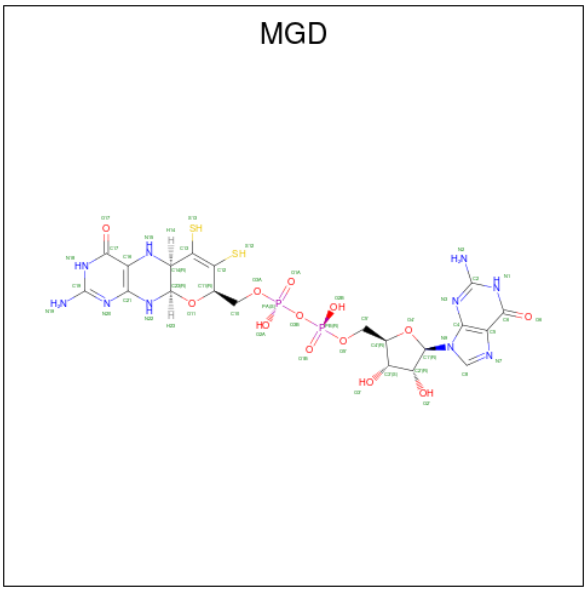
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	PHE	CYS	conflict	UNP Q7SIF3
B	80	GLY	CYS	conflict	UNP Q7SIF3
D	65	PHE	CYS	conflict	UNP Q7SIF3
D	80	GLY	CYS	conflict	UNP Q7SIF3
F	65	PHE	CYS	conflict	UNP Q7SIF3
F	80	GLY	CYS	conflict	UNP Q7SIF3
H	65	PHE	CYS	conflict	UNP Q7SIF3
H	80	GLY	CYS	conflict	UNP Q7SIF3

- Molecule 3 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

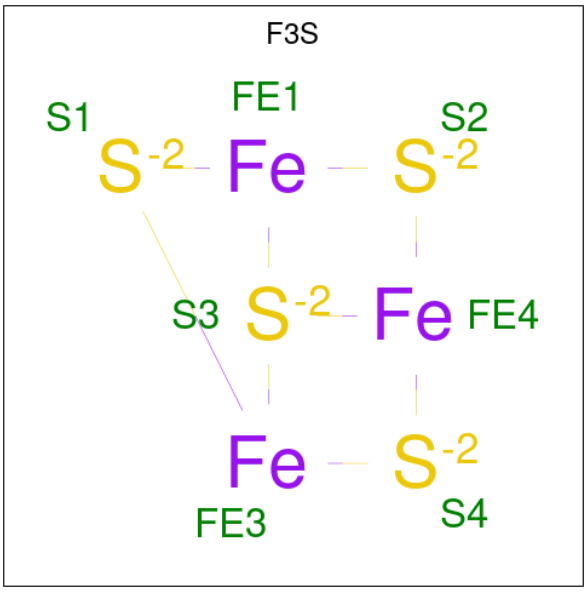
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mo	0	0
			1	1		

- Molecule 4 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).



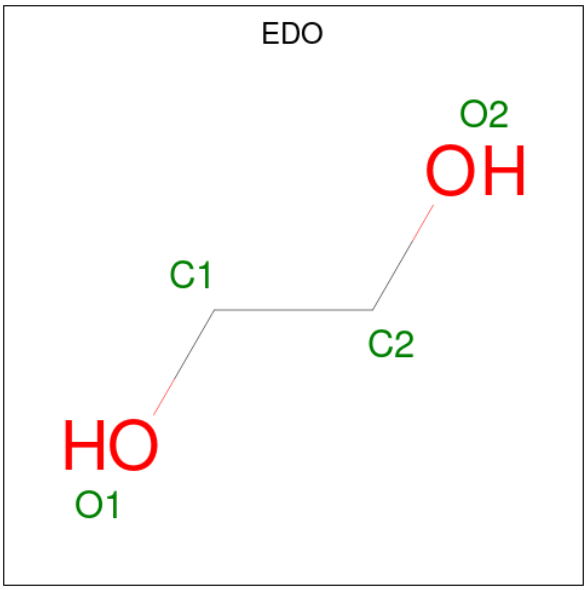
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P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

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



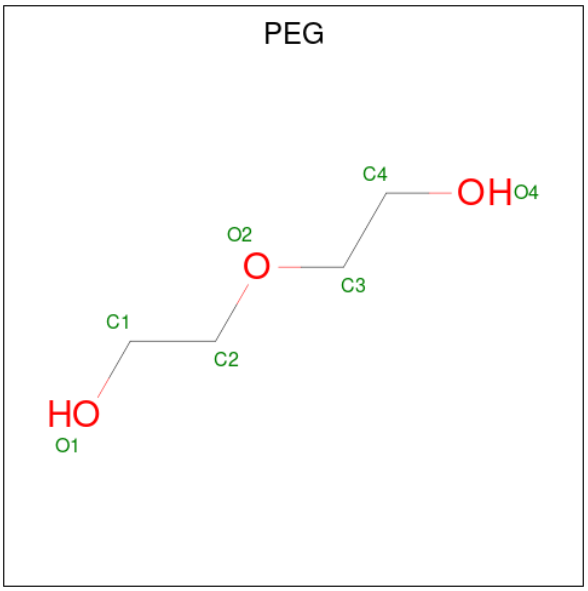
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 7 3 4	0	0
5	C	1	Total Fe S 7 3 4	0	0
5	E	1	Total Fe S 7 3 4	0	0
5	G	1	Total Fe S 7 3 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



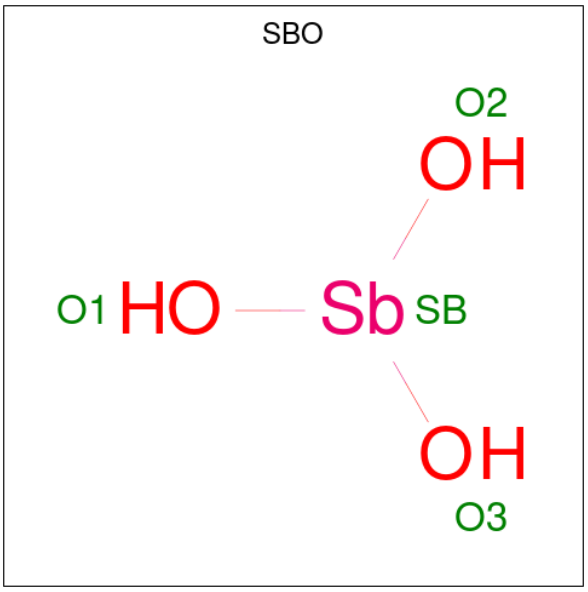
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total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

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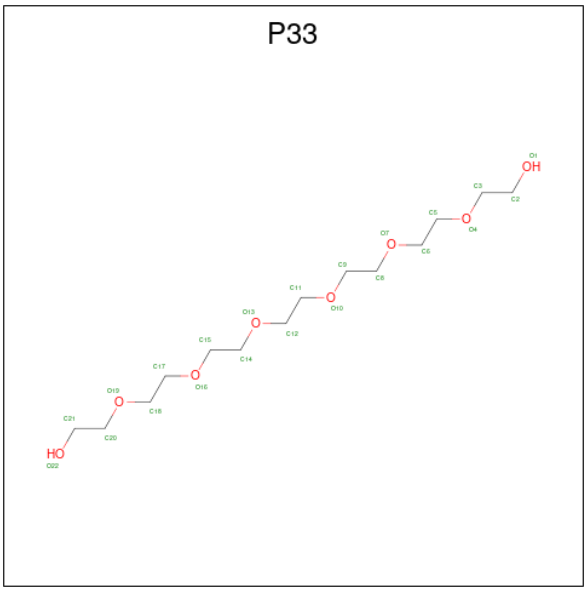
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0
7	F	1	Total C O 7 4 3	0	0
7	G	1	Total C O 7 4 3	0	0
7	G	1	Total C O 7 4 3	0	0
7	G	1	Total C O 7 4 3	0	0
7	G	1	Total C O 7 4 3	0	0
7	H	1	Total C O 7 4 3	0	0

- Molecule 8 is TRIHYDROXYANTIMONITE(III) (CCD ID: SBO) (formula: H_3O_3Sb) (labeled as "Ligand of Interest" by depositor).



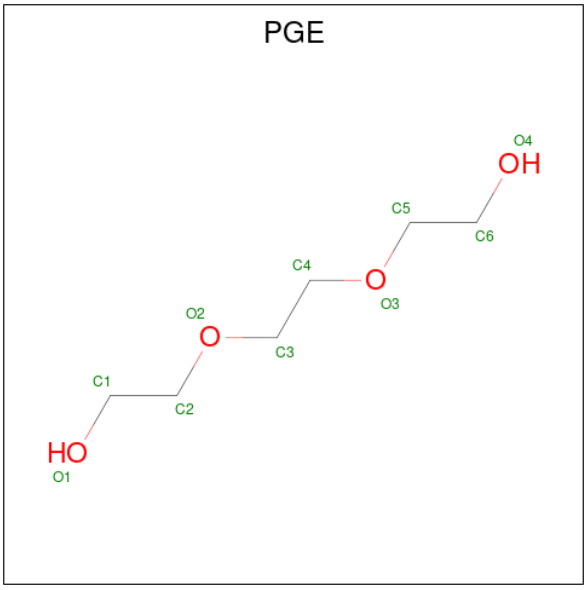
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O Sb 3 2 1	0	0
8	C	1	Total O Sb 4 3 1	0	0
8	E	1	Total O Sb 4 3 1	0	0
8	G	1	Total O Sb 3 2 1	0	0

- Molecule 9 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 22 14 8	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 11 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

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

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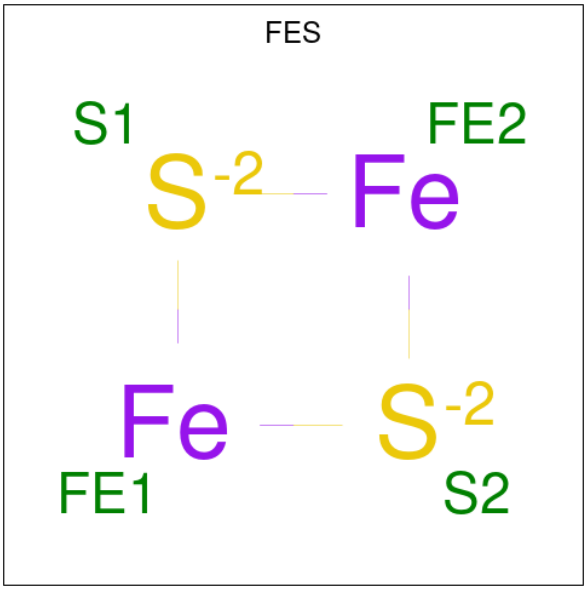
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	G	1	Total O 1 1	0	0

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

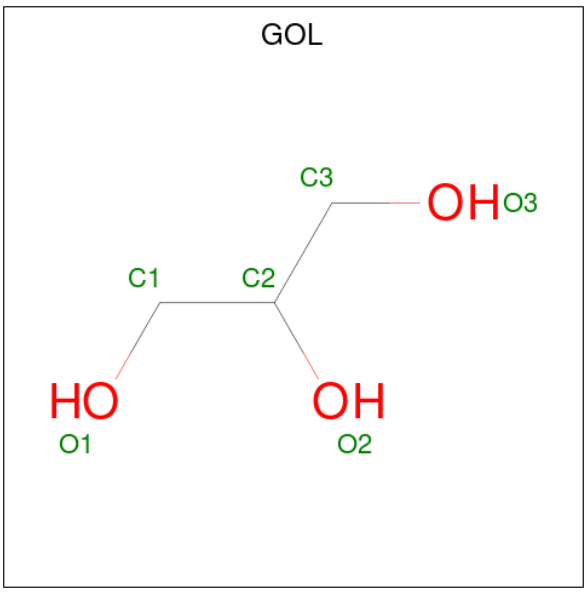
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Na 1 1	0	0
12	C	1	Total Na 1 1	0	0
12	E	1	Total Na 1 1	0	0
12	G	1	Total Na 1 1	0	0

- Molecule 13 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
13	B	1	Total Fe S 4 2 2	0	0
13	D	1	Total Fe S 4 2 2	0	0
13	F	1	Total Fe S 4 2 2	0	0
13	H	1	Total Fe S 4 2 2	0	0

- Molecule 14 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

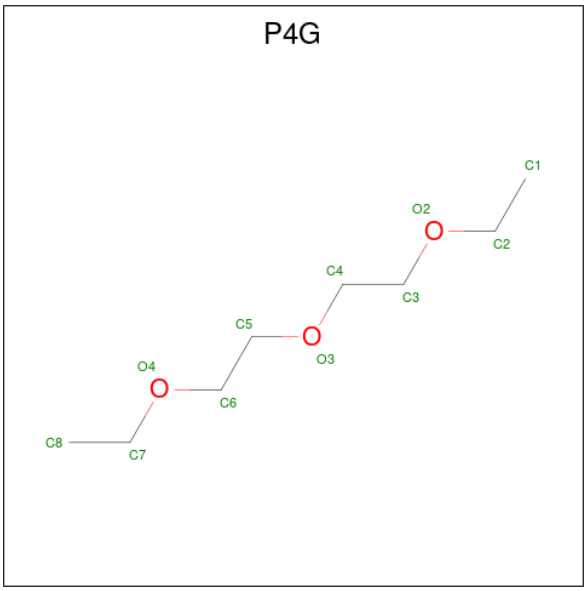


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C O 6 3 3	0	0
14	B	1	Total C O 6 3 3	0	0
14	E	1	Total C O 6 3 3	0	0

- Molecule 15 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

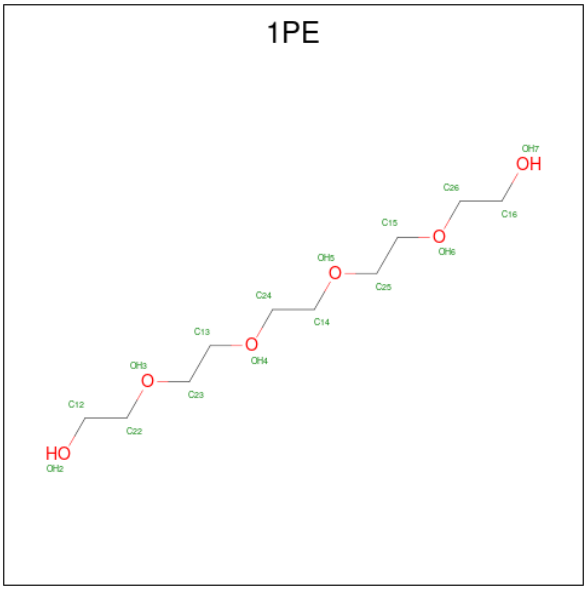
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Mo 1 1	0	0
15	E	1	Total Mo 1 1	0	0
15	G	1	Total Mo 1 1	0	0

- Molecule 16 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



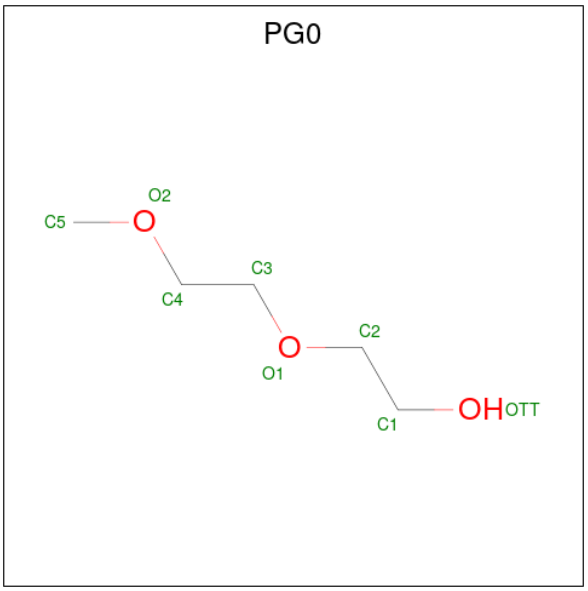
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 11 8 3	0	0

- Molecule 17 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 16 10 6	0	0
17	G	1	Total C O 16 10 6	0	0

- Molecule 18 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	1	Total C O 8 5 3	0	0

- Molecule 19 is water.

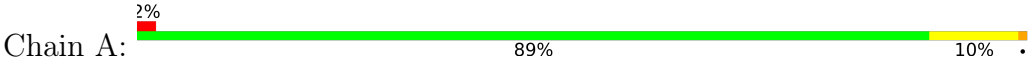
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	453	Total O 453 453	0	0
19	B	90	Total O 90 90	0	0
19	C	487	Total O 487 487	0	0
19	D	90	Total O 90 90	0	0
19	E	487	Total O 487 487	0	0
19	F	90	Total O 90 90	0	0
19	G	492	Total O 492 492	0	0
19	H	83	Total O 83 83	0	0

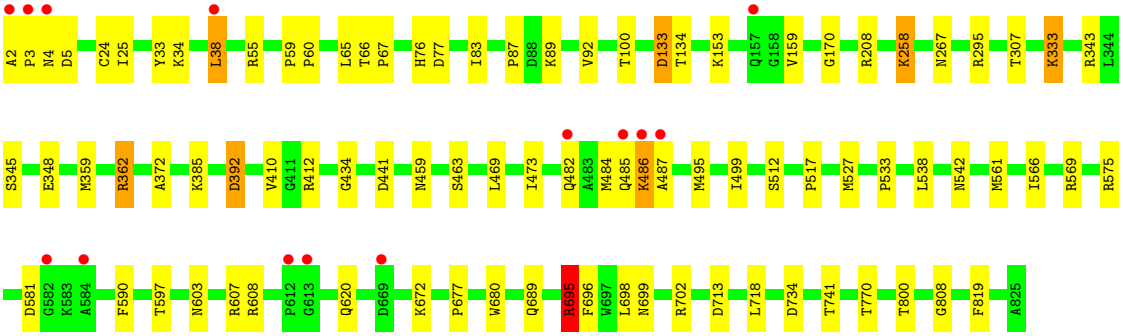
3 Residue-property plots (i)

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

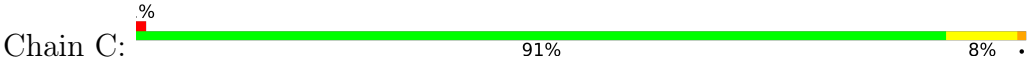
Chain A:

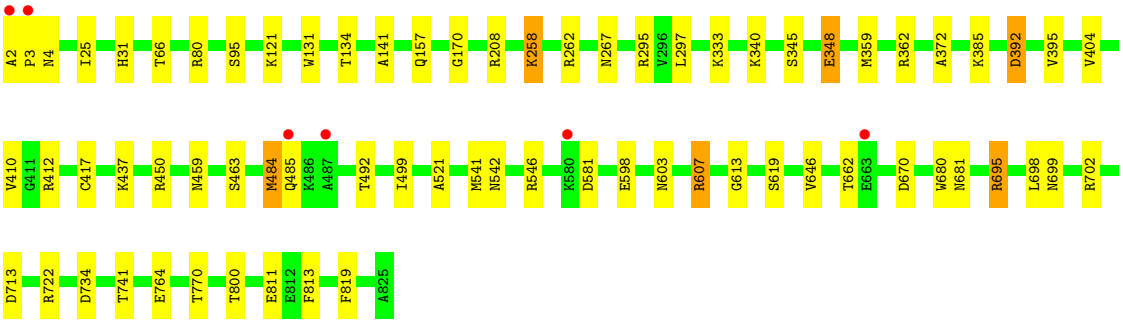




• Molecule 1: Arsenite oxidase subunit AioA

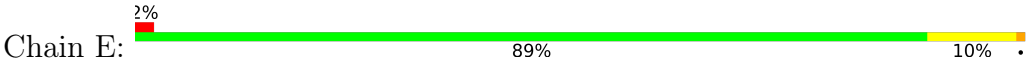
Chain C:

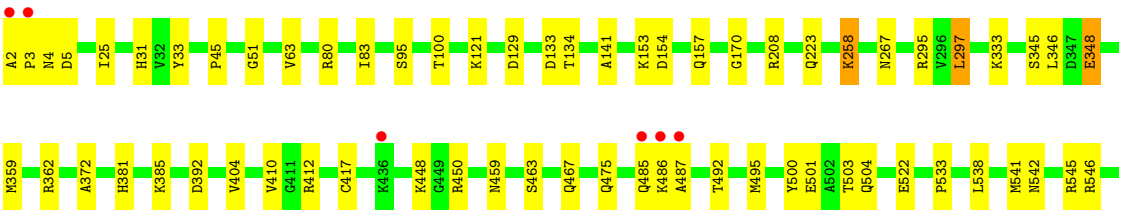


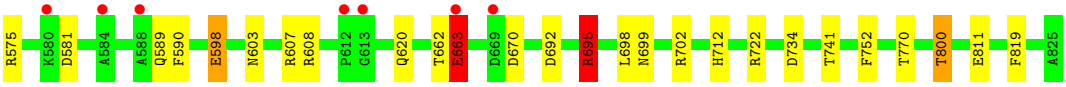


• Molecule 1: Arsenite oxidase subunit AioA

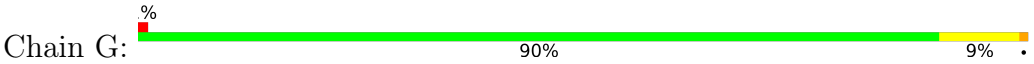
Chain E:

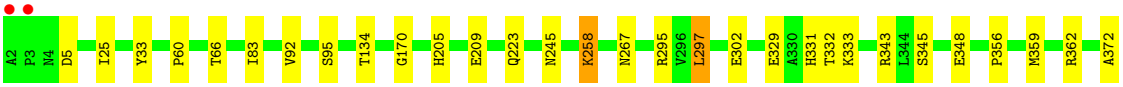


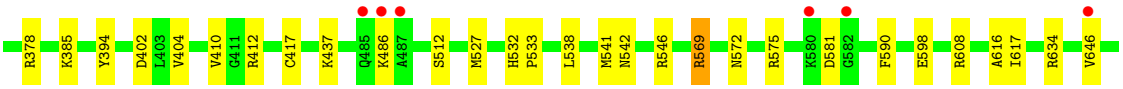




• Molecule 1: Arsenite oxidase subunit AioA

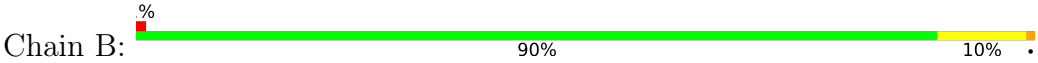


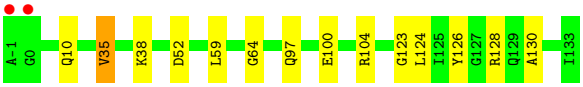




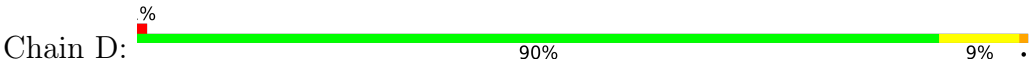


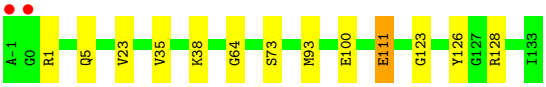
• Molecule 2: Arsenite oxidase subunit AioB



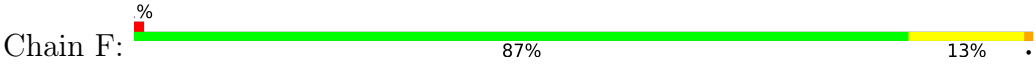


• Molecule 2: Arsenite oxidase subunit AioB



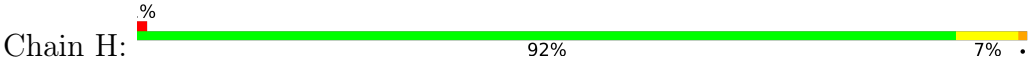


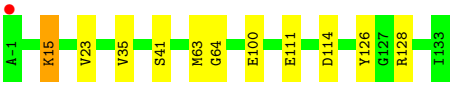
• Molecule 2: Arsenite oxidase subunit AioB





• Molecule 2: Arsenite oxidase subunit AioB





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.25Å 109.12Å 117.00Å 82.33° 89.68° 83.69°	Depositor
Resolution (Å)	48.94 – 1.87 48.94 – 1.87	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.94-1.87) 96.8 (48.94-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.179 , 0.214 0.191 , 0.223	Depositor DCC
R_{free} test set	17518 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.5	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	33119	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.77% 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: EDO, PEG, FES, P33, MO, PGE, SBO, GOL, 1PE, P4G, PG0, MGD, O, F3S, 4MO, NA

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	0.95	2/6661 (0.0%)	1.25	20/9029 (0.2%)
1	C	0.95	1/6661 (0.0%)	1.24	18/9029 (0.2%)
1	E	0.94	2/6653 (0.0%)	1.27	24/9018 (0.3%)
1	G	0.93	0/6653	1.25	22/9018 (0.2%)
2	B	1.00	2/1026 (0.2%)	1.27	0/1397
2	D	1.01	0/1026	1.31	4/1397 (0.3%)
2	F	0.98	0/1026	1.30	4/1397 (0.3%)
2	H	0.94	0/1026	1.27	2/1397 (0.1%)
All	All	0.95	7/30732 (0.0%)	1.26	94/41682 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	7
1	E	0	6
1	G	0	5
2	B	0	1
2	D	0	1
2	F	0	2
2	H	0	2
All	All	0	29

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	HIS	CG-CD2	-5.97	1.29	1.35
2	B	52	ASP	N-CA	-5.87	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	PRO	CA-CB	5.50	1.61	1.53
2	B	130	ALA	CA-CB	-5.14	1.44	1.53
1	E	712	HIS	CG-CD2	-5.12	1.30	1.35

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	295	ARG	CD-NE-CZ	9.31	137.43	124.40
1	E	295	ARG	CD-NE-CZ	9.01	137.02	124.40
1	E	412	ARG	CD-NE-CZ	8.32	136.05	124.40
1	E	741	THR	CA-CB-OG1	-8.20	97.30	109.60
2	D	111	GLU	CB-CG-CD	7.65	125.60	112.60

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	ARG	Sidechain
1	A	55	ARG	Sidechain
1	A	608	ARG	Sidechain
1	A	695	ARG	Sidechain
1	A	702	ARG	Sidechain

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	6500	0	6283	79	0
1	C	6500	0	6283	43	0
1	E	6492	0	6273	65	0
1	G	6492	0	6273	58	0
2	B	1004	0	986	20	0
2	D	1004	0	986	7	0
2	F	1004	0	986	9	0
2	H	1004	0	986	4	0
3	A	1	0	0	0	0
4	A	94	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	94	0	44	2	0
4	E	94	0	44	2	0
4	G	94	0	44	2	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	12	0	18	1	0
6	C	24	0	36	0	0
6	E	16	0	24	3	0
6	G	12	0	18	1	0
7	A	63	0	87	26	0
7	B	21	0	30	17	0
7	C	28	0	40	12	0
7	E	42	0	60	13	0
7	F	7	0	10	0	0
7	G	28	0	40	12	0
7	H	7	0	10	4	0
8	A	3	0	0	0	0
8	C	4	0	0	1	0
8	E	4	0	0	1	0
8	G	3	0	0	1	0
9	A	22	0	30	6	0
10	A	20	0	28	7	0
10	C	10	0	14	1	0
10	E	10	0	14	3	0
10	G	10	0	14	9	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	1	0
11	G	1	0	0	0	0
12	A	1	0	0	0	0
12	C	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
13	B	4	0	0	0	0
13	D	4	0	0	0	0
13	F	4	0	0	0	0
13	H	4	0	0	0	0
14	B	12	0	16	4	0
14	E	6	0	8	0	0
15	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	1	0	0	1	0
15	G	1	0	0	0	0
16	C	11	0	18	21	0
17	C	16	0	22	8	0
17	G	16	0	22	12	0
18	C	8	0	12	5	0
19	A	453	0	0	9	0
19	B	90	0	0	3	0
19	C	487	0	0	11	0
19	D	90	0	0	3	0
19	E	487	0	0	12	0
19	F	90	0	0	4	0
19	G	492	0	0	7	0
19	H	83	0	0	2	0
All	All	33119	0	29803	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 320 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)
7:A:914:PEG:H11	7:A:914:PEG:H41	1.32	1.11
1:A:620:GLN:HE21	7:A:915:PEG:H42	1.10	1.08
1:A:208:ARG:HH12	10:A:918:PGE:H42	1.27	0.99
1:A:208:ARG:HH12	10:A:918:PGE:C4	1.76	0.98
1:C:157:GLN:HG2	19:C:1336:HOH:O	1.64	0.98

There are no symmetry-related clashes.

