wwPDB X-ray Structure Validation Summary Report (i)

May 10, 2025 – 07:39 pm BST

PDB ID	:	8R3A / pdb_00008r3a
Title	:	NT-26 Arsenite oxidase B F108C-G123C
Authors	:	Engrola, F.; Santos-Silva, T.; Correia, M.A.S.; Romao, M.J.
Deposited on	:	2023-11-08
Resolution	:	1.89 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:

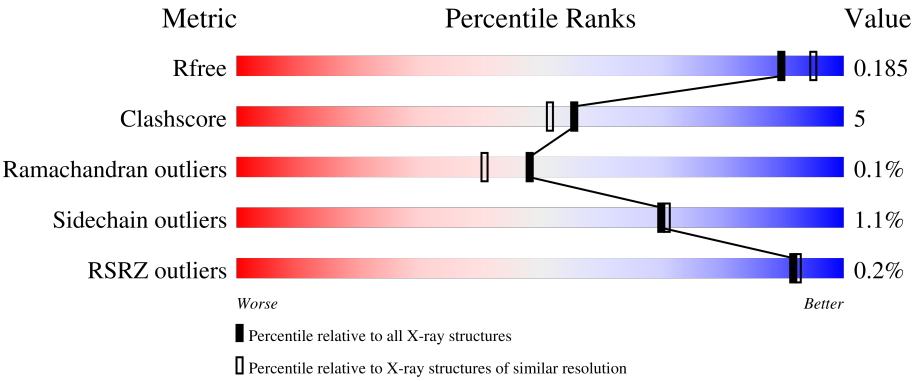
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	845	92% 8%
1	C	845	88% 11%
1	E	845	89% 9%
1	G	845	90% 8%
2	B	175	69% 6% 24%

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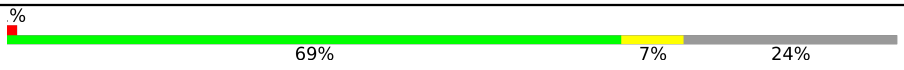
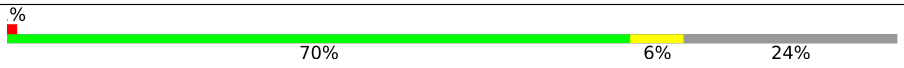
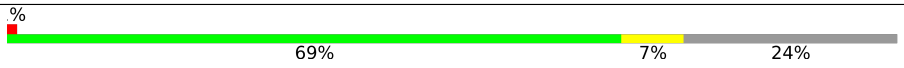
Mol	Chain	Length	Quality of chain
2	D	175	
2	F	175	
2	H	175	

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
11	GOL	G	914	-	-	X	-
13	FES	D	201	-	-	X	-
13	FES	F	201	-	-	X	-
13	FES	H	201	-	-	X	-
6	EDO	A	907	-	X	-	-
7	PEG	E	904	-	-	X	-
7	PEG	E	908	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 63455 atoms, of which 29455 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 AroA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	842	Total	C	H	N	O	S	0	24	0
			12927	4149	6279	1189	1267	43			
1	C	843	Total	C	H	N	O	S	0	28	0
			12947	4156	6287	1189	1273	42			
1	E	843	Total	C	H	N	O	S	0	20	0
			12891	4141	6261	1183	1265	41			
1	G	843	Total	C	H	N	O	S	0	28	0
			12980	4162	6310	1197	1269	42			

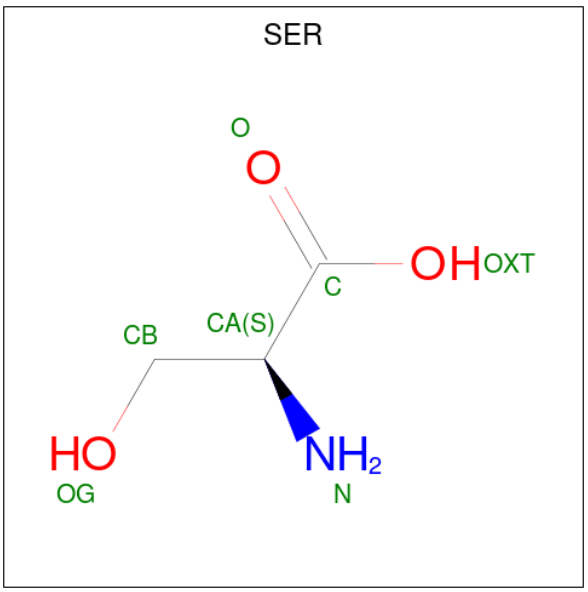
- Molecule 2 is a protein called Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	133	Total	C	H	N	O	S	0	5	0
			1969	639	952	170	202	6			
2	D	133	Total	C	H	N	O	S	0	3	0
			1949	633	940	169	201	6			
2	F	133	Total	C	H	N	O	S	0	3	0
			1949	633	940	169	201	6			
2	H	133	Total	C	H	N	O	S	0	5	0
			1969	639	952	170	202	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	CYS	PHE	engineered mutation	UNP L0NMC5
B	123	CYS	GLY	engineered mutation	UNP L0NMC5
D	108	CYS	PHE	engineered mutation	UNP L0NMC5
D	123	CYS	GLY	engineered mutation	UNP L0NMC5
F	108	CYS	PHE	engineered mutation	UNP L0NMC5
F	123	CYS	GLY	engineered mutation	UNP L0NMC5
H	108	CYS	PHE	engineered mutation	UNP L0NMC5
H	123	CYS	GLY	engineered mutation	UNP L0NMC5