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	824/824 (100%)	796 (97%)	27 (3%)	1 (0%)	48	37
1	C	824/824 (100%)	793 (96%)	30 (4%)	1 (0%)	48	37
1	E	823/824 (100%)	792 (96%)	30 (4%)	1 (0%)	48	37
1	G	823/824 (100%)	793 (96%)	30 (4%)	0	100	100
2	B	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	D	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	F	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
2	H	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
All	All	3826/3836 (100%)	3689 (96%)	134 (4%)	3 (0%)	48	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	392	ASP
1	A	392	ASP
1	C	392	ASP

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	678/676 (100%)	669 (99%)	9 (1%)	61	50
1	C	678/676 (100%)	674 (99%)	4 (1%)	78	72
1	E	677/676 (100%)	671 (99%)	6 (1%)	70	63
1	G	677/676 (100%)	669 (99%)	8 (1%)	63	53
2	B	110/110 (100%)	108 (98%)	2 (2%)	51	38
2	D	110/110 (100%)	108 (98%)	2 (2%)	51	38
2	F	110/110 (100%)	107 (97%)	3 (3%)	39	23
2	H	110/110 (100%)	107 (97%)	3 (3%)	39	23
All	All	3150/3144 (100%)	3113 (99%)	37 (1%)	65	53

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	329	GLU
2	H	35	VAL
1	G	410	VAL
1	G	652	LYS
1	C	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	270	GLN
1	G	461	GLN
1	G	688	GLN
1	C	611	GLN
1	C	461	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 12 are monoatomic - leaving 77 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	$\#\|Z\|>2$
4	MGD	G	901	15	45,52,52	1.13	3 (6%)	54,81,81	1.18	4 (7%)
7	PEG	C	909	-	6,6,6	0.25	0	5,5,5	0.39	0
6	EDO	G	906	-	3,3,3	0.39	0	2,2,2	1.00	0
7	PEG	E	912	-	6,6,6	0.47	0	5,5,5	0.21	0
7	PEG	A	907	-	6,6,6	0.72	0	5,5,5	0.43	0
7	PEG	A	921	-	6,6,6	0.45	0	5,5,5	0.36	0
18	PG0	C	916	-	7,7,7	1.19	0	6,6,6	0.90	0
10	PGE	G	913	-	9,9,9	0.92	0	8,8,8	1.18	2 (25%)
4	MGD	E	902	15	45,52,52	1.21	3 (6%)	54,81,81	1.24	7 (12%)
6	EDO	C	910	-	3,3,3	0.38	0	2,2,2	0.32	0
6	EDO	A	905	-	3,3,3	0.31	0	2,2,2	0.28	0
7	PEG	A	917	-	6,6,6	0.64	0	5,5,5	0.55	0
5	F3S	E	904	1	0,9,9	-	-	-		
7	PEG	A	910	-	6,6,6	0.74	0	5,5,5	0.63	0
7	PEG	F	202	-	6,6,6	0.47	0	5,5,5	0.48	0
14	GOL	B	2903	-	5,5,5	0.33	0	5,5,5	0.60	0
7	PEG	A	914	-	6,6,6	0.79	0	5,5,5	0.84	0
6	EDO	E	914	-	3,3,3	0.23	0	2,2,2	0.28	0
8	SBO	G	909	11	0,2,3	-	-	-		
6	EDO	E	915	-	3,3,3	1.17	0	2,2,2	0.90	0
6	EDO	E	905	-	3,3,3	0.21	0	2,2,2	0.31	0
7	PEG	E	910	-	6,6,6	0.50	0	5,5,5	0.51	0
7	PEG	G	911	-	6,6,6	0.58	0	5,5,5	0.36	0
7	PEG	G	907	-	6,6,6	0.70	0	5,5,5	0.50	0
7	PEG	E	907	-	6,6,6	0.37	0	5,5,5	0.13	0
4	MGD	A	902	3	45,52,52	0.83	0	54,81,81	1.10	4 (7%)
10	PGE	C	917	-	9,9,9	1.38	1 (11%)	8,8,8	0.93	0
7	PEG	C	919	-	6,6,6	1.10	0	5,5,5	0.61	0
16	P4G	C	911	-	10,10,10	0.45	0	9,9,9	0.69	0
4	MGD	C	904	15	45,52,52	1.05	3 (6%)	54,81,81	1.07	3 (5%)
9	P33	A	912	-	21,21,21	1.19	3 (14%)	20,20,20	1.01	1 (5%)
7	PEG	A	908	-	6,6,6	0.96	0	5,5,5	0.64	0
6	EDO	C	907	-	3,3,3	0.90	0	2,2,2	0.51	0
4	MGD	A	903	3	45,52,52	0.89	1 (2%)	54,81,81	1.15	4 (7%)
7	PEG	B	2904	-	6,6,6	0.38	0	5,5,5	0.45	0
8	SBO	A	911	19,11	0,2,3	-	-	-		
13	FES	H	2202	2	0,4,4	-	-	-		
7	PEG	E	911	-	6,6,6	0.37	0	5,5,5	0.42	0
7	PEG	H	2201	-	6,6,6	0.74	0	5,5,5	0.51	0
7	PEG	E	909	-	6,6,6	0.44	0	5,5,5	0.58	0
17	1PE	G	910	-	15,15,15	0.80	0	14,14,14	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SBO	C	918	19,11	0,3,3	-	-	-		
10	PGE	A	918	-	9,9,9	0.93	0	8,8,8	0.84	0
6	EDO	C	906	-	3,3,3	0.18	0	2,2,2	0.32	0
7	PEG	A	909	-	6,6,6	0.37	0	5,5,5	0.53	0
4	MGD	G	902	15	45,52,52	1.06	4 (8%)	54,81,81	1.34	3 (5%)
6	EDO	C	905	-	3,3,3	0.46	0	2,2,2	0.14	0
14	GOL	E	908	-	5,5,5	0.23	0	5,5,5	0.53	0
6	EDO	C	908	-	3,3,3	0.56	0	2,2,2	0.69	0
7	PEG	C	913	-	6,6,6	1.09	1 (16%)	5,5,5	0.56	0
7	PEG	C	914	-	6,6,6	0.44	0	5,5,5	0.92	0
7	PEG	G	908	-	6,6,6	0.46	0	5,5,5	0.55	0
14	GOL	B	2905	-	5,5,5	0.23	0	5,5,5	0.82	0
6	EDO	G	905	-	3,3,3	0.46	0	2,2,2	0.47	0
7	PEG	B	2901	-	6,6,6	0.69	0	5,5,5	0.53	0
13	FES	D	201	2	0,4,4	-	-	-		
17	1PE	C	912	-	15,15,15	1.11	2 (13%)	14,14,14	1.04	0
7	PEG	G	912	-	6,6,6	0.75	0	5,5,5	0.91	0
5	F3S	C	901	1	0,9,9	-	-	-		
7	PEG	A	913	-	6,6,6	0.46	0	5,5,5	0.30	0
4	MGD	E	901	15	45,52,52	0.77	1 (2%)	54,81,81	1.13	5 (9%)
5	F3S	A	904	1	0,9,9	-	-	-		
13	FES	B	2902	2	0,4,4	-	-	-		
5	F3S	G	903	1	0,9,9	-	-	-		
6	EDO	E	906	-	3,3,3	0.52	0	2,2,2	0.58	0
8	SBO	E	917	11	0,3,3	-	-	-		
7	PEG	A	915	-	6,6,6	1.00	0	5,5,5	0.86	0
7	PEG	B	2906	-	6,6,6	2.04	3 (50%)	5,5,5	1.74	1 (20%)
7	PEG	E	913	-	6,6,6	1.15	1 (16%)	5,5,5	0.83	0
10	PGE	E	916	-	9,9,9	1.30	1 (11%)	8,8,8	1.14	1 (12%)
4	MGD	C	902	15	45,52,52	0.87	1 (2%)	54,81,81	1.11	4 (7%)
6	EDO	A	919	-	3,3,3	0.41	0	2,2,2	0.39	0
6	EDO	G	914	-	3,3,3	0.62	0	2,2,2	0.58	0
6	EDO	C	915	-	3,3,3	0.33	0	2,2,2	0.88	0
13	FES	F	201	2	0,4,4	-	-	-		
6	EDO	A	906	-	3,3,3	0.56	0	2,2,2	0.63	0
10	PGE	A	916	-	9,9,9	0.98	1 (11%)	8,8,8	1.23	1 (12%)

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
4	MGD	G	901	15	-	4/22/66/66	0/6/6/6
7	PEG	B	2901	-	-	2/4/4/4	-
7	PEG	C	909	-	-	3/4/4/4	-
7	PEG	E	910	-	-	4/4/4/4	-
4	MGD	A	903	3	-	5/22/66/66	0/6/6/6
7	PEG	B	2904	-	-	4/4/4/4	-
7	PEG	G	911	-	-	3/4/4/4	-
13	FES	D	201	2	-	-	0/1/1/1
17	1PE	C	912	-	-	8/13/13/13	-
6	EDO	G	906	-	-	1/1/1/1	-
13	FES	H	2202	2	-	-	0/1/1/1
7	PEG	G	912	-	-	0/4/4/4	-
5	F3S	C	901	1	-	-	0/3/3/3
7	PEG	A	913	-	-	0/4/4/4	-
4	MGD	E	901	15	-	4/22/66/66	0/6/6/6
7	PEG	G	907	-	-	3/4/4/4	-
7	PEG	E	911	-	-	4/4/4/4	-
7	PEG	E	907	-	-	3/4/4/4	-
4	MGD	A	902	3	-	4/22/66/66	0/6/6/6
7	PEG	H	2201	-	-	2/4/4/4	-
5	F3S	A	904	1	-	-	0/3/3/3
13	FES	B	2902	2	-	-	0/1/1/1
7	PEG	E	909	-	-	1/4/4/4	-
17	1PE	G	910	-	-	7/13/13/13	-
5	F3S	G	903	1	-	-	0/3/3/3
7	PEG	E	912	-	-	3/4/4/4	-
7	PEG	A	907	-	-	1/4/4/4	-
10	PGE	A	918	-	-	4/7/7/7	-
10	PGE	C	917	-	-	5/7/7/7	-
6	EDO	E	906	-	-	1/1/1/1	-
6	EDO	C	906	-	-	1/1/1/1	-
7	PEG	A	909	-	-	3/4/4/4	-
7	PEG	A	915	-	-	1/4/4/4	-
7	PEG	A	921	-	-	2/4/4/4	-
7	PEG	B	2906	-	-	3/4/4/4	-
7	PEG	E	913	-	-	3/4/4/4	-
18	PG0	C	916	-	-	2/5/5/5	-
4	MGD	G	902	15	-	3/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGE	G	913	-	-	3/7/7/7	-
4	MGD	E	902	15	-	4/22/66/66	0/6/6/6
6	EDO	C	910	-	-	1/1/1/1	-
6	EDO	A	905	-	-	1/1/1/1	-
7	PEG	C	919	-	-	2/4/4/4	-
7	PEG	A	917	-	-	2/4/4/4	-
6	EDO	C	905	-	-	0/1/1/1	-
7	PEG	A	910	-	-	2/4/4/4	-
5	F3S	E	904	1	-	-	0/3/3/3
10	PGE	E	916	-	-	5/7/7/7	-
7	PEG	F	202	-	-	2/4/4/4	-
14	GOL	B	2903	-	-	0/4/4/4	-
14	GOL	E	908	-	-	0/4/4/4	-
16	P4G	C	911	-	-	6/8/8/8	-
7	PEG	A	914	-	-	2/4/4/4	-
6	EDO	C	908	-	-	0/1/1/1	-
6	EDO	E	914	-	-	0/1/1/1	-
7	PEG	C	913	-	-	3/4/4/4	-
7	PEG	C	914	-	-	1/4/4/4	-
4	MGD	C	902	15	-	5/22/66/66	0/6/6/6
4	MGD	C	904	15	-	4/22/66/66	0/6/6/6
6	EDO	A	919	-	-	1/1/1/1	-
9	P33	A	912	-	-	8/19/19/19	-
7	PEG	G	908	-	-	3/4/4/4	-
14	GOL	B	2905	-	-	4/4/4/4	-
6	EDO	G	914	-	-	1/1/1/1	-
7	PEG	A	908	-	-	3/4/4/4	-
6	EDO	E	915	-	-	1/1/1/1	-
6	EDO	C	915	-	-	1/1/1/1	-
13	FES	F	201	2	-	-	0/1/1/1
6	EDO	A	906	-	-	1/1/1/1	-
6	EDO	G	905	-	-	0/1/1/1	-
6	EDO	C	907	-	-	1/1/1/1	-
6	EDO	E	905	-	-	1/1/1/1	-
10	PGE	A	916	-	-	4/7/7/7	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	902	MGD	C10-C11	-4.98	1.45	1.52
4	G	901	MGD	C23-C14	-4.25	1.50	1.53
10	C	917	PGE	C4-C3	3.71	1.68	1.49
4	E	902	MGD	C23-C14	3.52	1.56	1.53
4	C	904	MGD	C10-C11	-3.31	1.47	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	902	MGD	O11-C23-C14	5.82	112.85	108.96
4	G	901	MGD	O11-C23-N22	-3.67	104.79	108.57
4	A	903	MGD	O11-C23-C14	3.52	111.31	108.96
4	G	902	MGD	C19-N20-C21	3.43	119.62	113.43
4	G	901	MGD	C4'-O4'-C1'	-3.42	101.92	109.47

There are no chirality outliers.

5 of 166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	MGD	PA-O3B-PB-O5'
4	A	902	MGD	C5'-O5'-PB-O1B
4	A	902	MGD	C5'-O5'-PB-O3B
4	A	903	MGD	C5'-O5'-PB-O1B
4	A	903	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	909	PEG	2	0
18	C	916	PG0	5	0
10	G	913	PGE	9	0
4	E	902	MGD	2	0
7	A	917	PEG	4	0
14	B	2903	GOL	1	0
7	A	914	PEG	9	0
6	E	914	EDO	1	0
8	G	909	SBO	1	0
6	E	905	EDO	1	0
7	E	910	PEG	1	0
7	G	911	PEG	2	0
7	G	907	PEG	1	0

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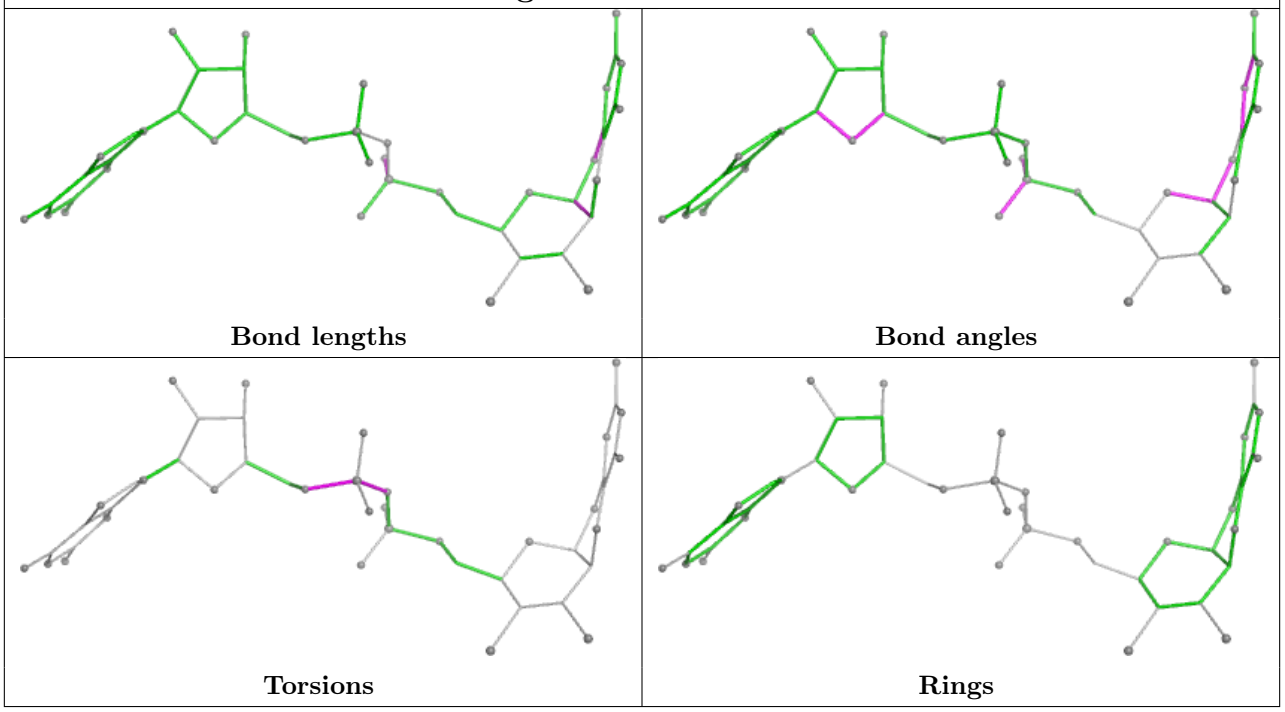
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	907	PEG	4	0
10	C	917	PGE	1	0
7	C	919	PEG	3	0
16	C	911	P4G	21	0
4	C	904	MGD	2	0
9	A	912	P33	6	0
7	A	908	PEG	1	0
4	A	903	MGD	2	0
7	E	911	PEG	3	0
7	H	2201	PEG	4	0
7	E	909	PEG	4	0
17	G	910	1PE	12	0
8	C	918	SBO	1	0
10	A	918	PGE	6	0
7	A	909	PEG	7	0
4	G	902	MGD	2	0
7	C	913	PEG	3	0
7	C	914	PEG	4	0
7	G	908	PEG	5	0
14	B	2905	GOL	3	0
6	G	905	EDO	1	0
7	B	2901	PEG	3	0
17	C	912	1PE	8	0
7	G	912	PEG	4	0
7	A	913	PEG	1	0
6	E	906	EDO	2	0
8	E	917	SBO	1	0
7	A	915	PEG	4	0
7	B	2906	PEG	14	0
7	E	913	PEG	2	0
10	E	916	PGE	3	0
6	A	919	EDO	1	0
6	G	914	EDO	1	0
10	A	916	PGE	1	0

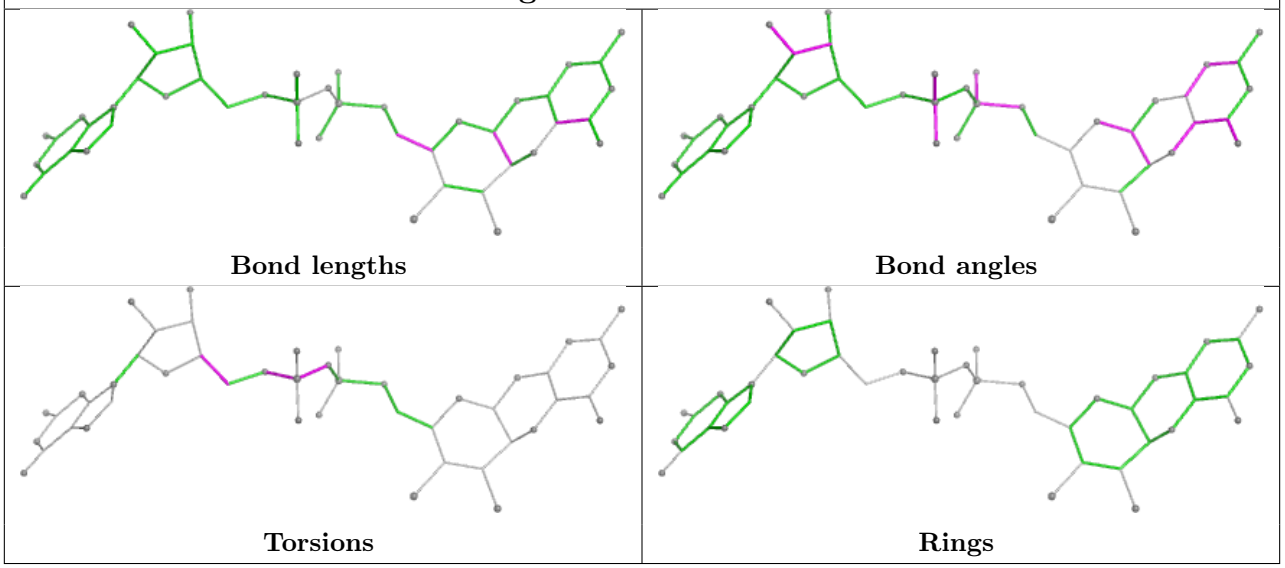
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

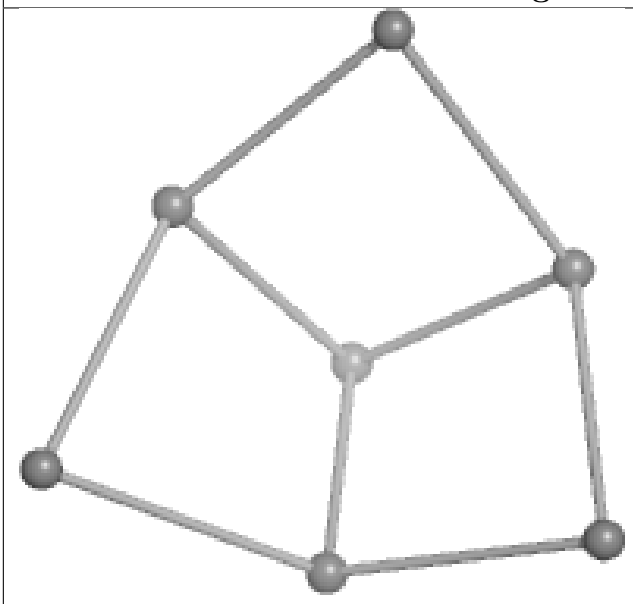
Ligand MGD G 901



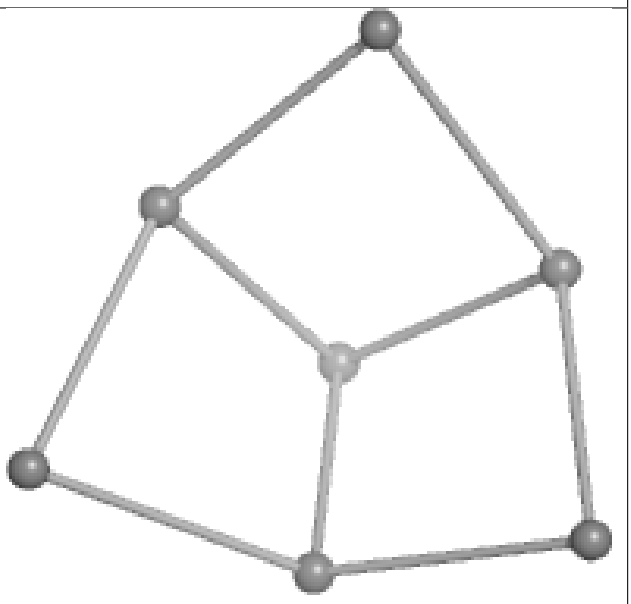
Ligand MGD E 902



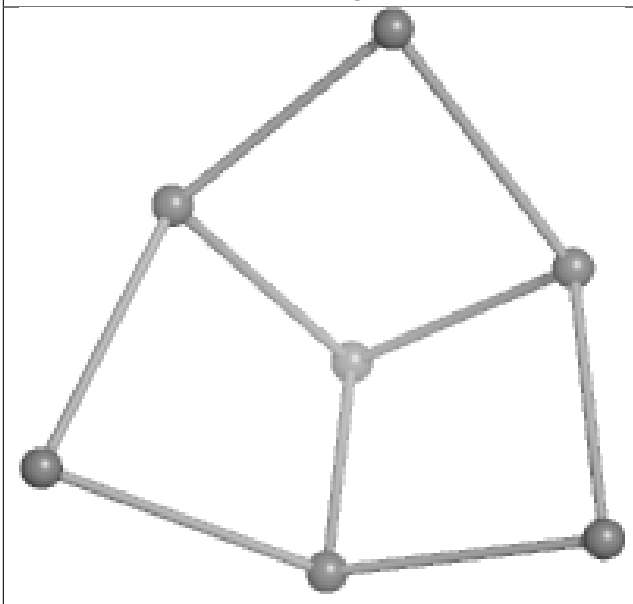
Ligand F3S E 904



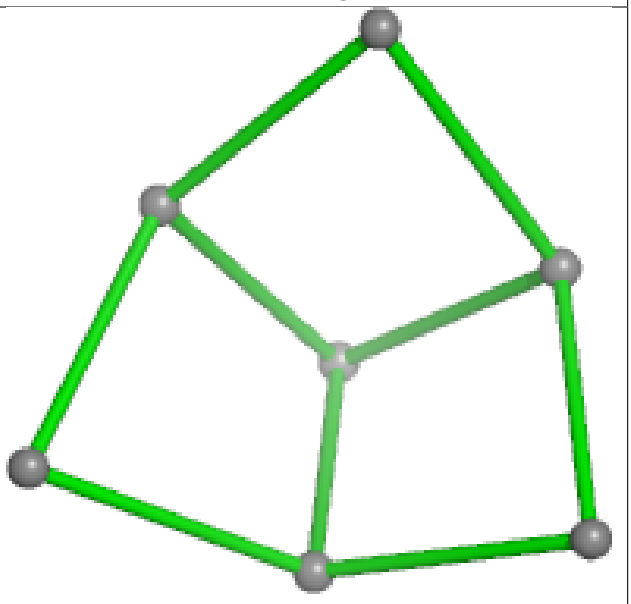
Bond lengths



Bond angles

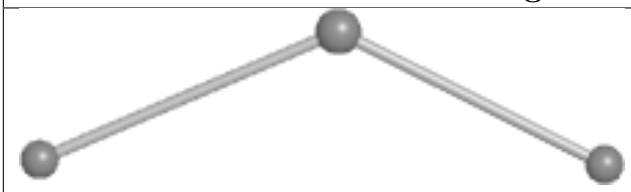


Torsions

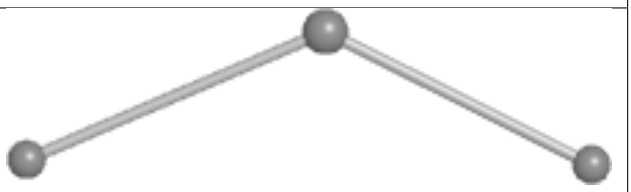


Rings

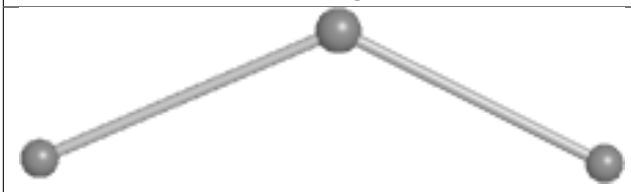
Ligand SBO G 909



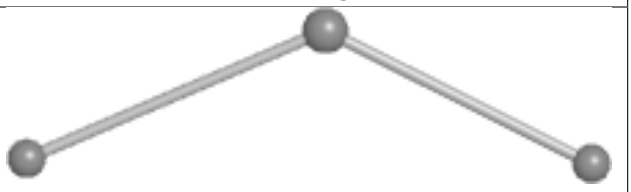
Bond lengths



Bond angles

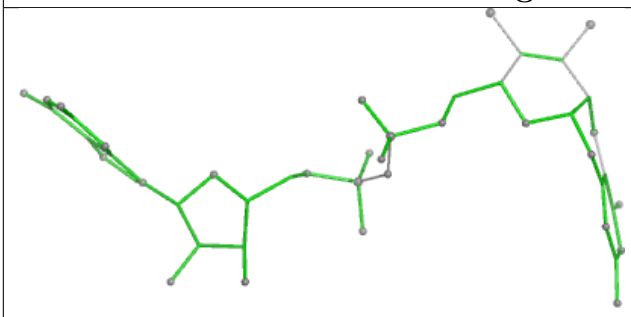


Torsions

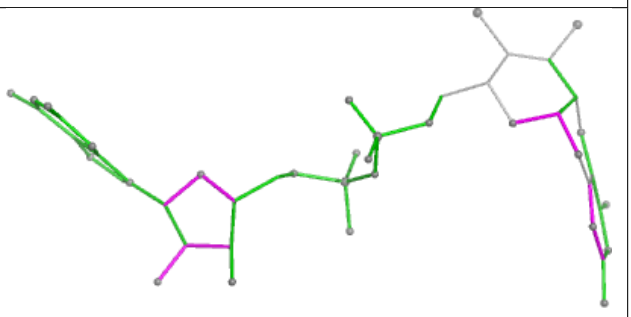


Rings

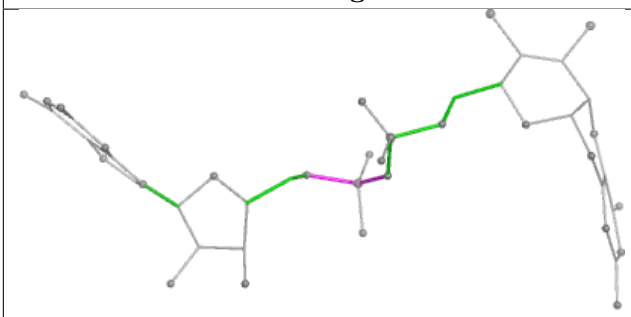
Ligand MGD A 902



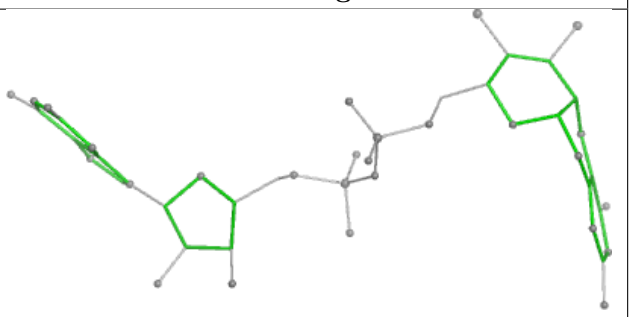
Bond lengths



Bond angles

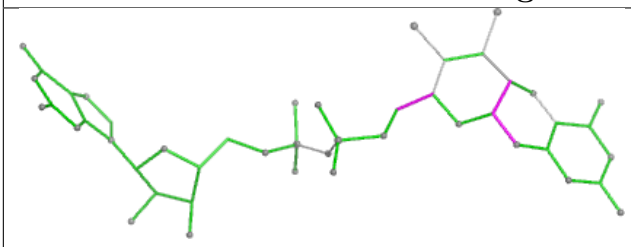


Torsions

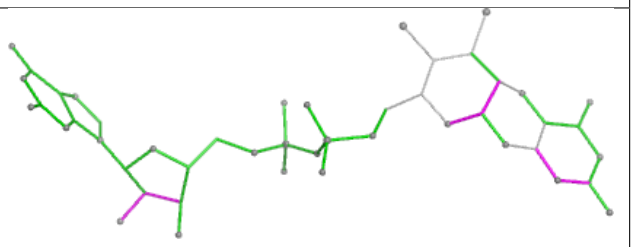


Rings

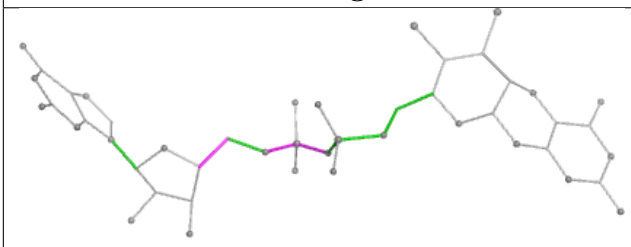
Ligand MGD C 904



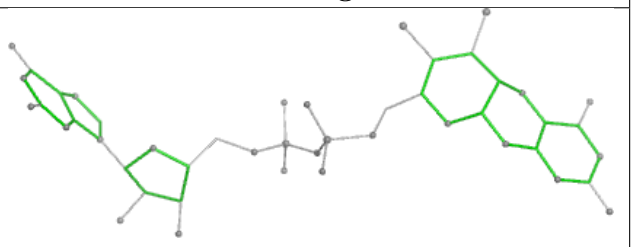
Bond lengths



Bond angles

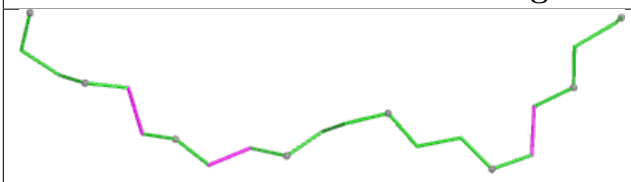


Torsions

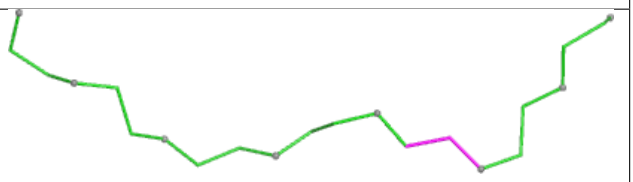


Rings

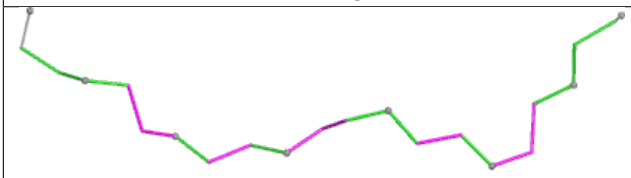
Ligand P33 A 912



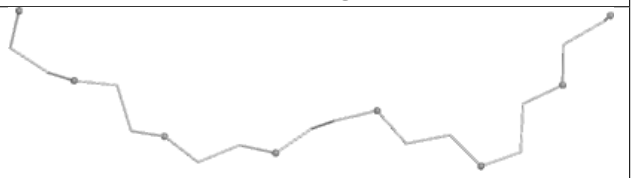
Bond lengths



Bond angles

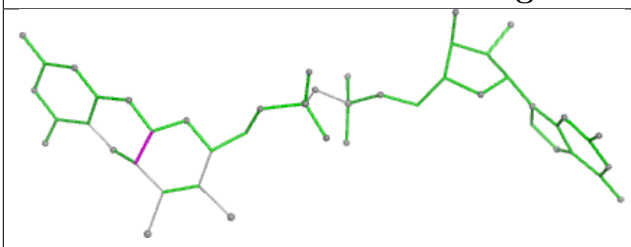


Torsions

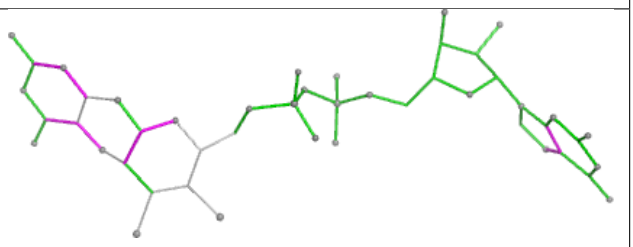


Rings

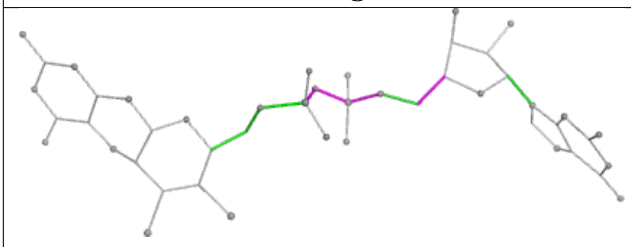
Ligand MGD A 903



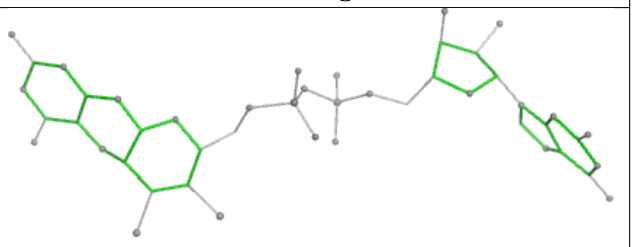
Bond lengths



Bond angles

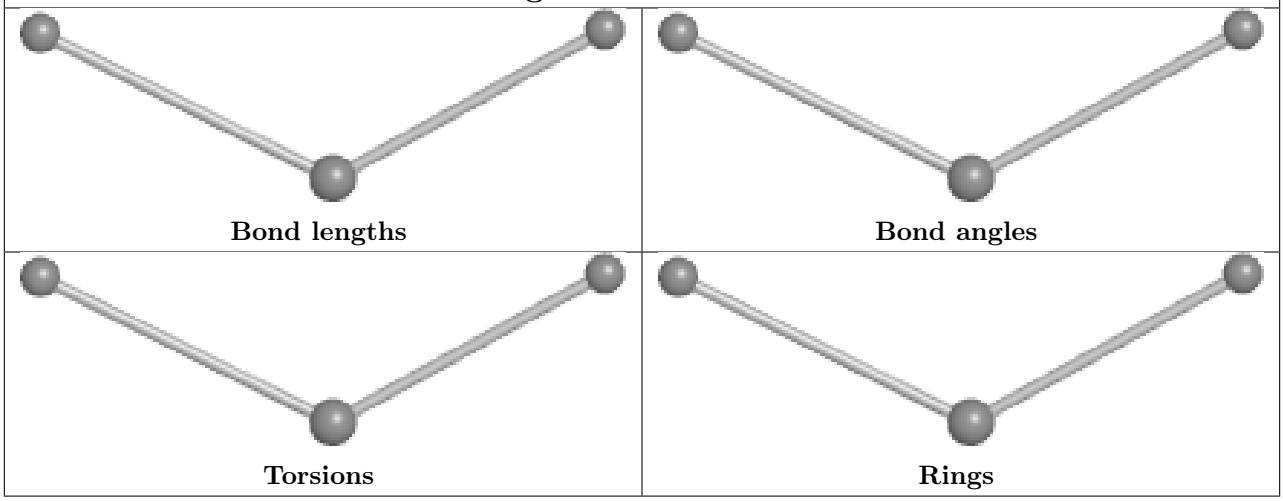


Torsions

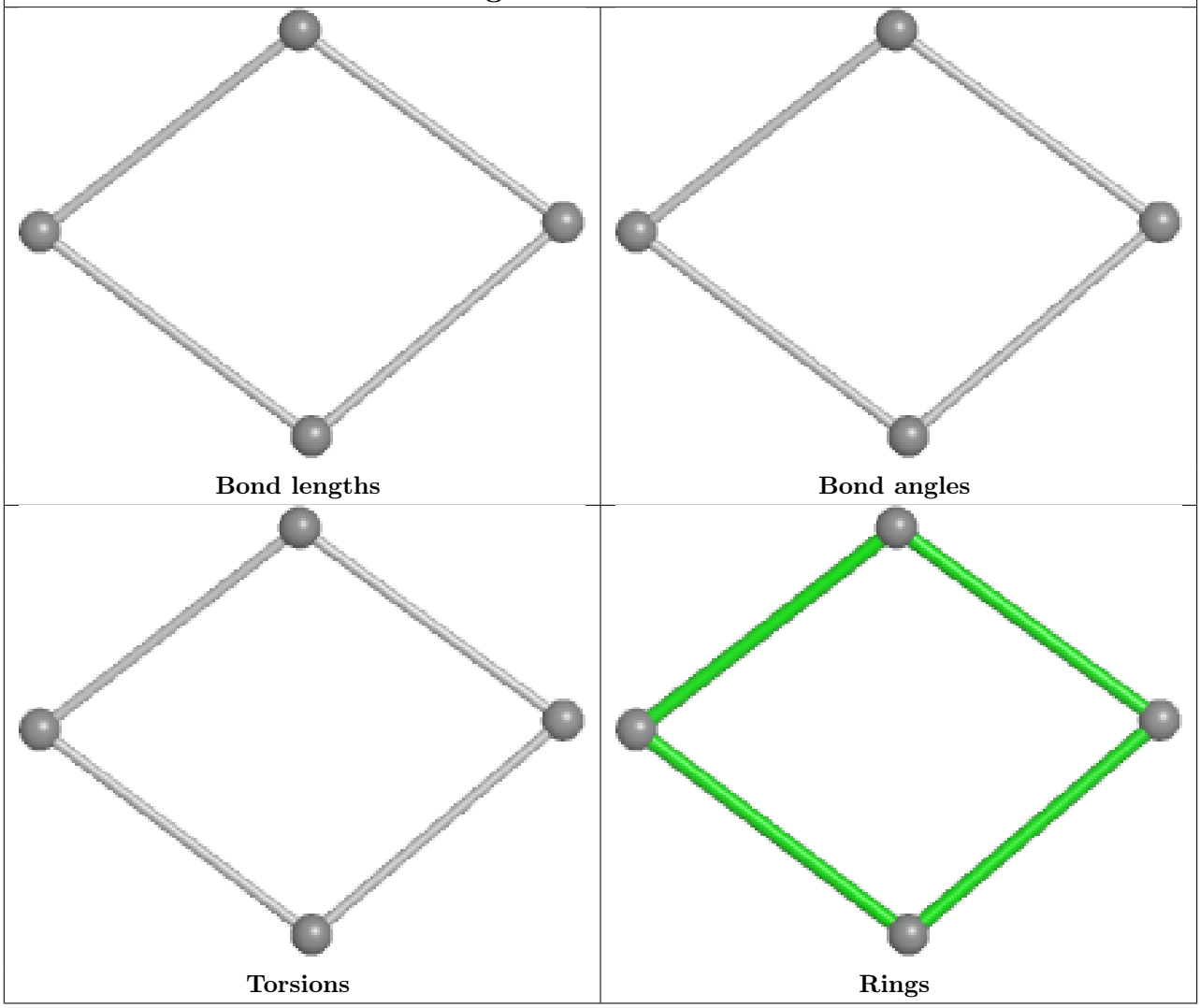


Rings

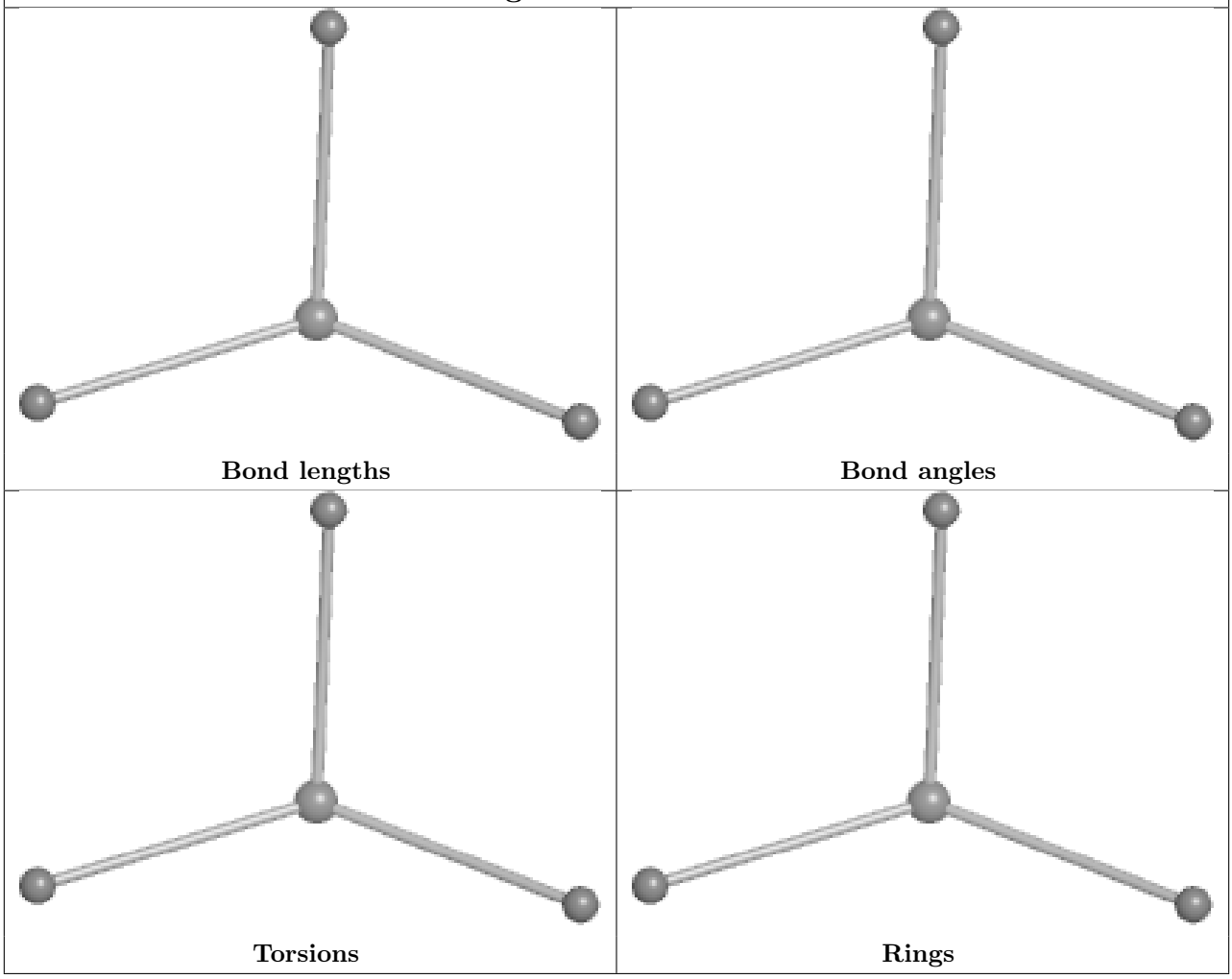
Ligand SBO A 911



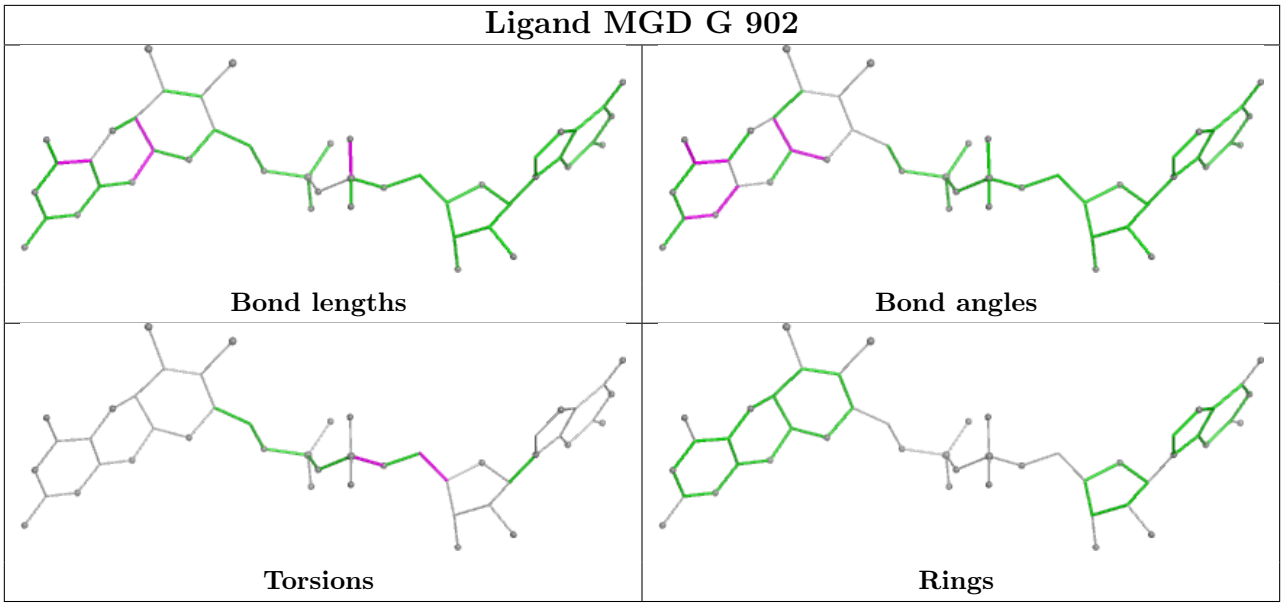
Ligand FES H 2202



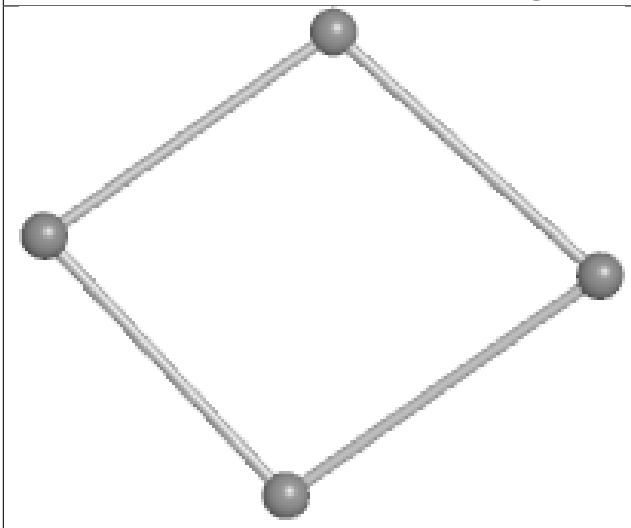
Ligand SBO C 918



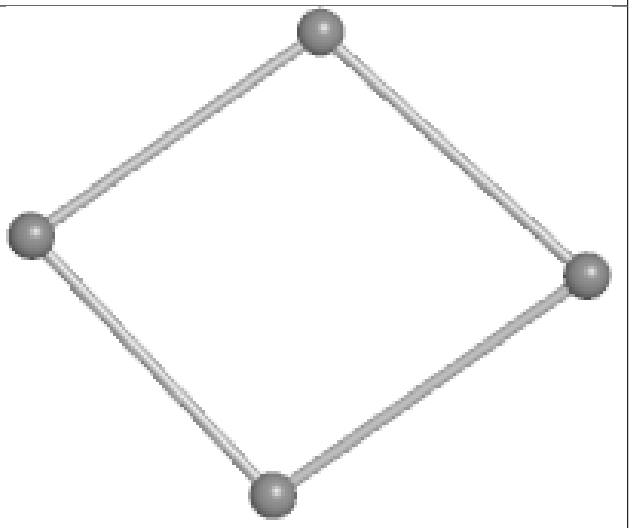
Ligand MGD G 902



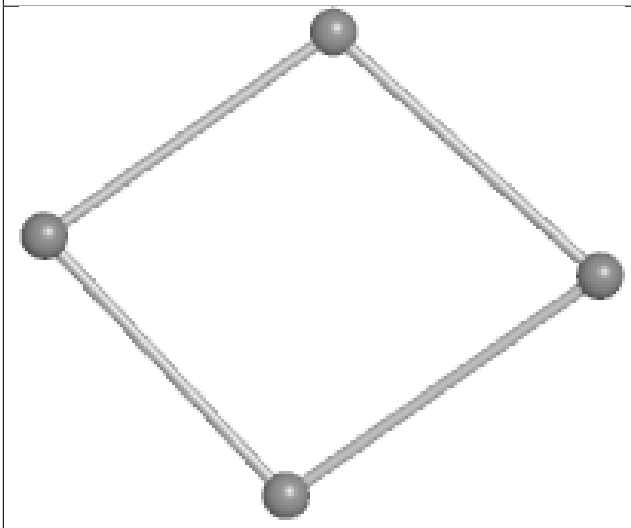
Ligand FES D 201



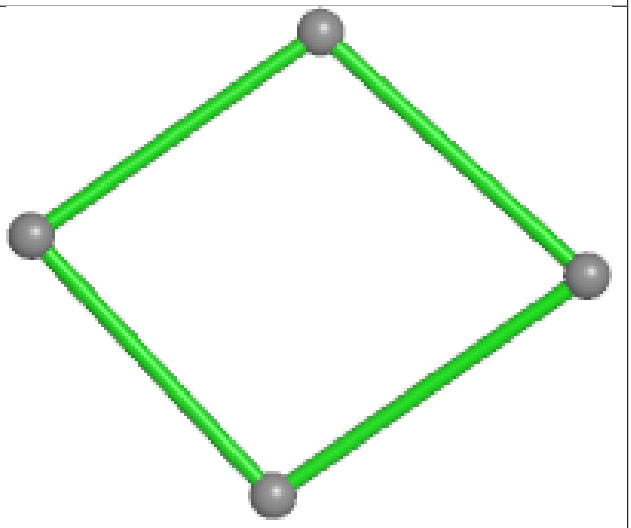
Bond lengths



Bond angles

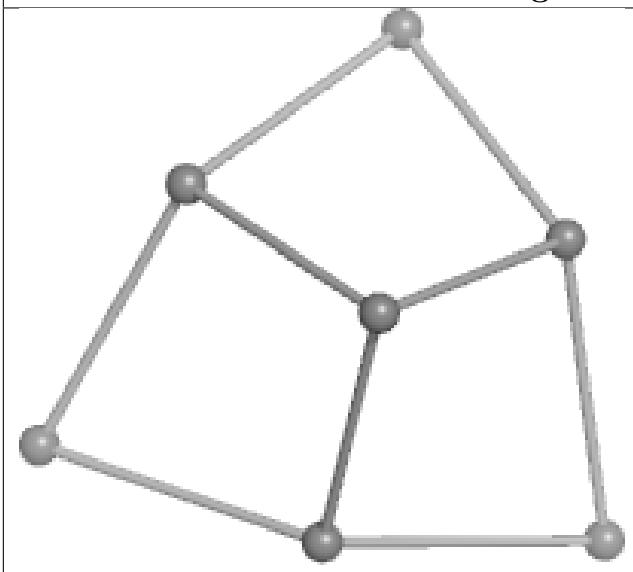


Torsions

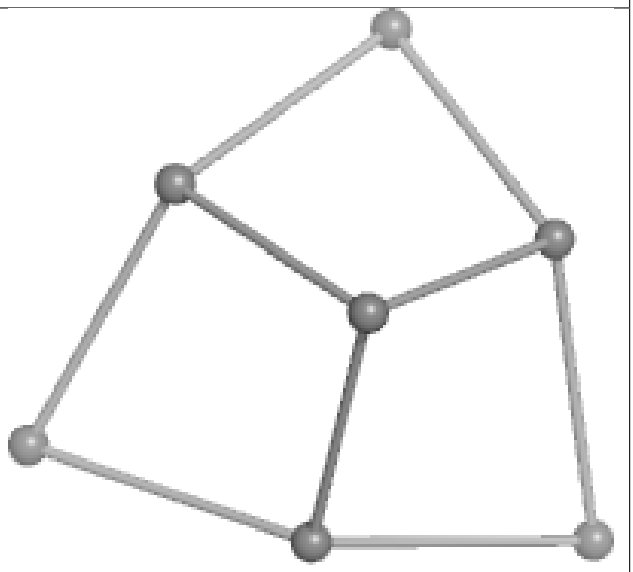


Rings

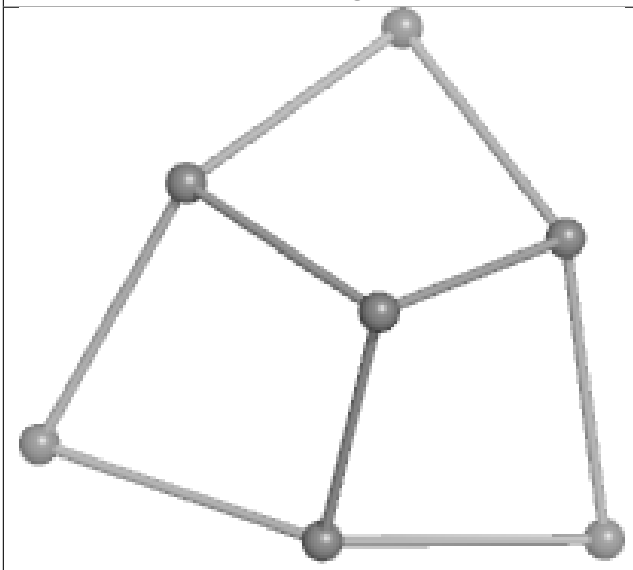
Ligand F3S C 901



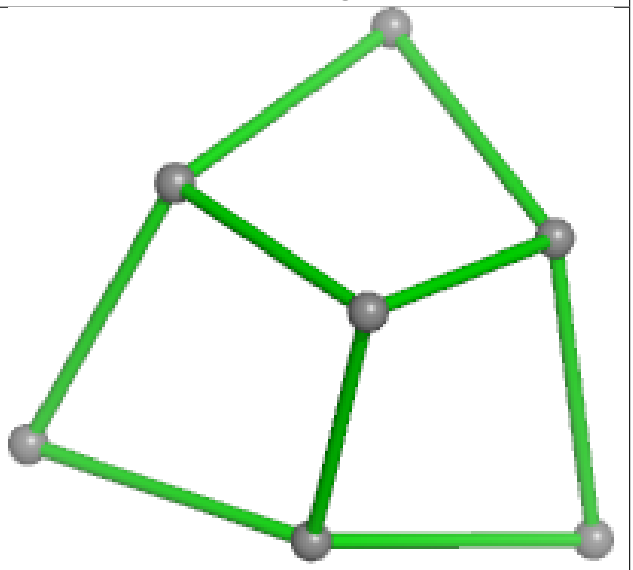
Bond lengths



Bond angles

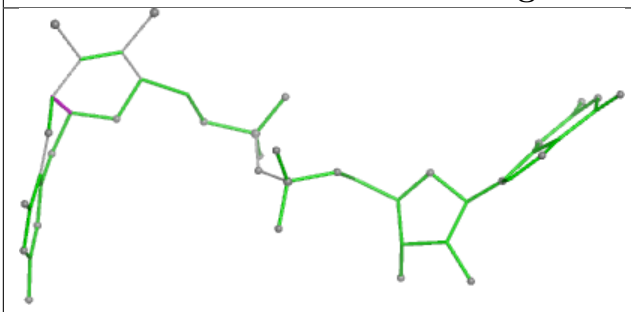


Torsions

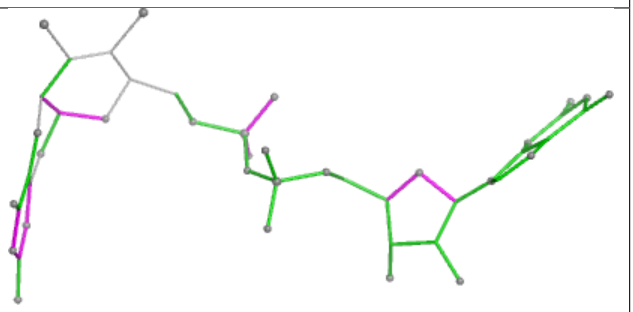


Rings

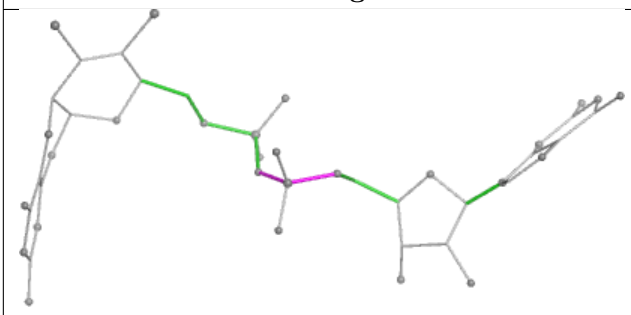
Ligand MGD E 901



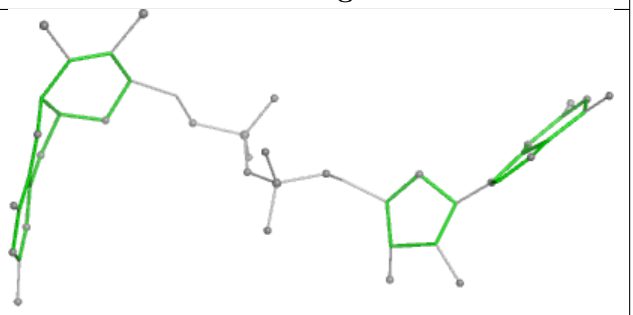
Bond lengths



Bond angles

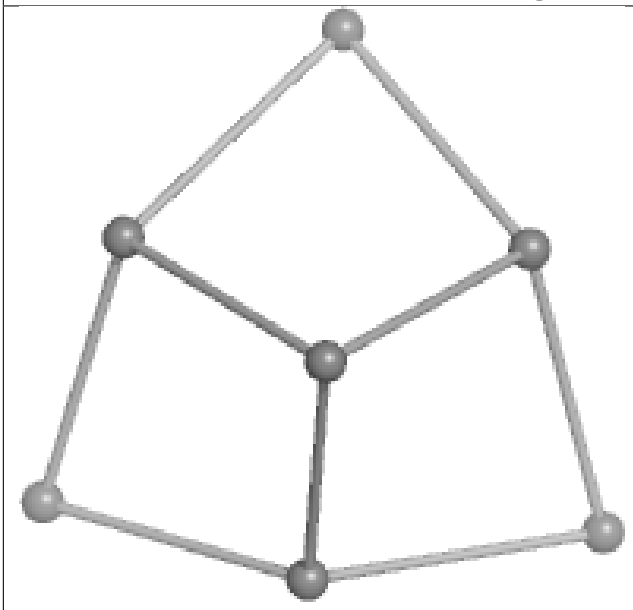


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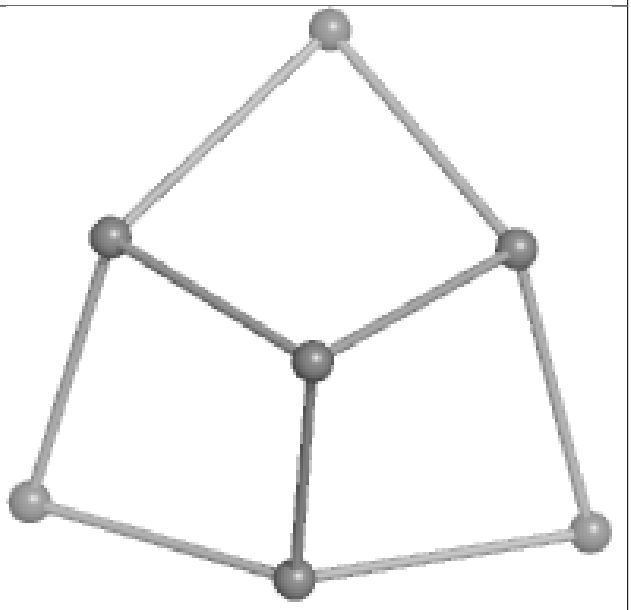


Rings

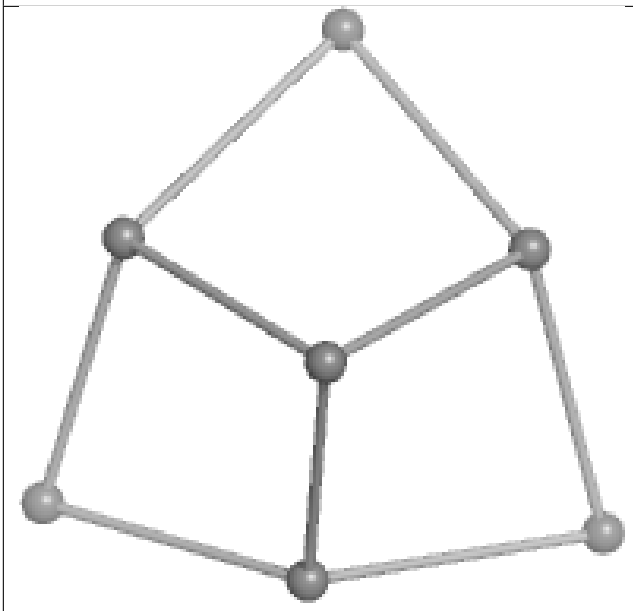
Ligand F3S A 904



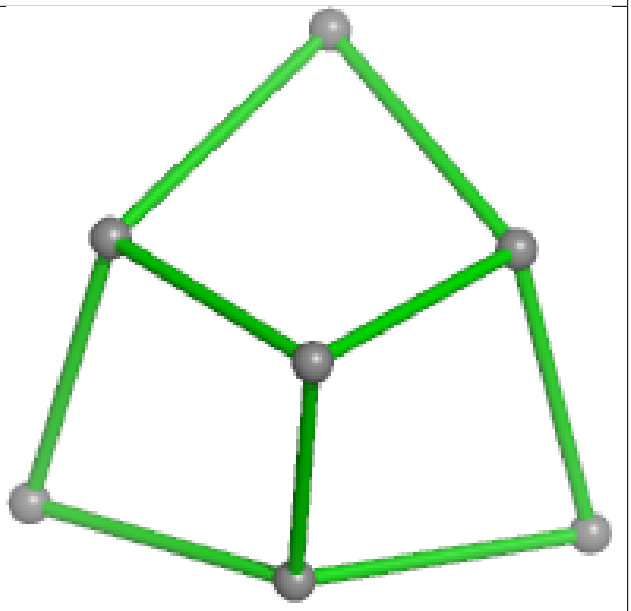
Bond lengths



Bond angles

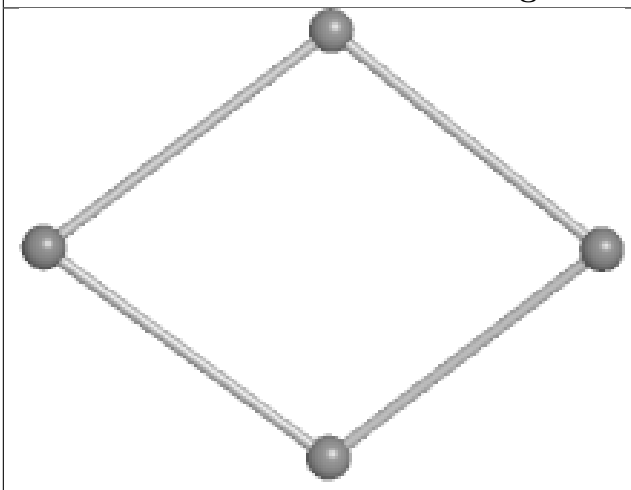


Torsions

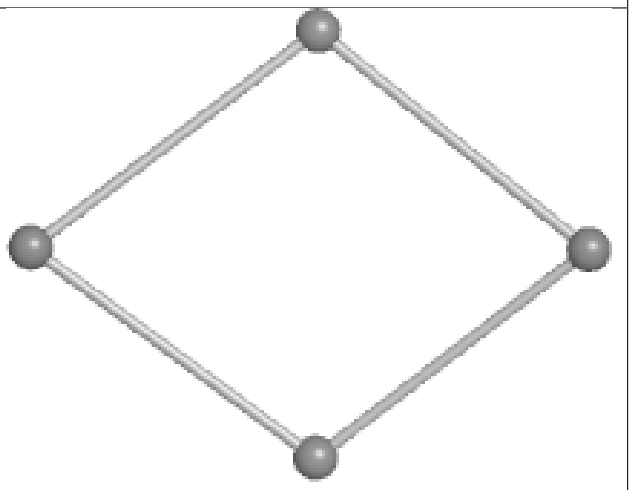


Rings

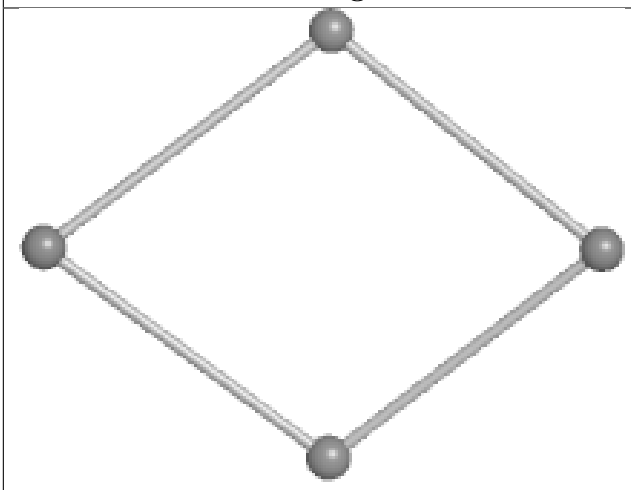
Ligand FES B 2902



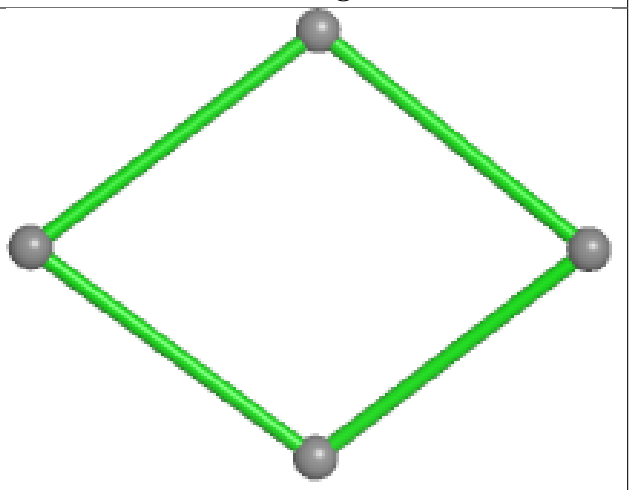
Bond lengths



Bond angles

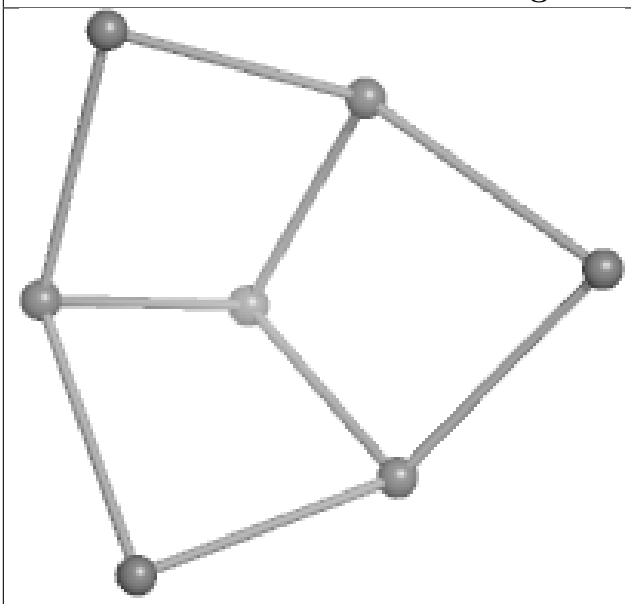


Torsions

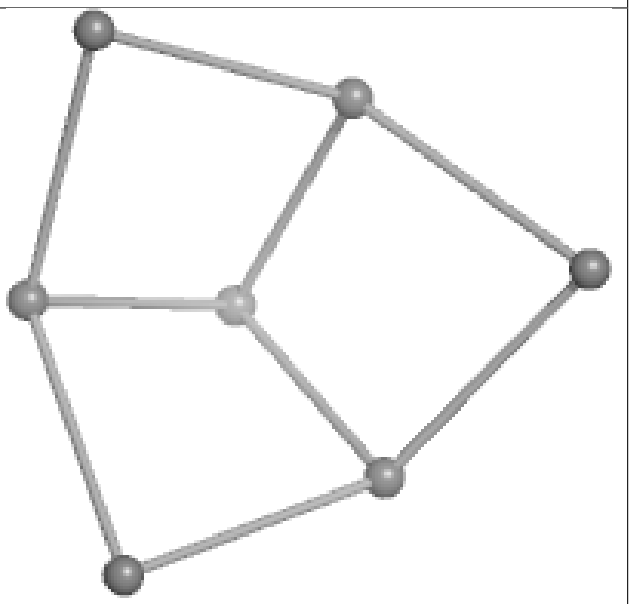


Rings

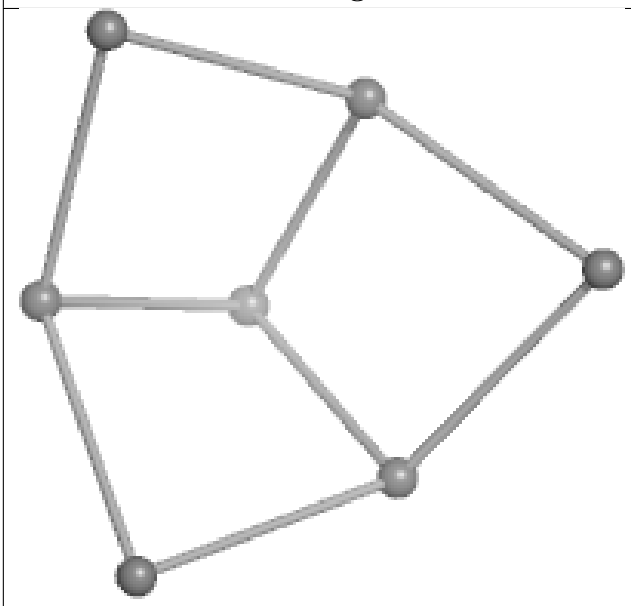
Ligand F3S G 903



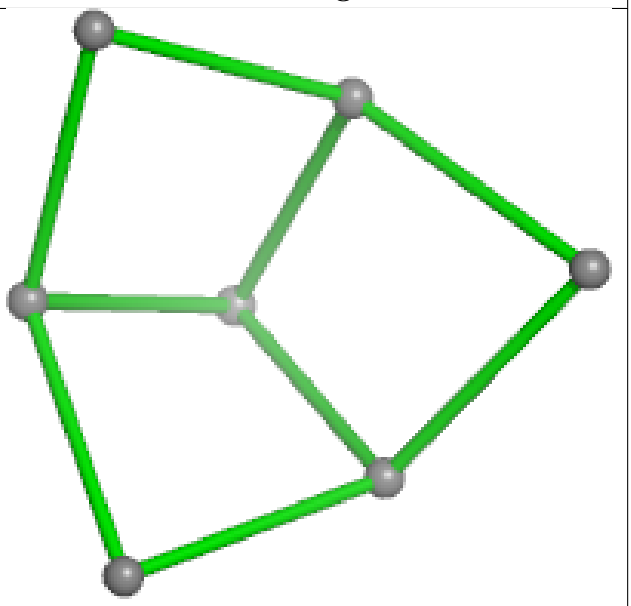
Bond lengths



Bond angles

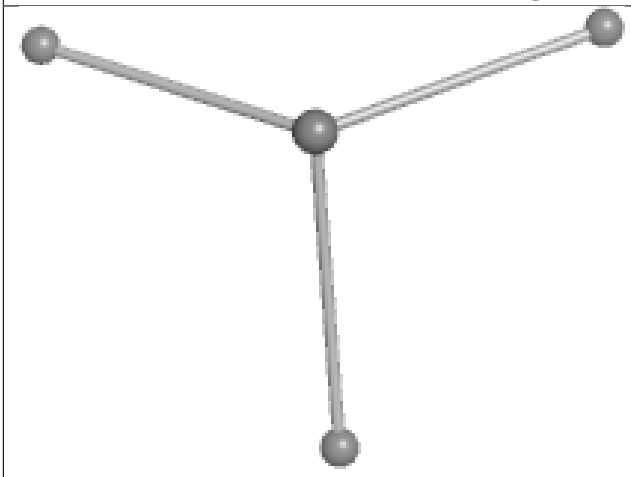


Torsions

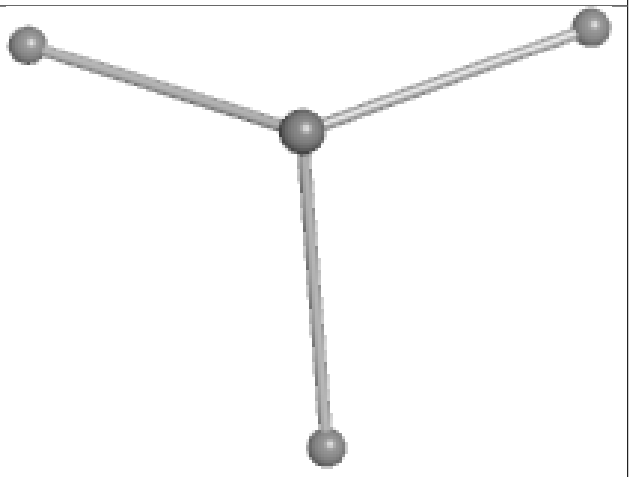


Rings

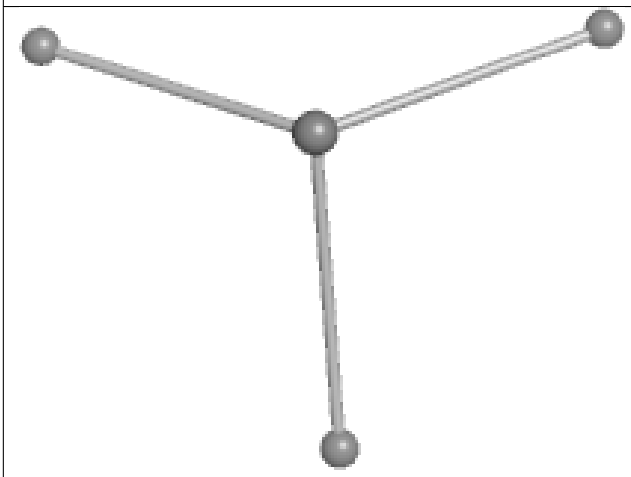
Ligand SBO E 917



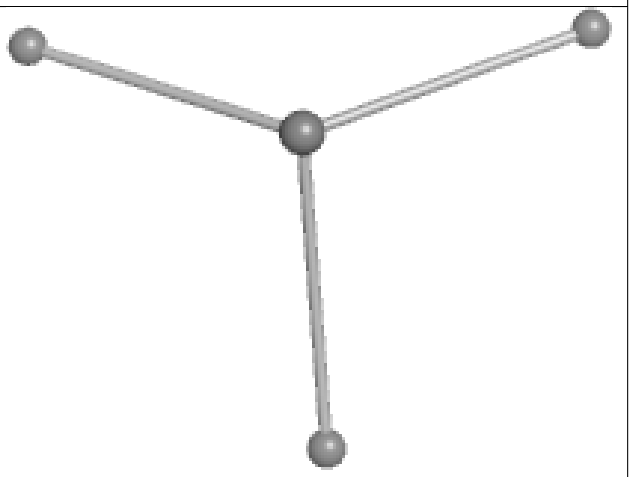
Bond lengths



Bond angles

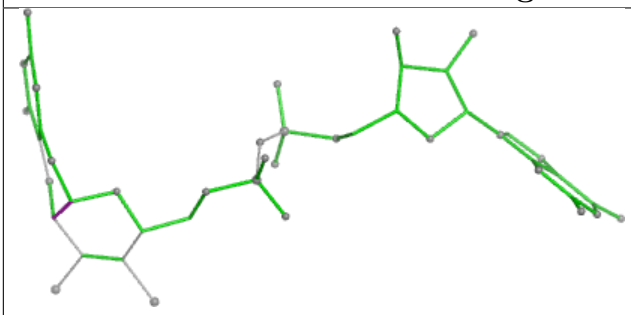


Torsions

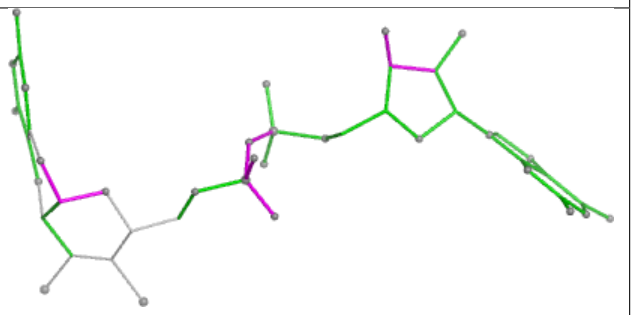


Rings

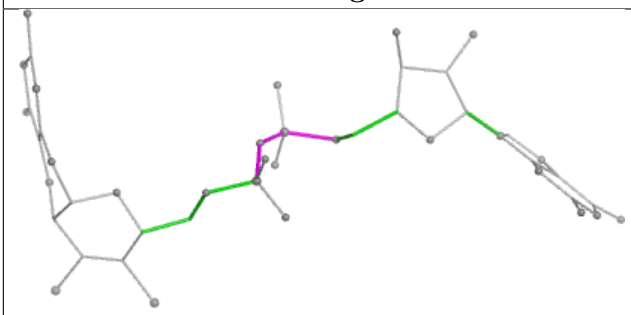
Ligand MGD C 902



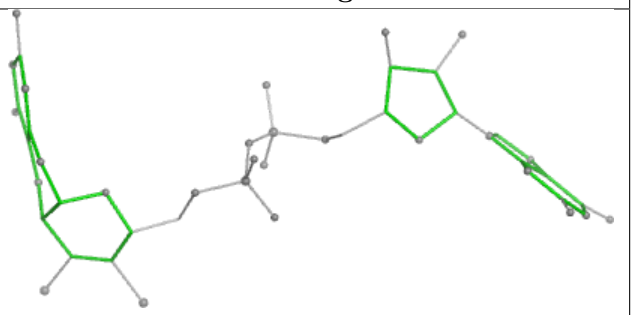
Bond lengths



Bond angles

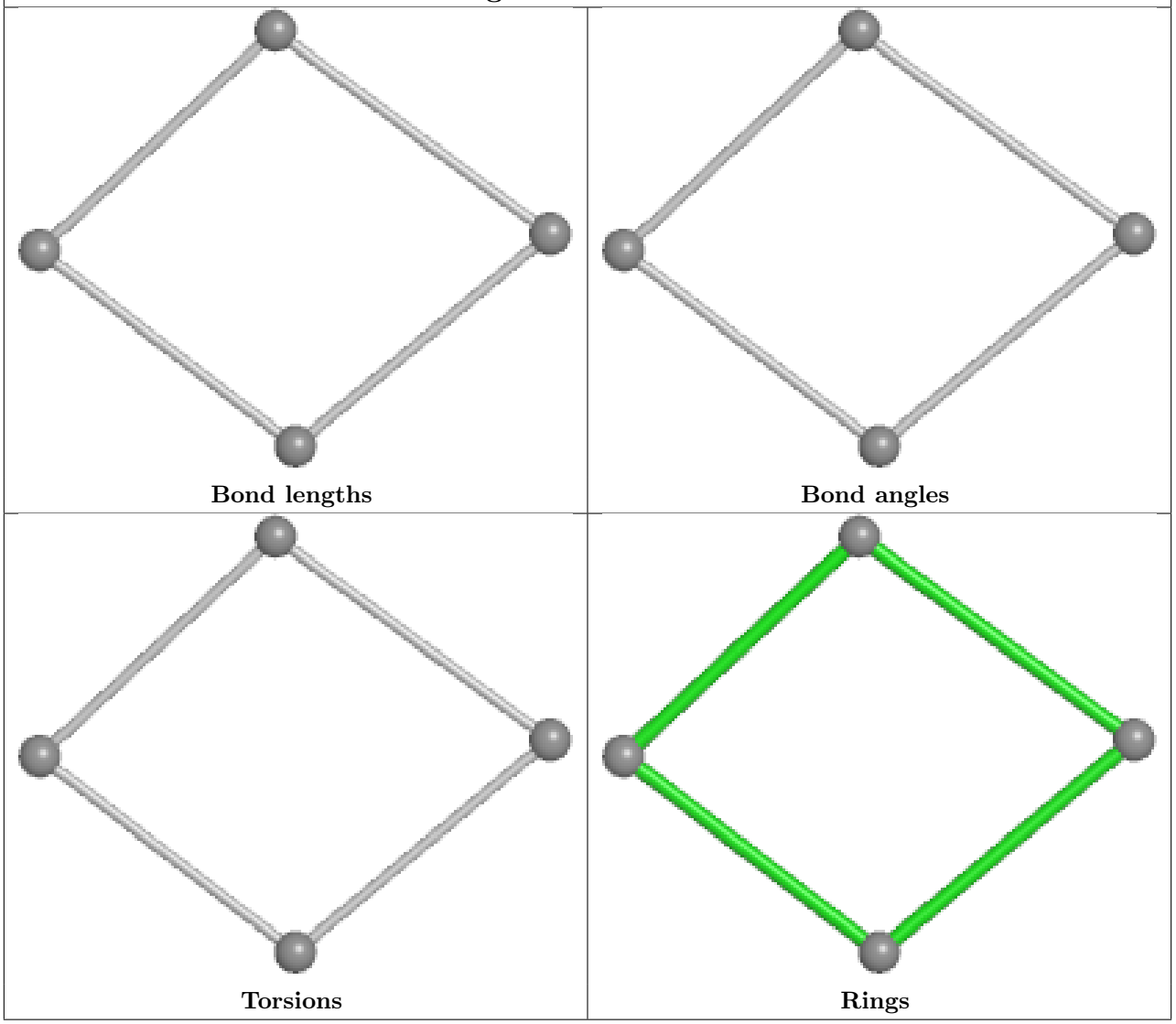


Torsions



Rings

Ligand FES F 201



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	824/824 (100%)	-0.09	14 (1%) 69 74	11, 19, 34, 70	3 (0%)
1	C	824/824 (100%)	-0.15	6 (0%) 84 88	10, 18, 33, 57	3 (0%)
1	E	824/824 (100%)	-0.05	13 (1%) 70 75	10, 19, 34, 62	2 (0%)
1	G	824/824 (100%)	-0.13	8 (0%) 79 83	10, 18, 33, 62	2 (0%)
2	B	135/135 (100%)	-0.01	2 (1%) 72 77	12, 19, 30, 52	0
2	D	135/135 (100%)	0.01	2 (1%) 72 77	12, 19, 31, 56	0
2	F	135/135 (100%)	0.07	2 (1%) 72 77	13, 19, 33, 68	0
2	H	135/135 (100%)	-0.01	1 (0%) 84 88	12, 19, 32, 55	0
All	All	3836/3836 (100%)	-0.09	48 (1%) 75 80	10, 18, 34, 70	10 (0%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	-1	ALA	6.0
1	G	2	ALA	5.7
1	E	2	ALA	5.6
1	C	2	ALA	5.6
1	A	2	ALA	5.5

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 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, 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
10	PGE	C	917	10/10	0.66	0.29	22,38,42,45	0
10	PGE	E	916	10/10	0.67	0.25	24,37,42,44	0
7	PEG	G	907	7/7	0.72	0.23	37,45,54,59	0
7	PEG	E	907	7/7	0.73	0.26	45,55,63,67	0
7	PEG	A	907	7/7	0.75	0.20	32,37,42,43	0
7	PEG	H	2201	7/7	0.75	0.18	33,38,42,44	0
6	EDO	C	915	4/4	0.76	0.15	26,34,34,38	0
6	EDO	E	915	4/4	0.76	0.19	34,34,40,41	0
17	1PE	C	912	16/16	0.76	0.19	31,38,44,46	0
7	PEG	A	915	7/7	0.77	0.21	32,39,41,51	0
9	P33	A	912	22/22	0.78	0.20	29,41,50,74	0
7	PEG	C	909	7/7	0.78	0.18	37,40,49,53	0
10	PGE	A	918	10/10	0.79	0.21	27,44,51,52	0
6	EDO	A	919	4/4	0.79	0.18	31,36,37,43	0
10	PGE	A	916	10/10	0.80	0.22	27,35,47,65	0
7	PEG	E	913	7/7	0.80	0.17	23,33,38,42	0
7	PEG	A	917	7/7	0.80	0.17	31,37,51,52	0
7	PEG	A	921	7/7	0.80	0.18	16,24,41,42	0
7	PEG	E	909	7/7	0.80	0.19	43,51,56,62	0
7	PEG	G	912	7/7	0.81	0.19	29,38,46,52	0
10	PGE	G	913	10/10	0.82	0.20	21,33,41,45	0
17	1PE	G	910	16/16	0.82	0.20	31,44,56,69	0
7	PEG	F	202	7/7	0.83	0.19	41,44,50,52	0
6	EDO	G	914	4/4	0.83	0.17	33,41,44,48	0
7	PEG	G	908	7/7	0.83	0.15	39,45,48,49	0
7	PEG	G	911	7/7	0.83	0.19	37,46,60,62	0
6	EDO	C	910	4/4	0.83	0.16	42,45,48,50	0
16	P4G	C	911	11/11	0.83	0.15	30,36,41,44	0
7	PEG	E	910	7/7	0.83	0.15	26,36,45,45	0
7	PEG	C	913	7/7	0.83	0.18	24,41,47,50	0
18	PG0	C	916	8/8	0.83	0.18	26,39,46,51	0
7	PEG	A	909	7/7	0.84	0.14	36,41,48,50	0
6	EDO	E	905	4/4	0.84	0.23	41,42,48,49	0
14	GOL	B	2903	6/6	0.84	0.14	31,41,41,51	0
14	GOL	E	908	6/6	0.84	0.13	36,41,44,46	0
7	PEG	A	910	7/7	0.85	0.17	24,31,45,47	0
7	PEG	E	912	7/7	0.85	0.17	35,44,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	B	2904	7/7	0.85	0.16	31,50,59,66	0
7	PEG	B	2901	7/7	0.86	0.15	20,36,39,42	0
6	EDO	A	905	4/4	0.86	0.14	30,36,37,40	0
6	EDO	G	905	4/4	0.86	0.13	27,29,31,33	0
6	EDO	C	905	4/4	0.86	0.14	27,35,41,44	0
7	PEG	C	914	7/7	0.86	0.17	25,32,40,62	0
6	EDO	C	908	4/4	0.86	0.16	19,33,34,38	0
7	PEG	A	908	7/7	0.86	0.13	23,27,41,44	0
7	PEG	E	911	7/7	0.87	0.17	40,52,56,58	0
7	PEG	A	913	7/7	0.87	0.14	29,40,46,47	0
6	EDO	E	914	4/4	0.87	0.15	38,40,41,43	0
7	PEG	B	2906	7/7	0.88	0.17	18,27,40,46	0
7	PEG	C	919	7/7	0.89	0.13	21,26,34,35	0
6	EDO	E	906	4/4	0.89	0.12	20,23,25,29	0
6	EDO	C	906	4/4	0.89	0.12	30,37,41,51	0
7	PEG	A	914	7/7	0.89	0.15	29,35,44,51	0
14	GOL	B	2905	6/6	0.89	0.13	21,33,46,46	0
6	EDO	C	907	4/4	0.91	0.12	19,24,26,27	0
6	EDO	A	906	4/4	0.93	0.11	19,21,24,24	0
8	SBO	C	918	4/4	0.94	0.11	26,29,36,41	1
8	SBO	E	917	4/4	0.94	0.10	21,28,33,33	2
6	EDO	G	906	4/4	0.94	0.09	21,22,27,29	0
8	SBO	G	909	3/4	0.95	0.07	20,20,25,32	1
8	SBO	A	911	3/4	0.96	0.08	27,27,33,37	1
11	O	C	920	1/1	0.97	0.08	17,17,17,17	0
4	MGD	G	901	47/47	0.98	0.05	10,13,17,20	0
11	O	G	915	1/1	0.98	0.07	19,19,19,19	0
4	MGD	G	902	47/47	0.98	0.04	8,14,16,17	0
4	MGD	A	902	47/47	0.98	0.05	10,13,17,18	0
4	MGD	A	903	47/47	0.98	0.05	11,14,17,18	0
4	MGD	C	902	47/47	0.98	0.04	10,13,15,17	0
4	MGD	C	904	47/47	0.98	0.05	9,14,17,18	0
4	MGD	E	901	47/47	0.98	0.05	11,15,17,18	0
4	MGD	E	902	47/47	0.98	0.05	12,15,17,19	0
13	FES	H	2202	4/4	0.99	0.03	16,18,18,19	0
12	NA	A	922	1/1	0.99	0.05	9,9,9,9	0
12	NA	C	921	1/1	0.99	0.05	12,12,12,12	0
12	NA	E	919	1/1	0.99	0.05	12,12,12,12	0
12	NA	G	916	1/1	0.99	0.07	11,11,11,11	0
13	FES	B	2902	4/4	0.99	0.03	16,16,17,18	0
13	FES	D	201	4/4	0.99	0.03	14,15,16,16	0
13	FES	F	201	4/4	0.99	0.02	11,13,15,15	0

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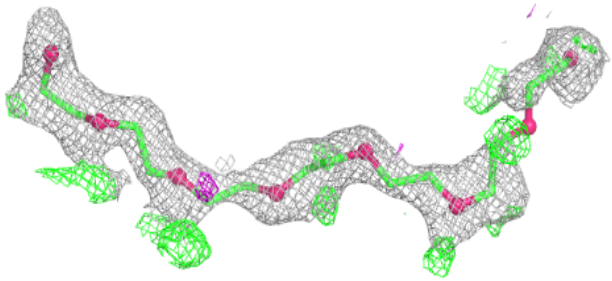
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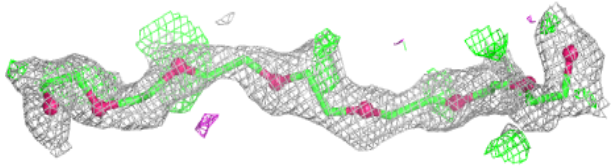
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	F3S	C	901	7/7	1.00	0.02	13,14,15,15	0
5	F3S	E	904	7/7	1.00	0.02	13,13,14,14	0
11	O	A	920	1/1	1.00	0.04	19,19,19,19	0
15	4MO	C	903	1/1	1.00	0.02	15,15,15,15	0
15	4MO	E	903	1/1	1.00	0.01	16,16,16,16	0
15	4MO	G	904	1/1	1.00	0.02	16,16,16,16	0
5	F3S	G	903	7/7	1.00	0.02	11,13,13,14	0
11	O	E	918	1/1	1.00	0.03	16,16,16,16	0
3	MO	A	901	1/1	1.00	0.02	15,15,15,15	0
5	F3S	A	904	7/7	1.00	0.02	12,14,15,15	0

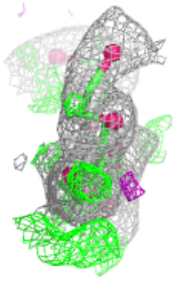
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P33 A 912:

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

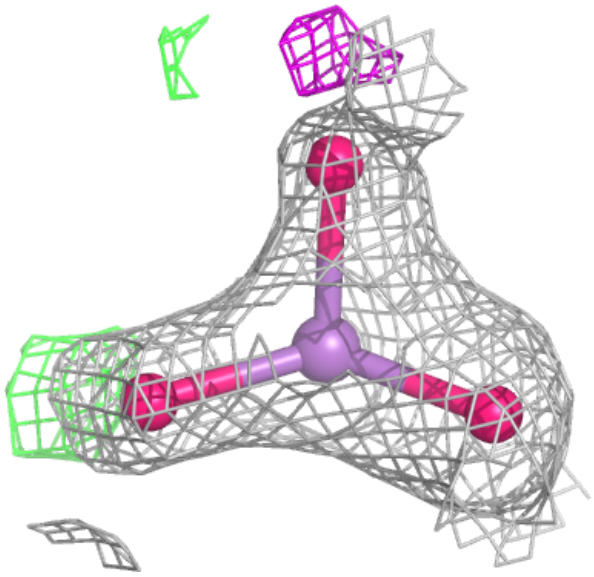


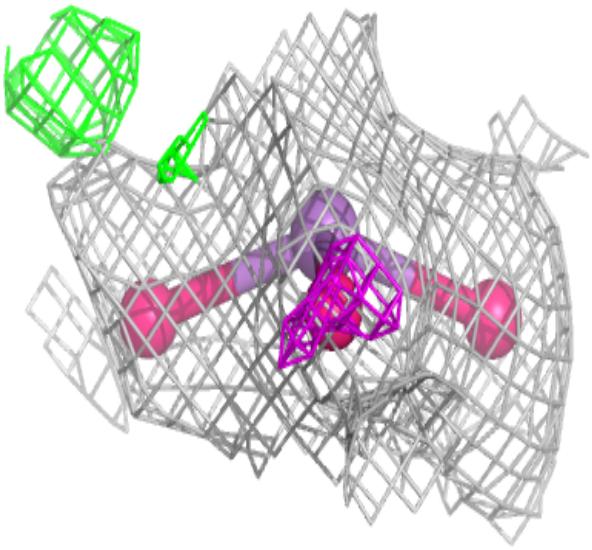


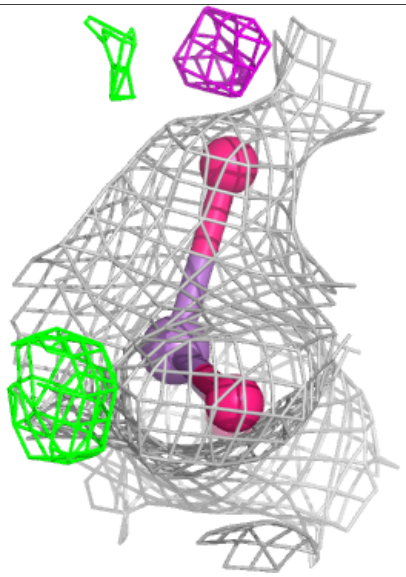


Electron density around SBO C 918:

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

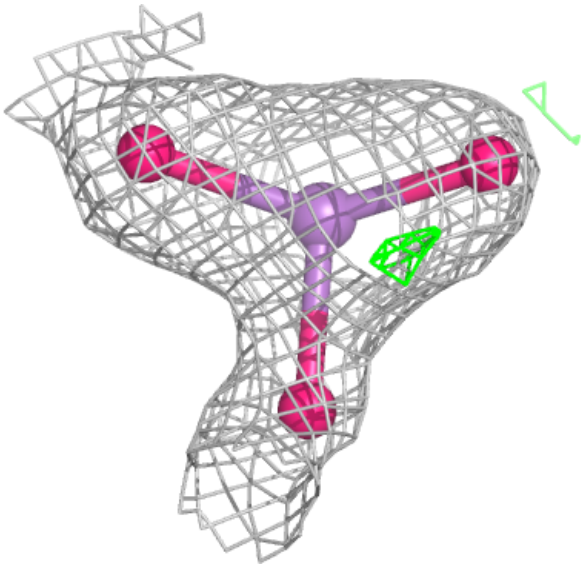


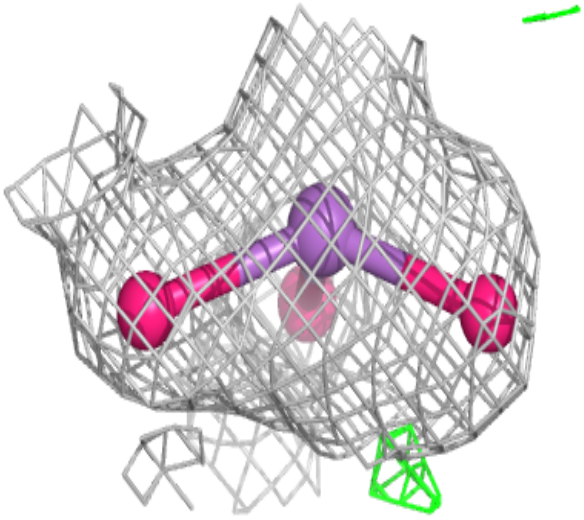


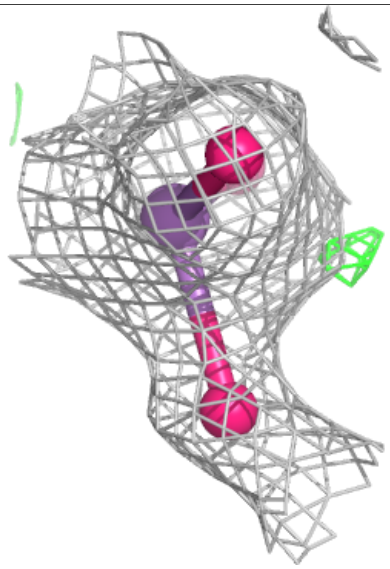


Electron density around SBO E 917:

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

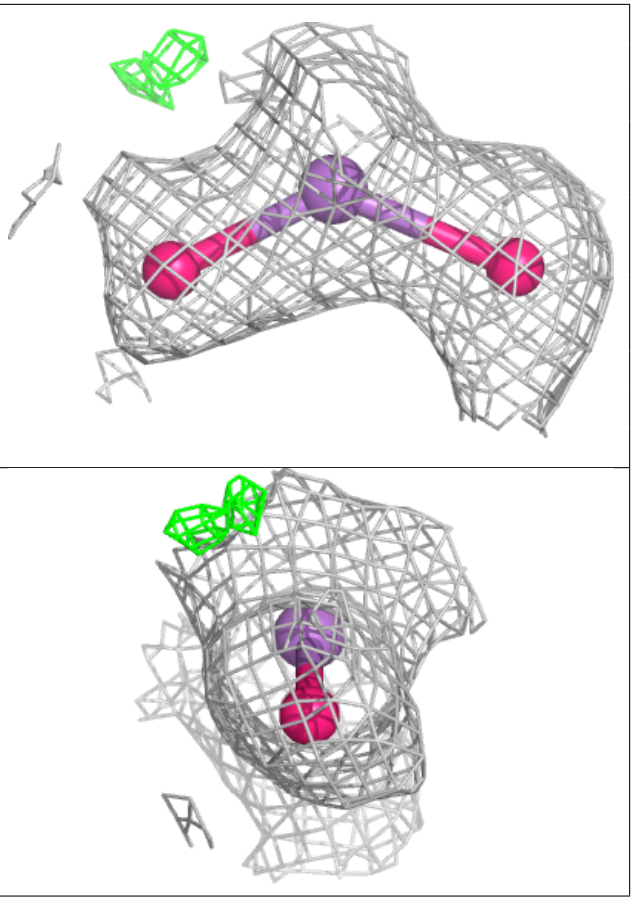






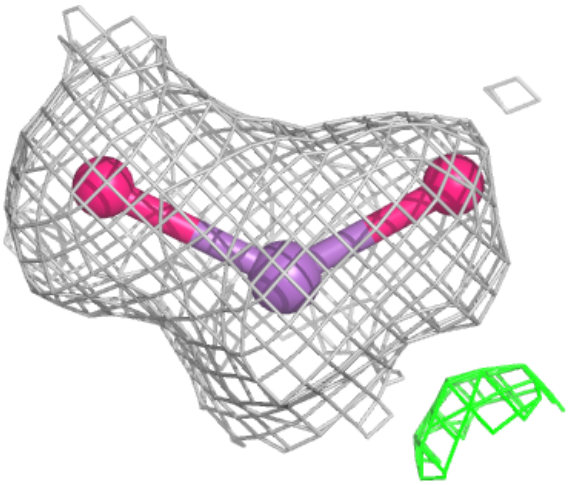
Electron density around SBO G 909:

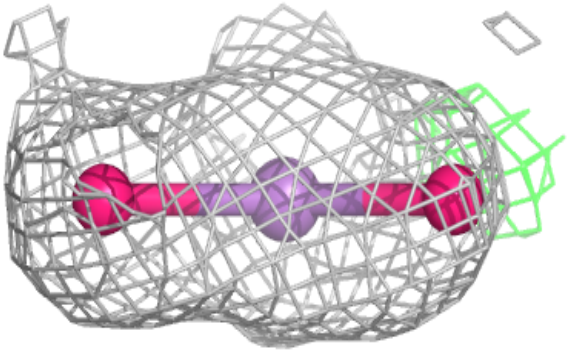
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

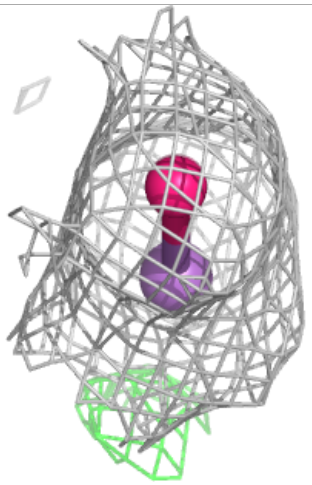


Electron density around SBO A 911:

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

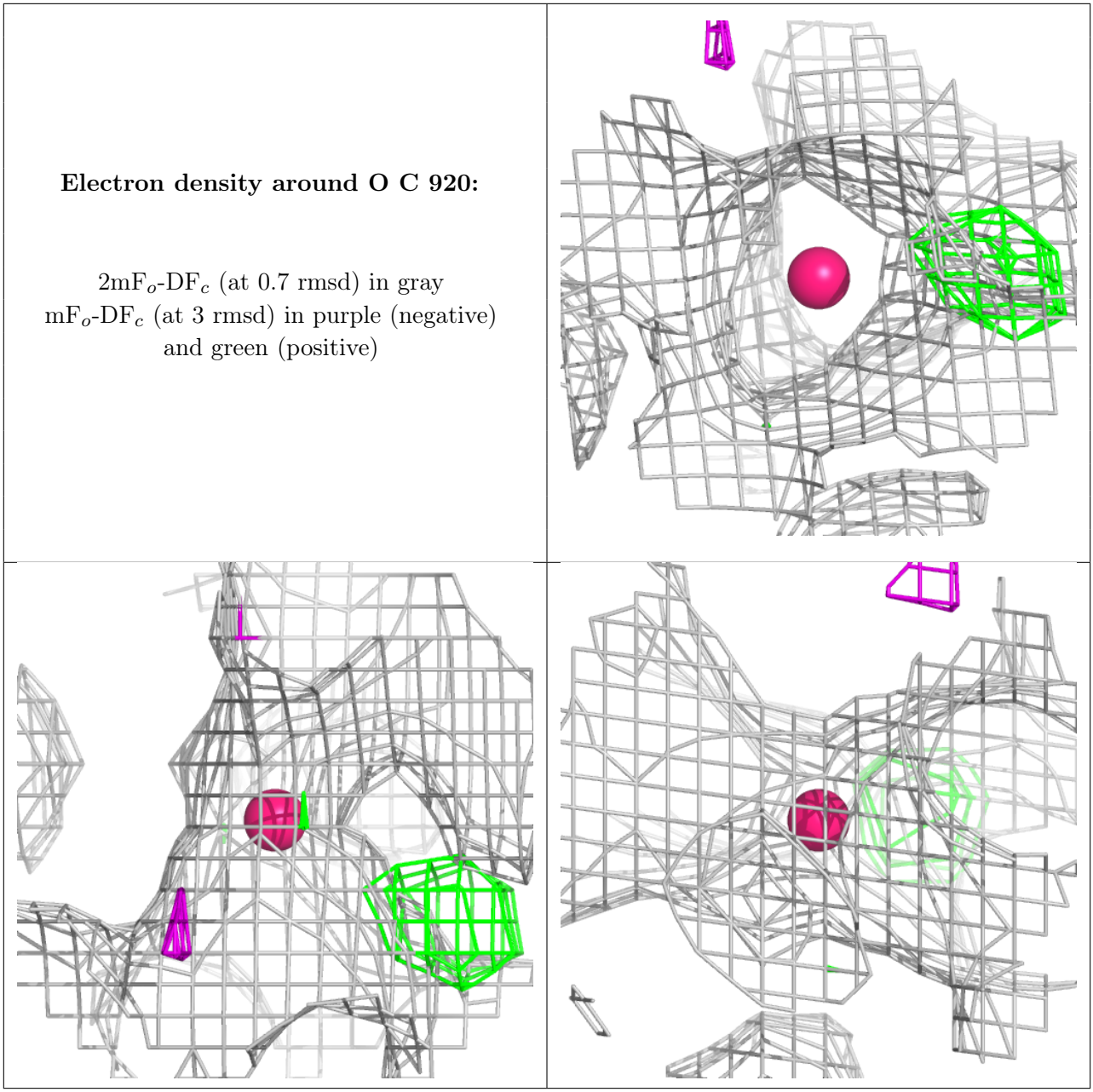






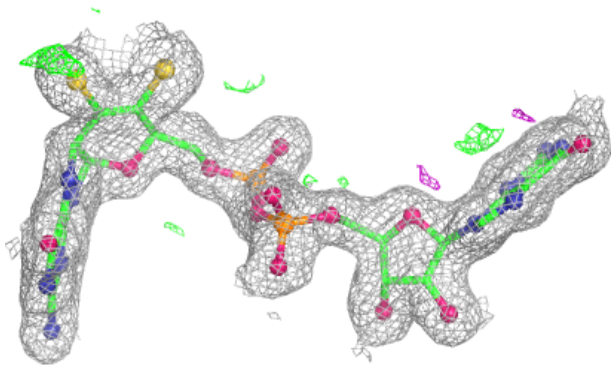
Electron density around O C 920:

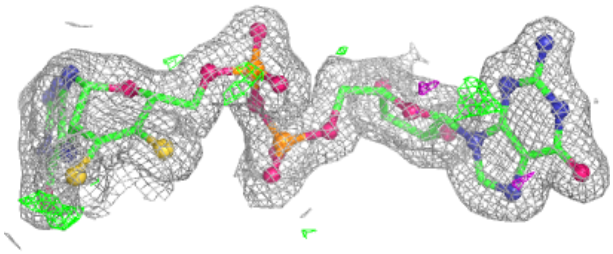
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

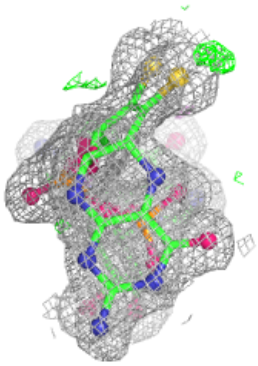


Electron density around MGD G 901:

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

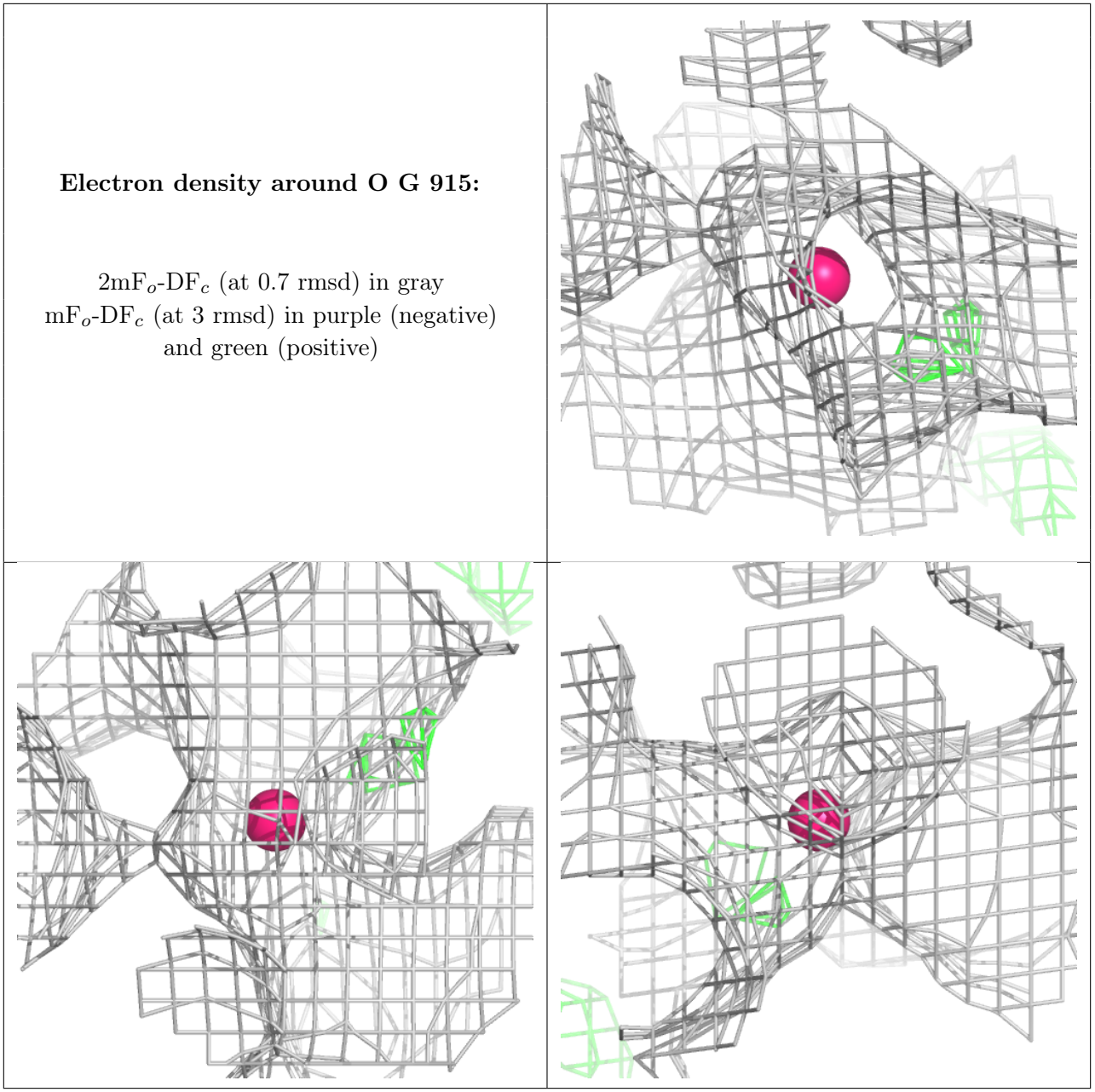






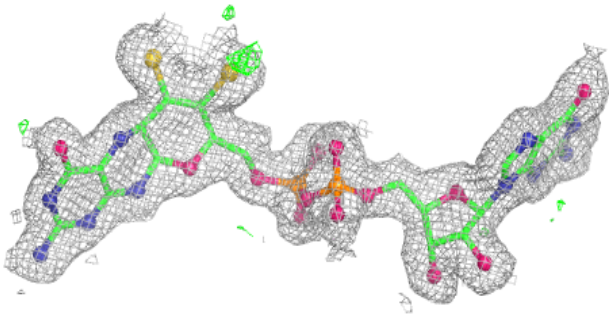
Electron density around O G 915:

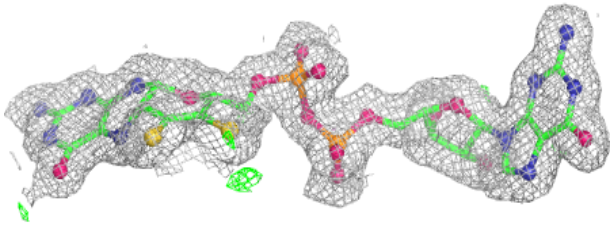
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

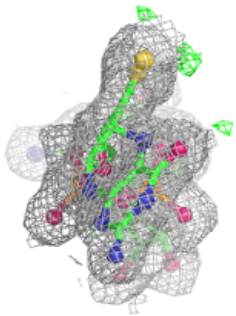


Electron density around MGD G 902:

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

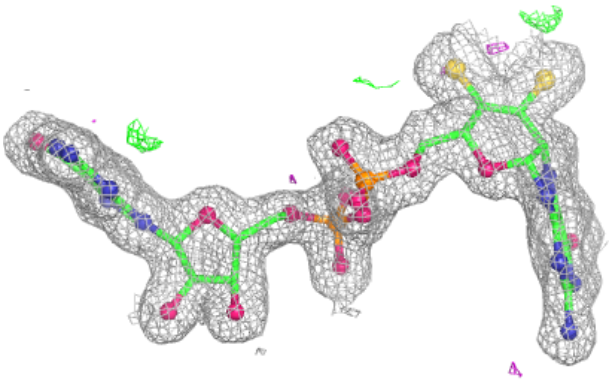


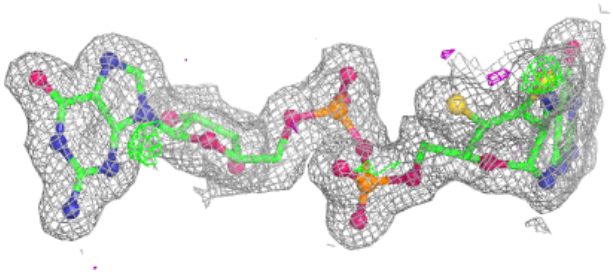


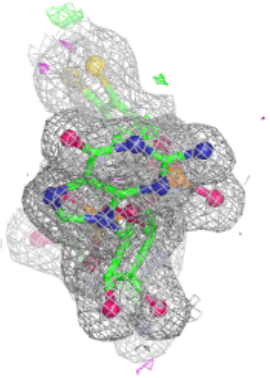


Electron density around MGD A 902:

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

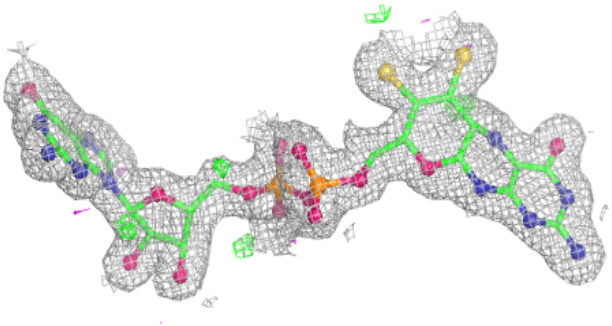


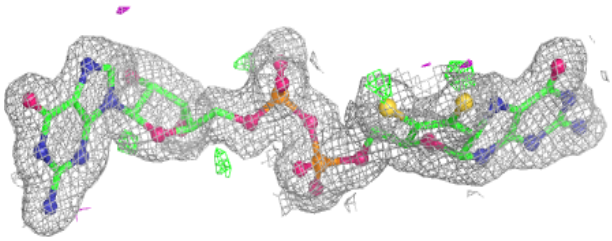


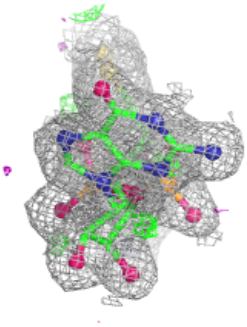


Electron density around MGD A 903:

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

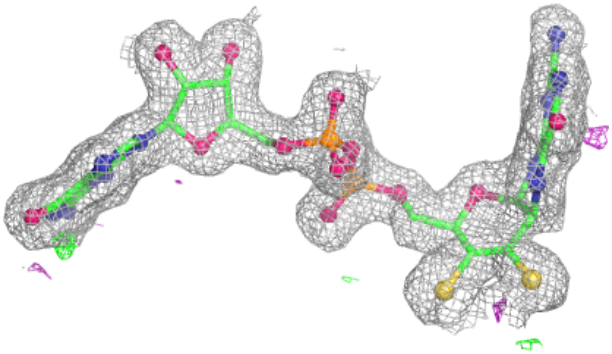


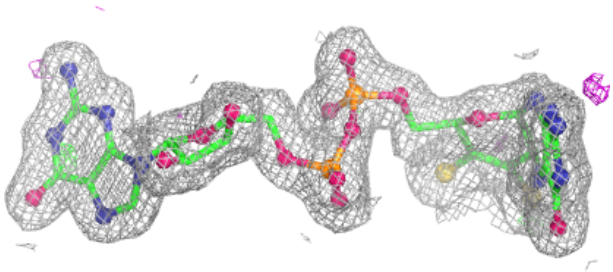


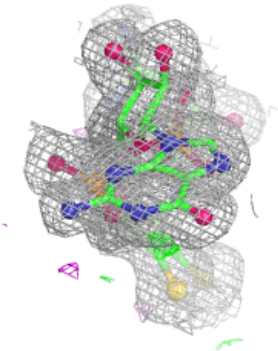


Electron density around MGD C 902:

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

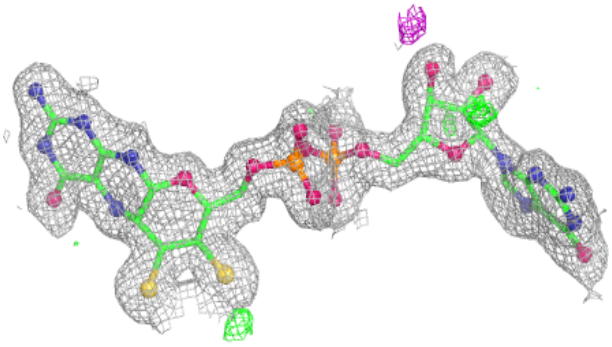


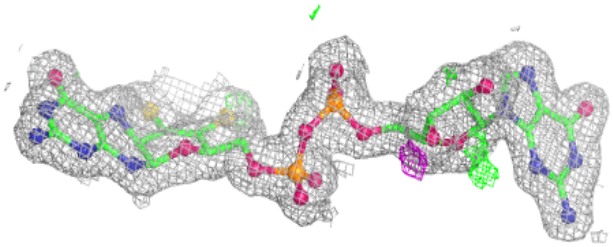


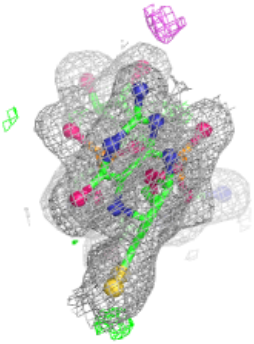


Electron density around MGD C 904:

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

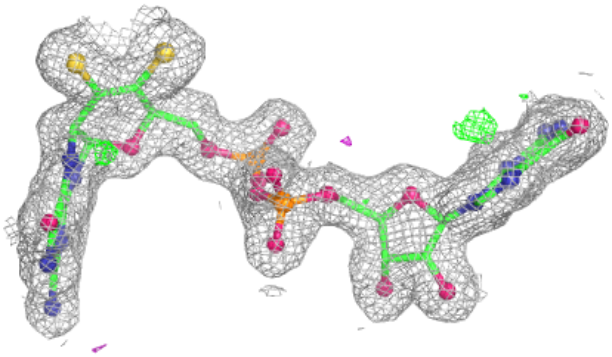


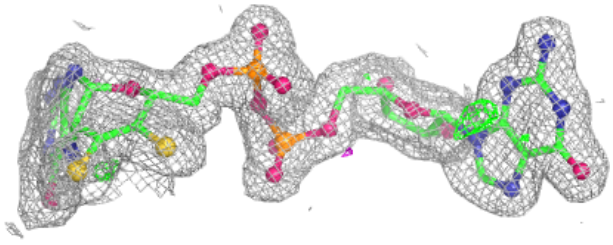


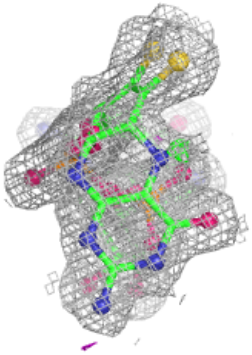


Electron density around MGD E 901:

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

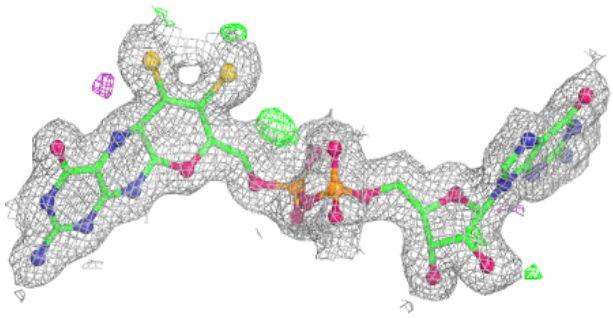


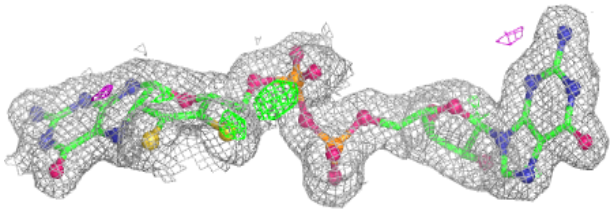


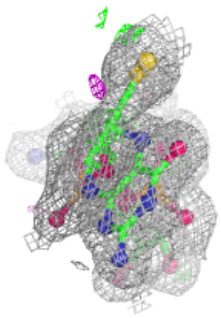


Electron density around MGD E 902:

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

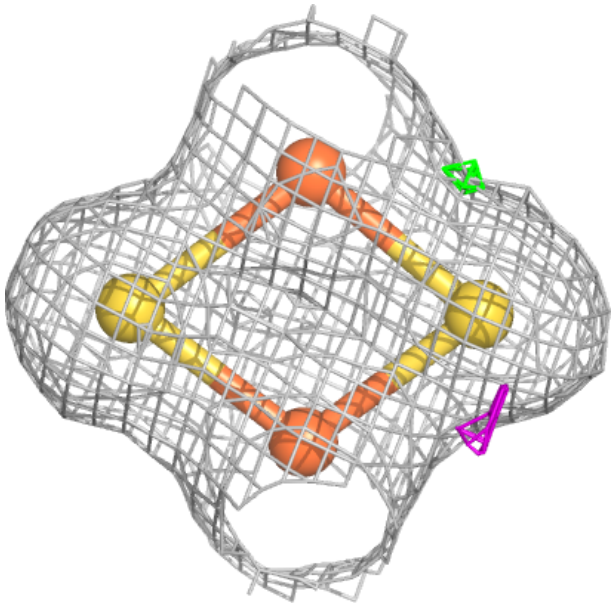


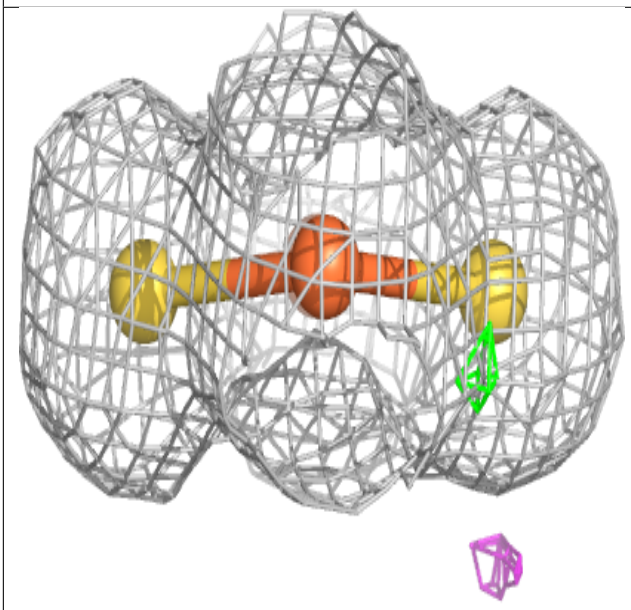


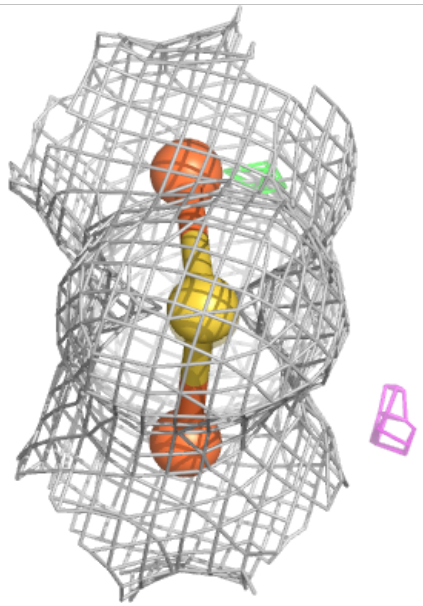


Electron density around FES H 2202:

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

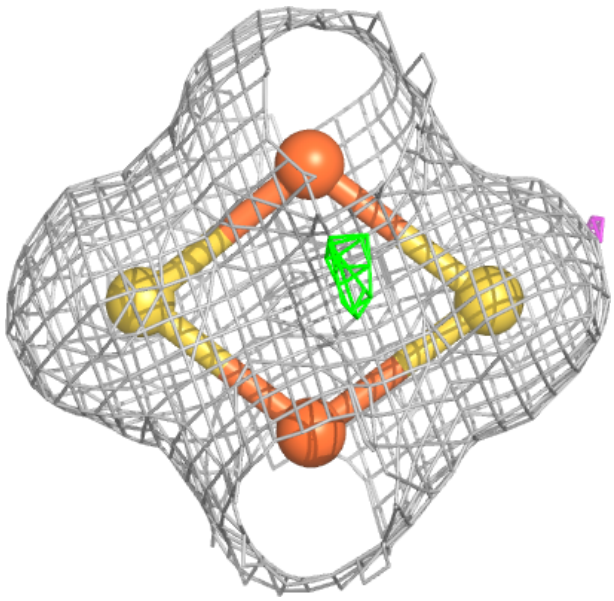


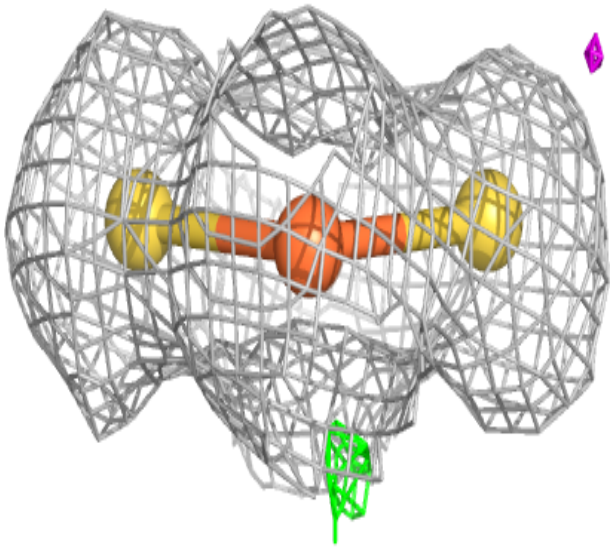


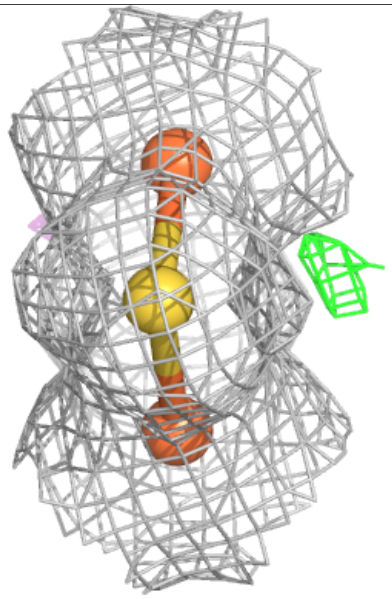


Electron density around FES B 2902:

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

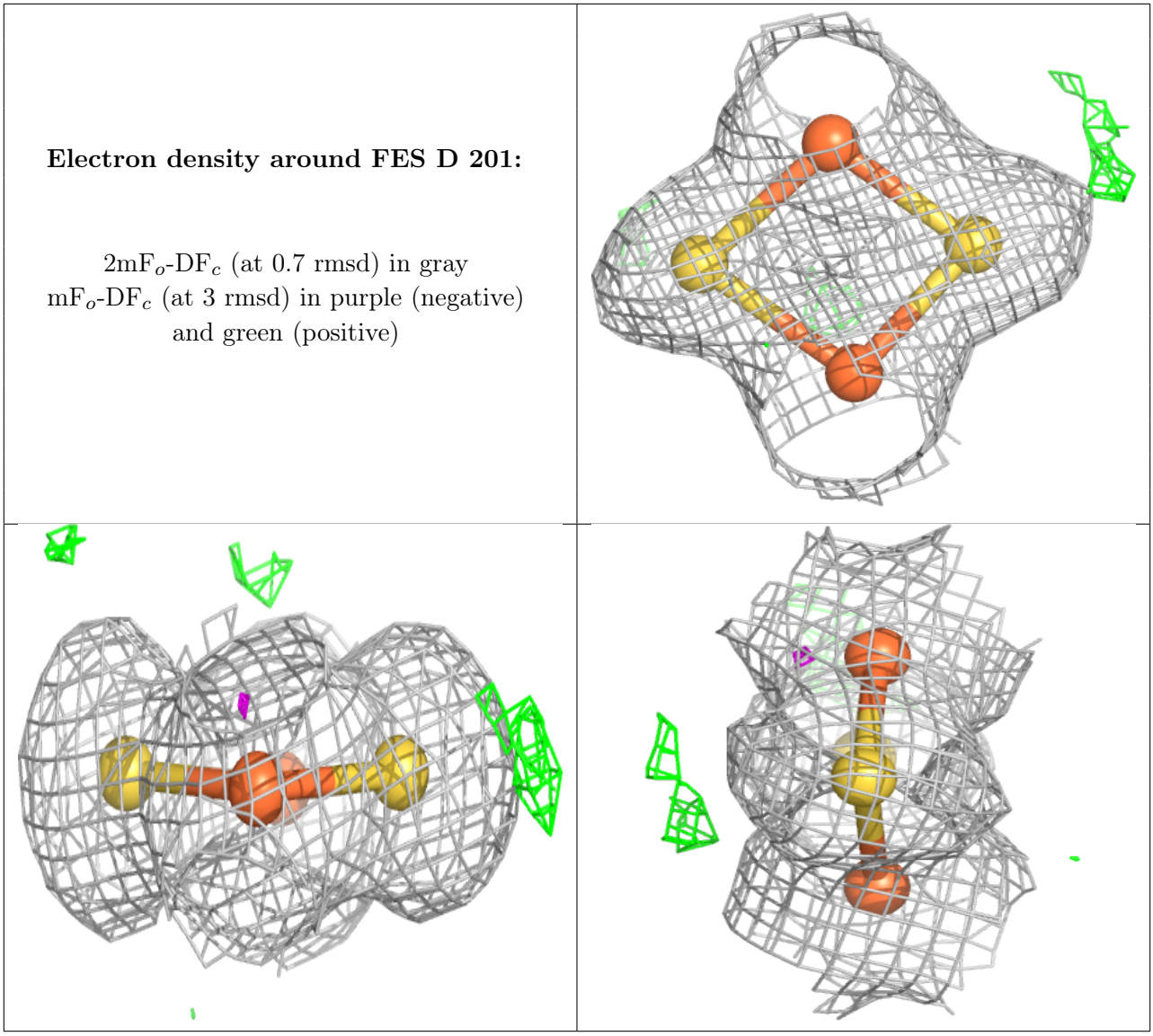






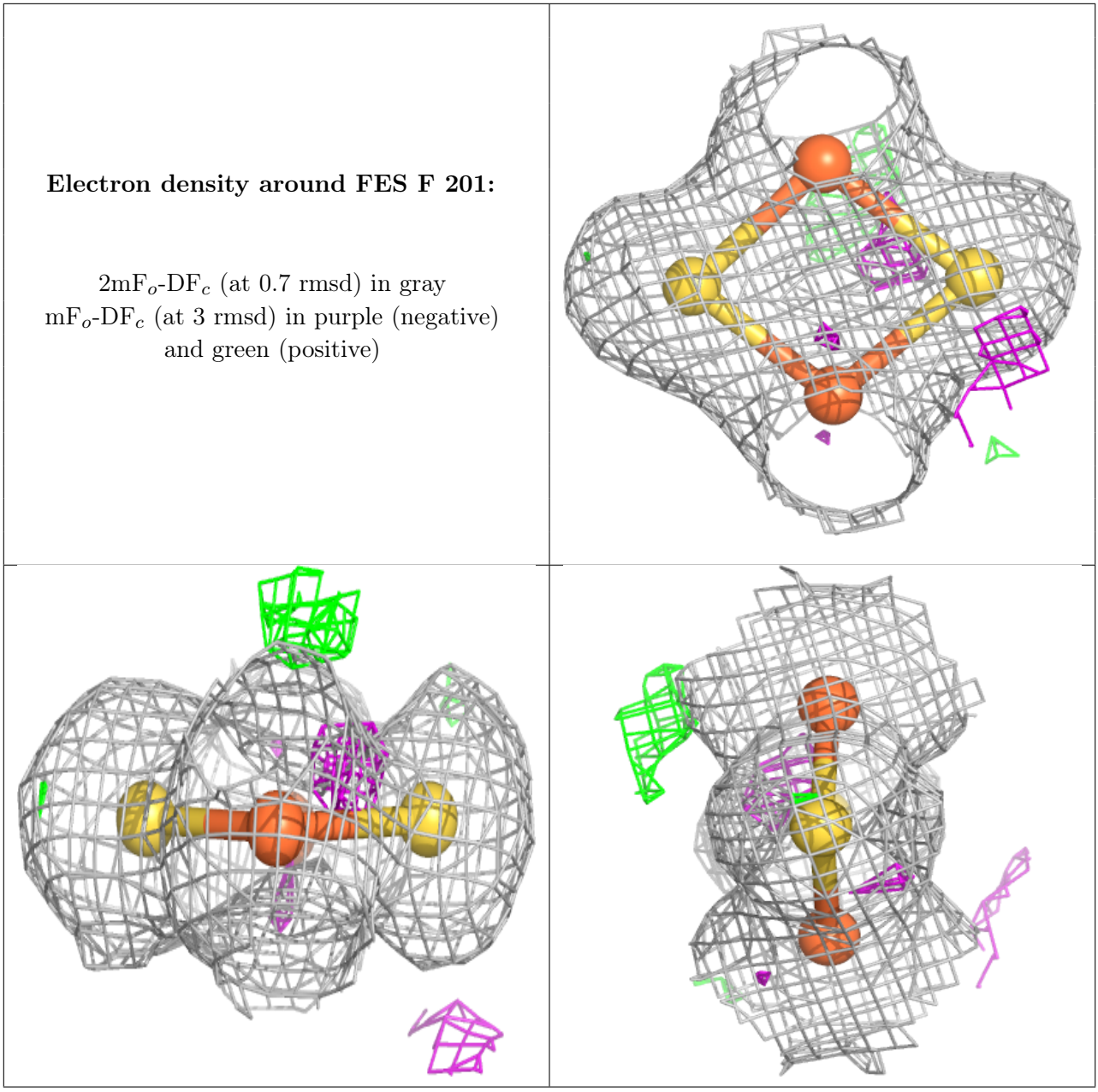
Electron density around FES D 201:

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



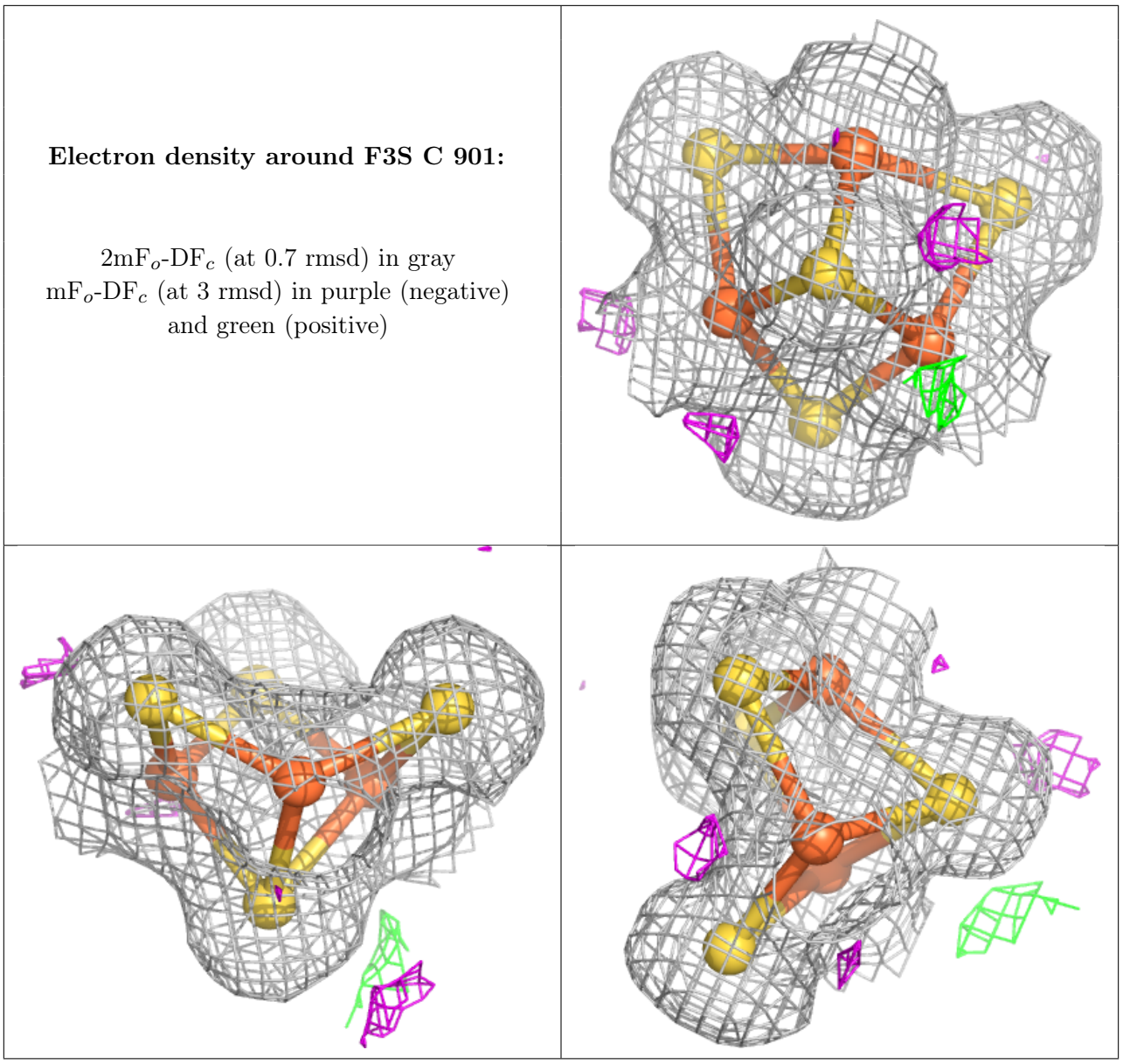
Electron density around FES F 201:

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



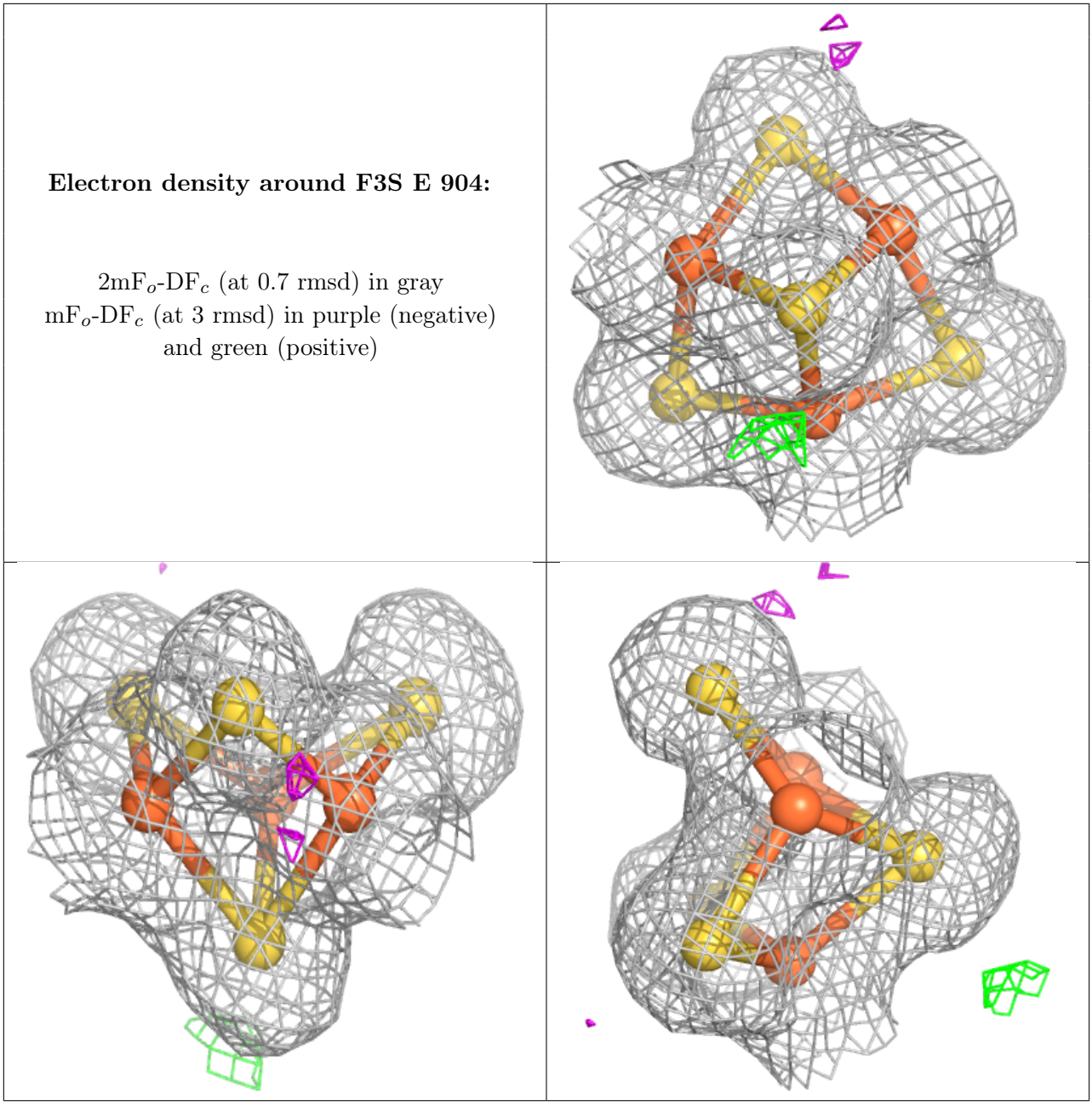
Electron density around F3S C 901:

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



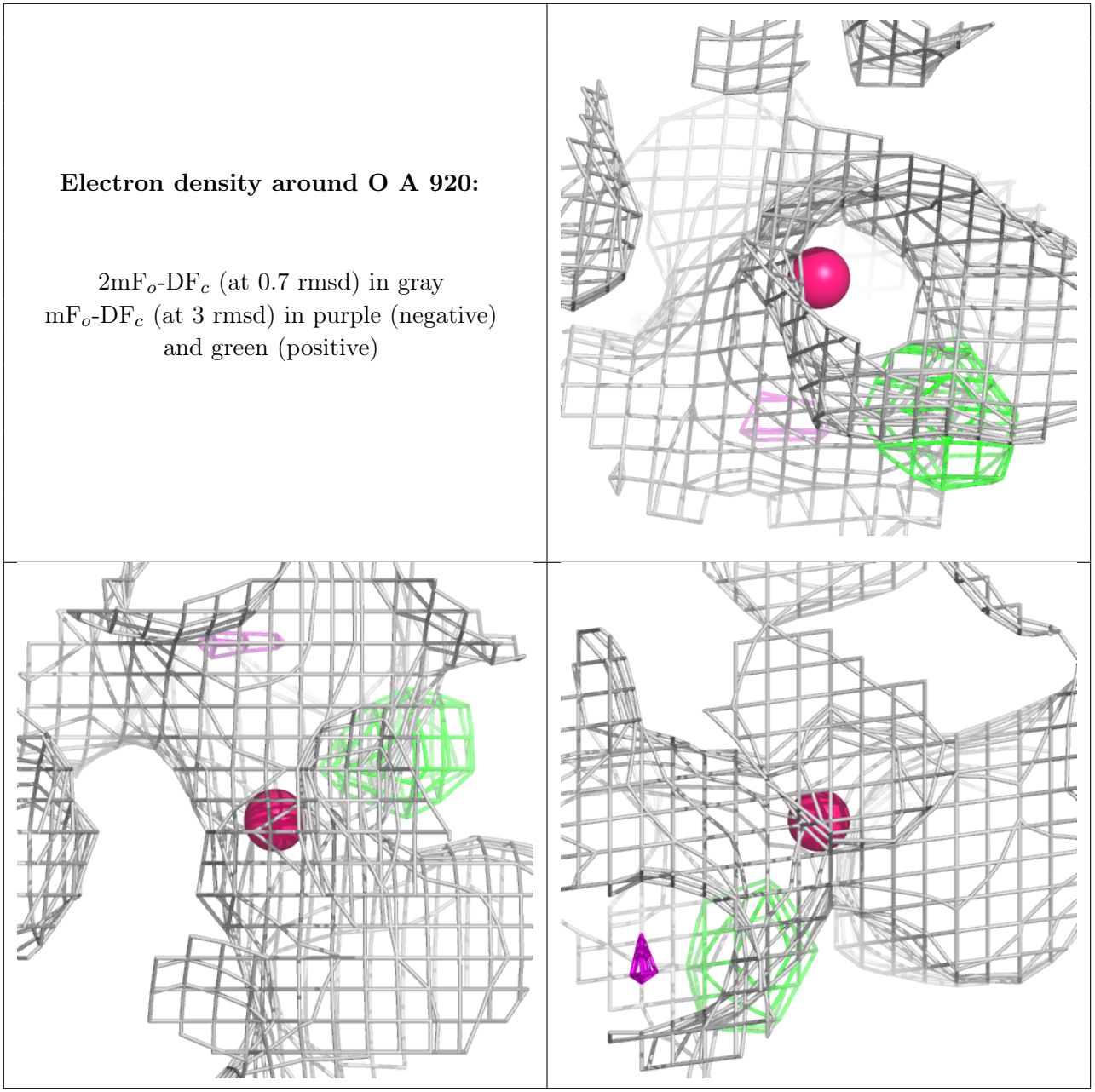
Electron density around F3S E 904:

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



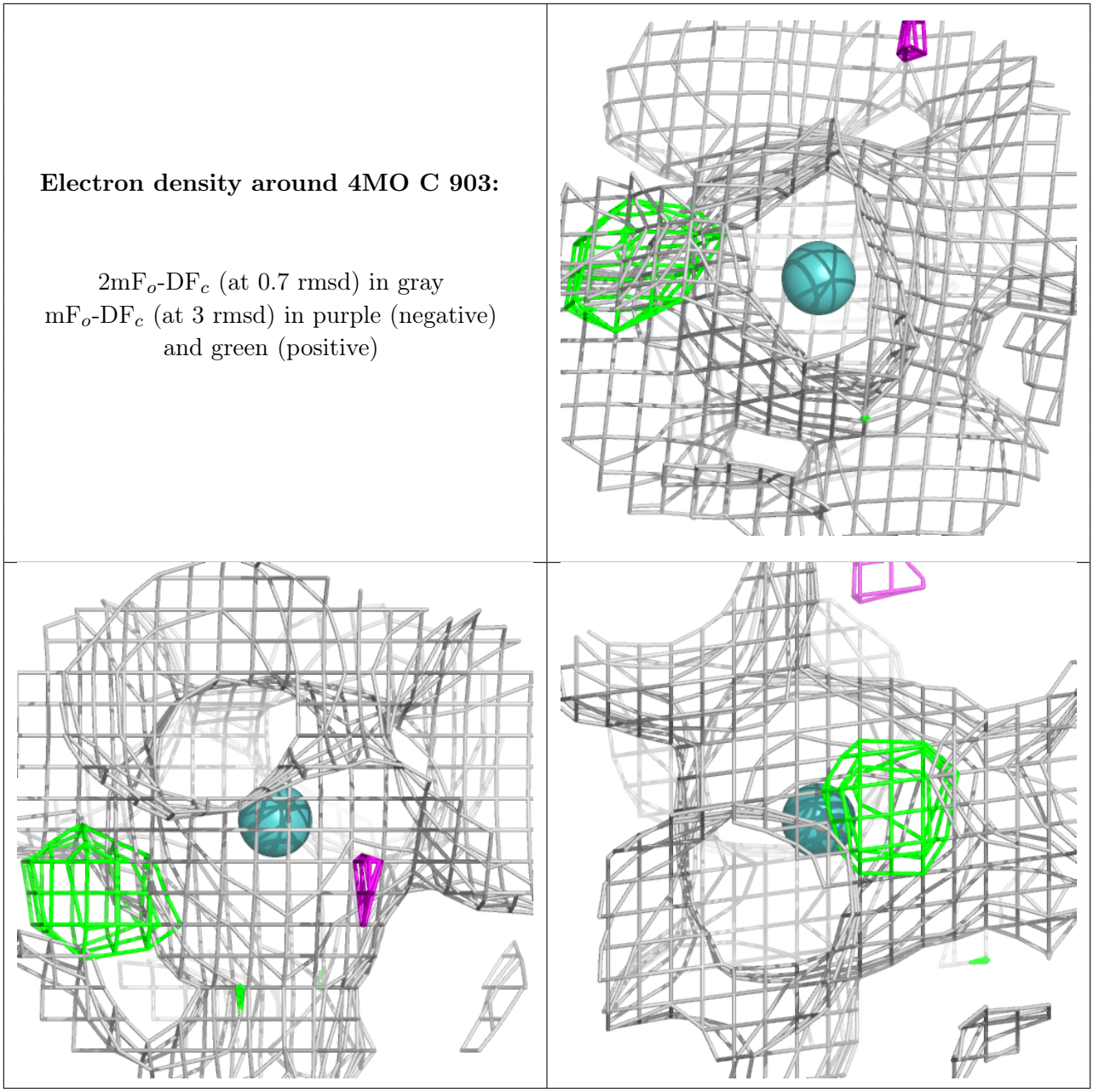
Electron density around O A 920:

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



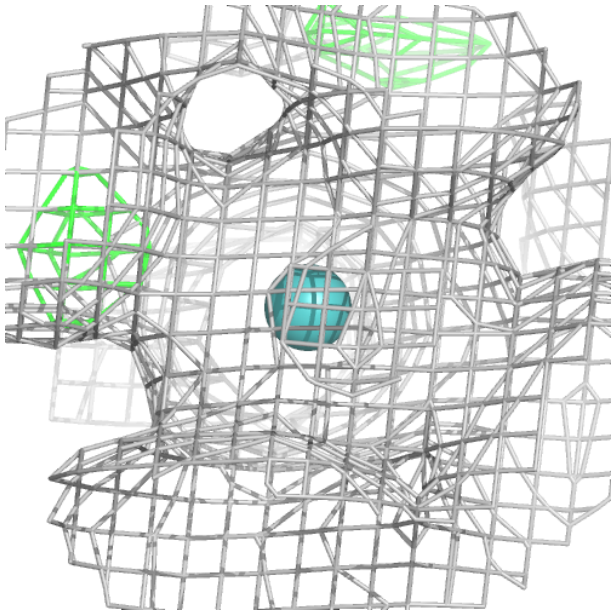
Electron density around 4MO C 903:

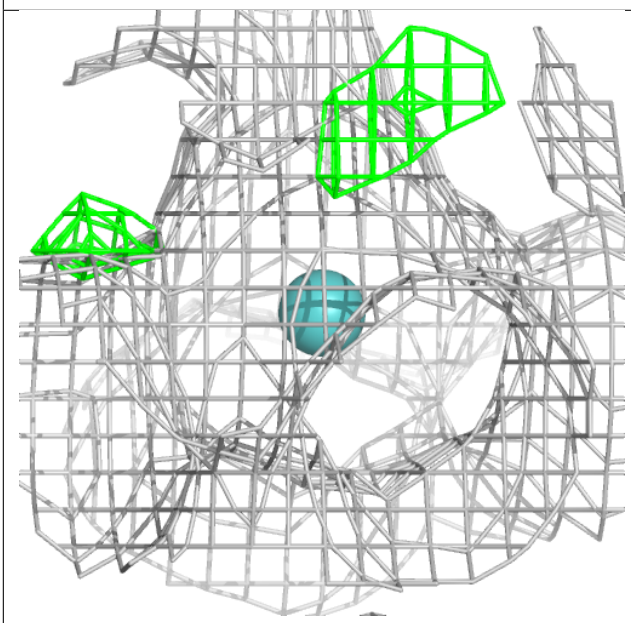
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

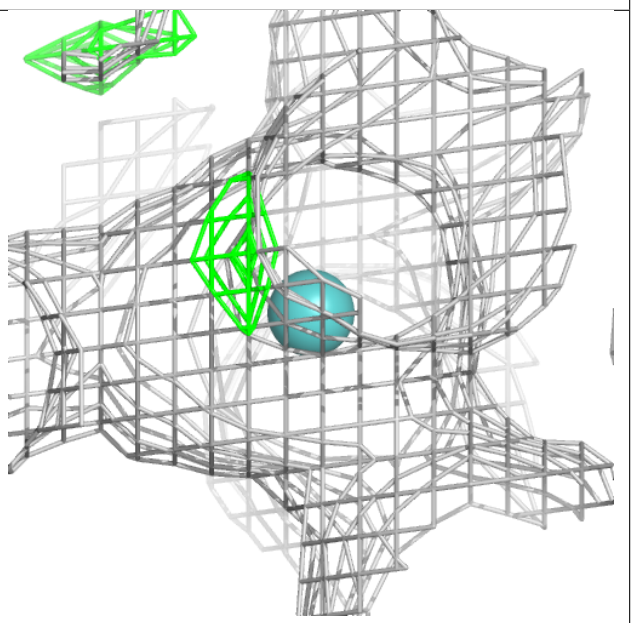


Electron density around 4MO E 903:

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

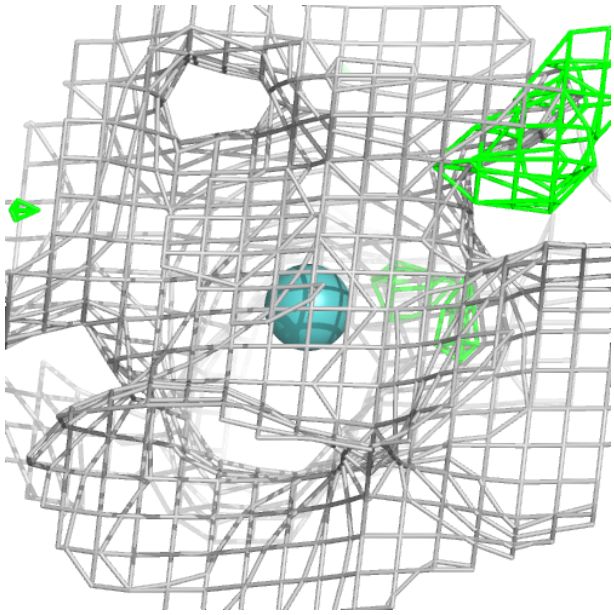


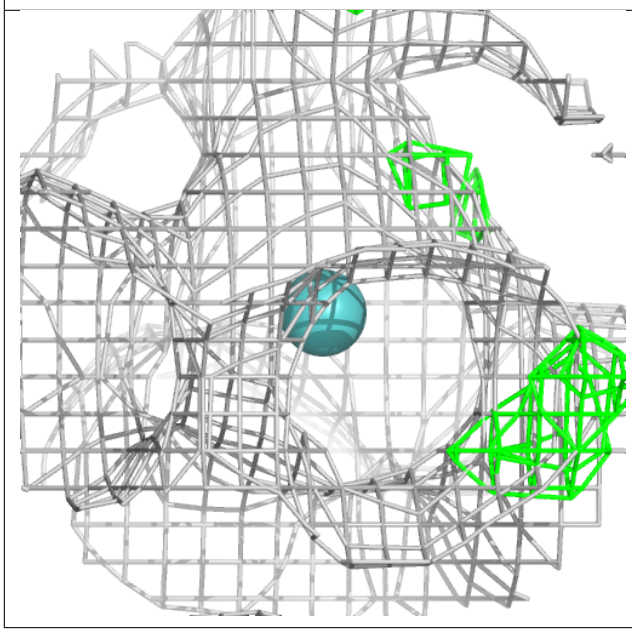


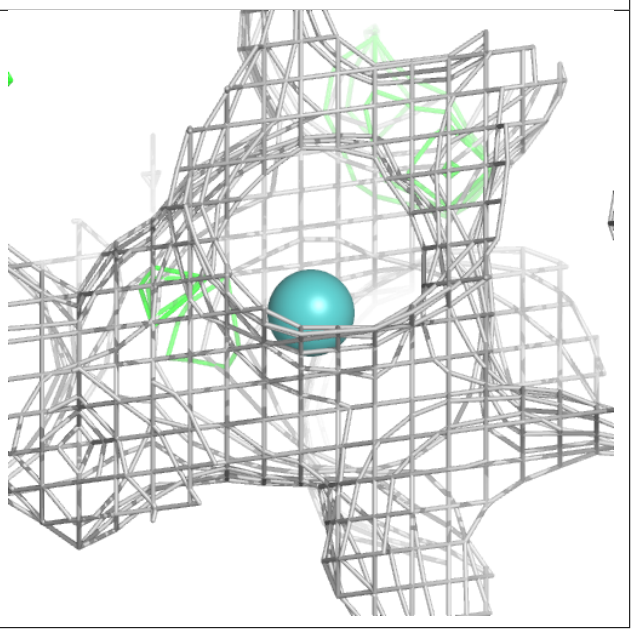


Electron density around 4MO G 904:

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

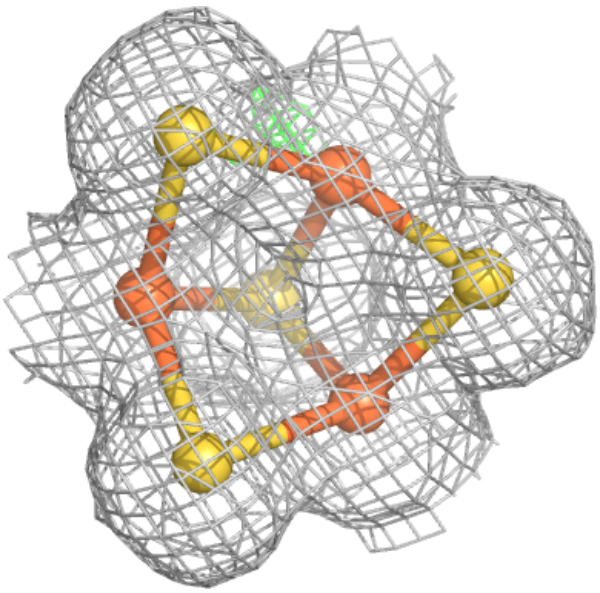


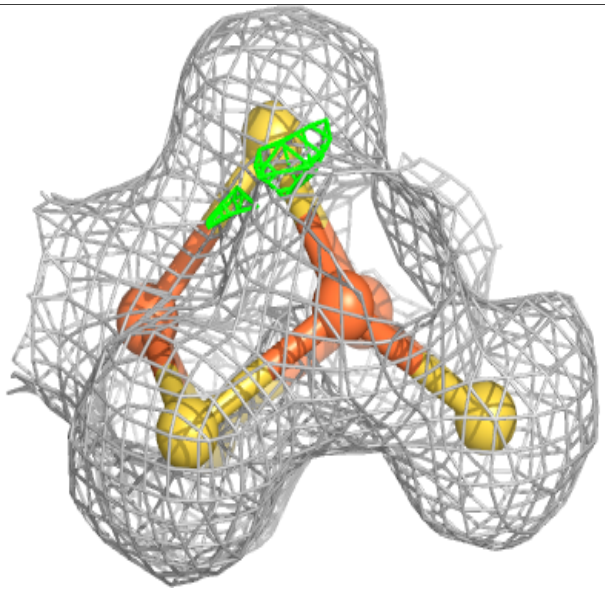


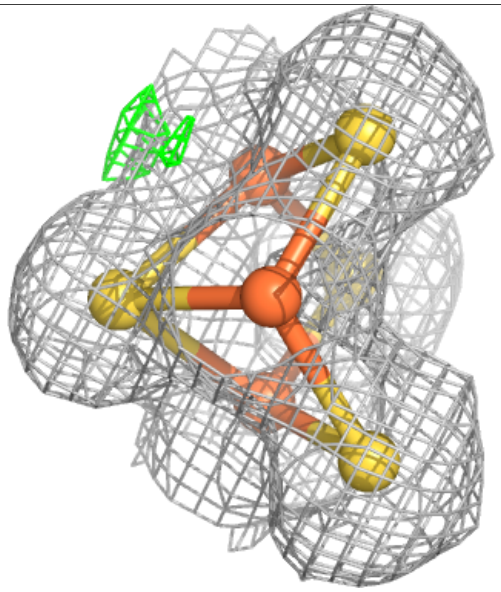


Electron density around F3S G 903:

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

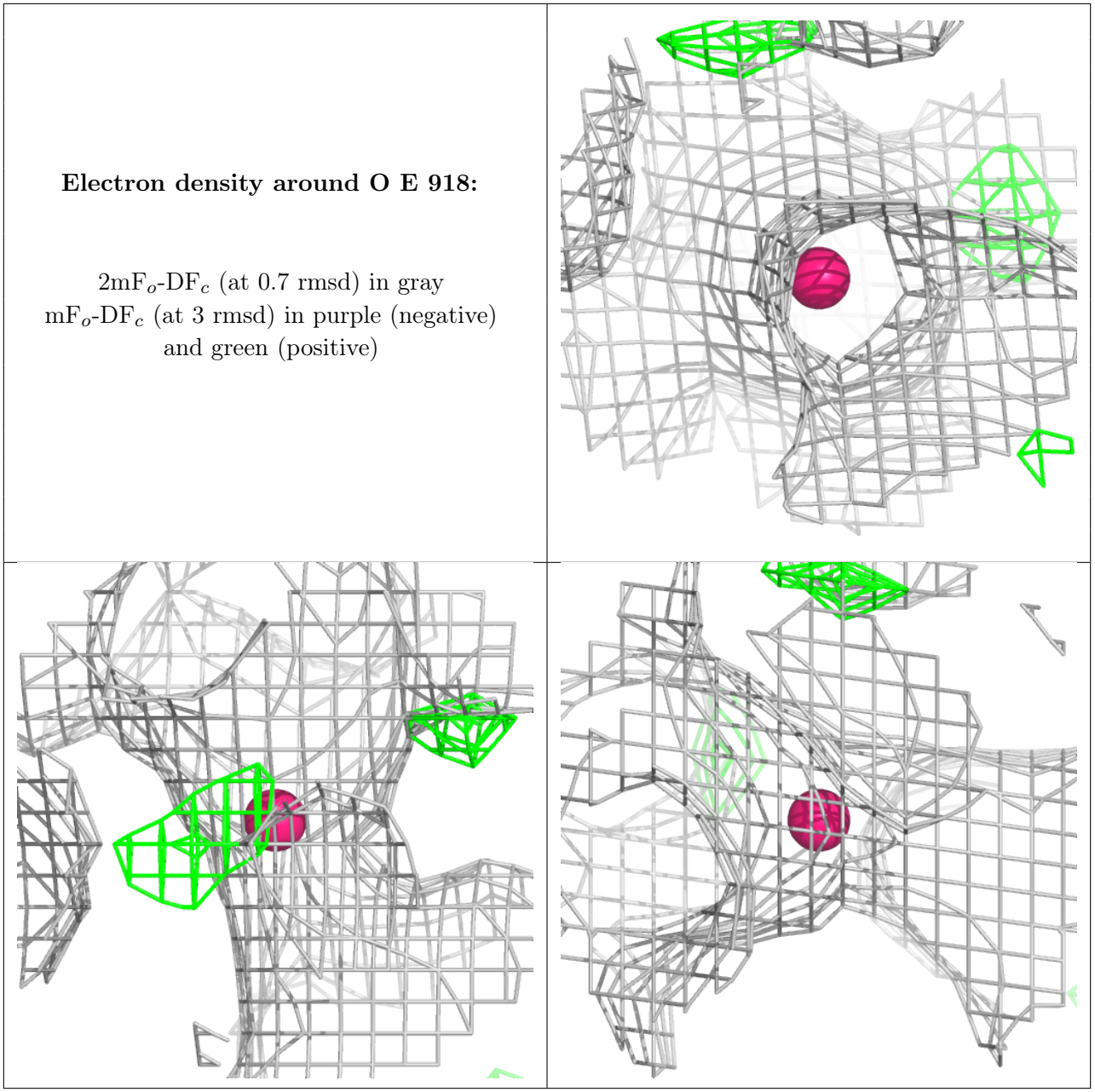






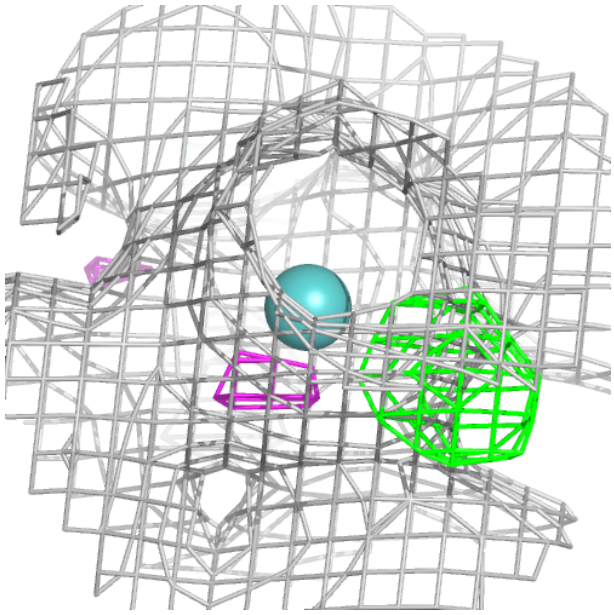
Electron density around O E 918:

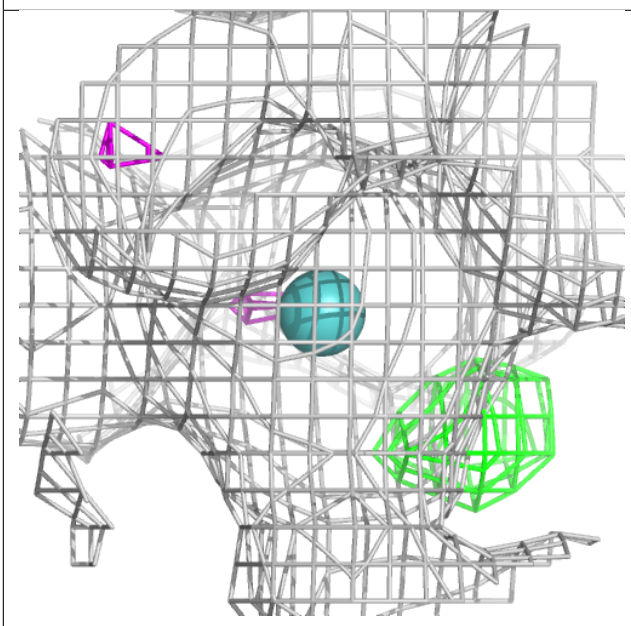
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

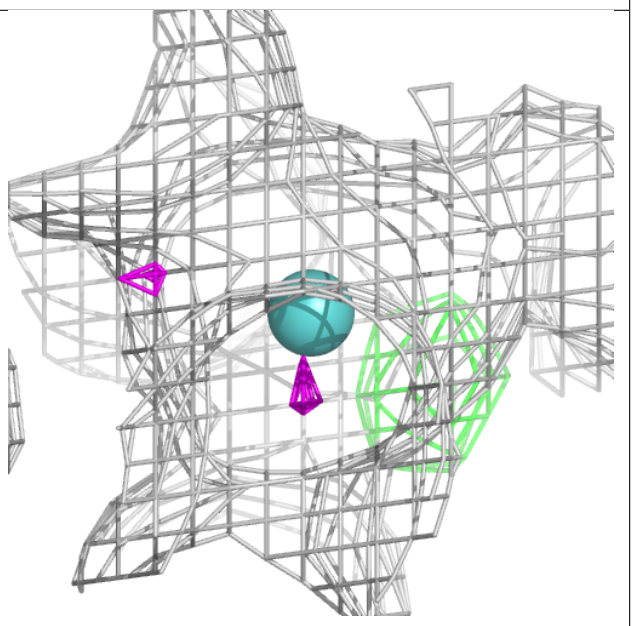


Electron density around MO A 901:

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

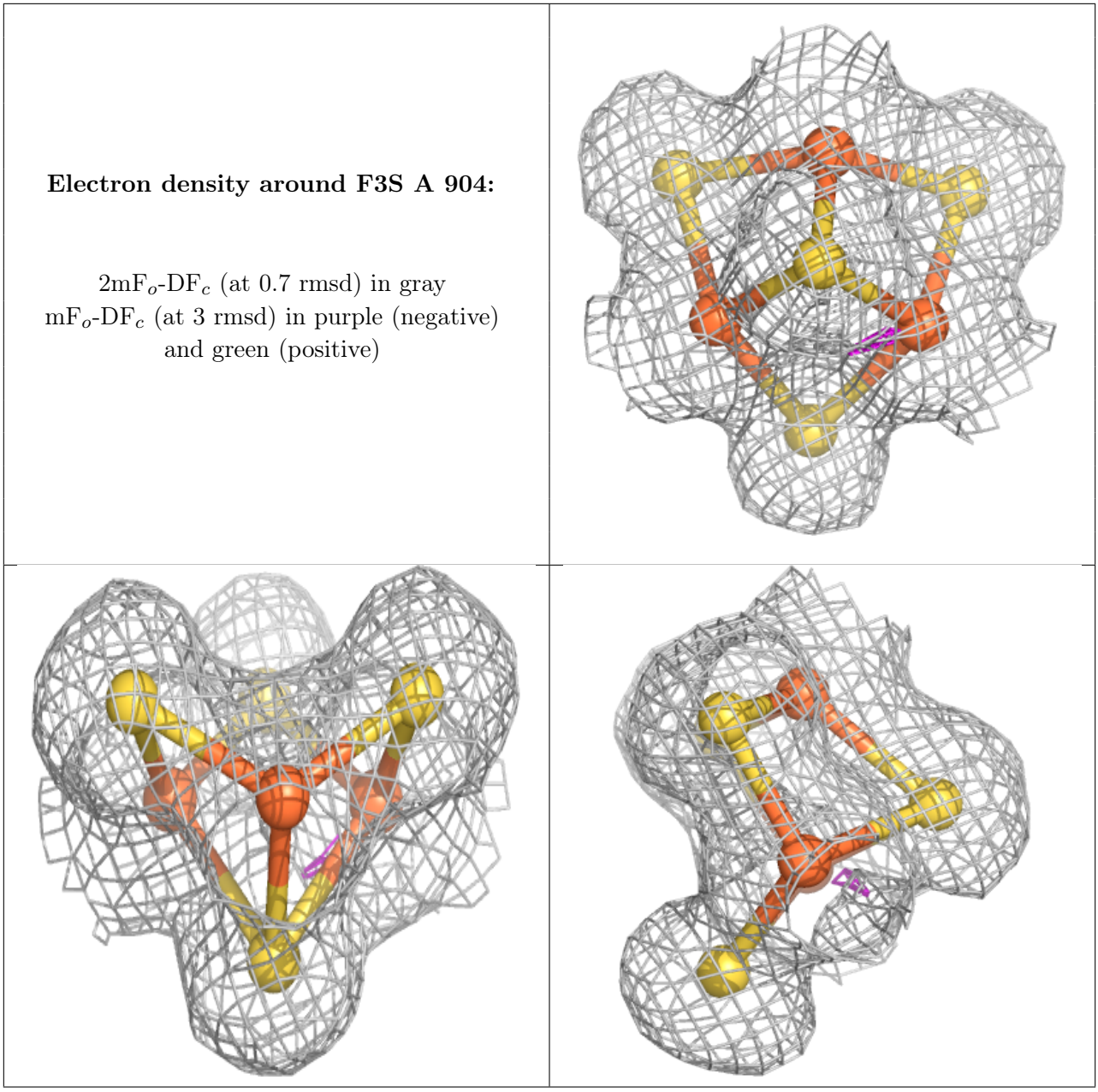






Electron density around F3S A 904:

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



6.5 Other polymers

There are no such residues in this entry.