- Molecule 3 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).

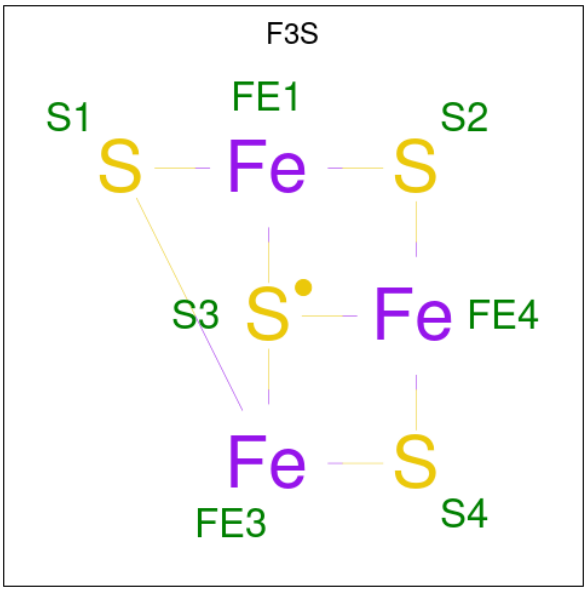


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			12	3	6	1	2		

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

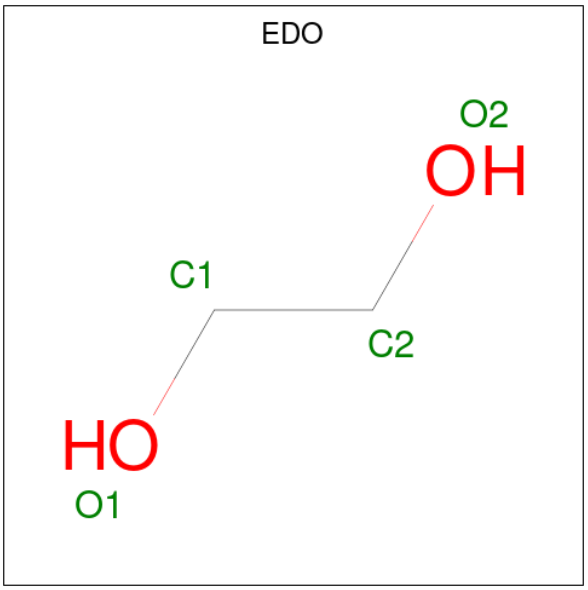
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		
4	C	1	Total	Mo	0	0
			1	1		
4	E	1	Total	Mo	0	0
			1	1		
4	G	1	Total	Mo	0	0
			1	1		

- 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 H O 8 2 4 2	0	0
6	A	1	Total C H O 8 2 4 2	0	0
6	A	1	Total C H O 8 2 4 2	0	0
6	A	1	Total C H O 16 4 8 4	0	1
6	A	1	Total C H O 8 2 4 2	0	0
6	C	1	Total C H O 8 2 4 2	0	0
6	C	1	Total C H O 8 2 4 2	0	0
6	C	1	Total C H O 8 2 4 2	0	0
6	C	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	E	1	Total C H O 8 2 4 2	0	0
6	G	1	Total C H O 8 2 4 2	0	0
6	G	1	Total C H O 8 2 4 2	0	0
6	G	1	Total C H O 8 2 4 2	0	0
6	G	1	Total C H O 8 2 4 2	0	0
6	G	1	Total C H O 8 2 4 2	0	0

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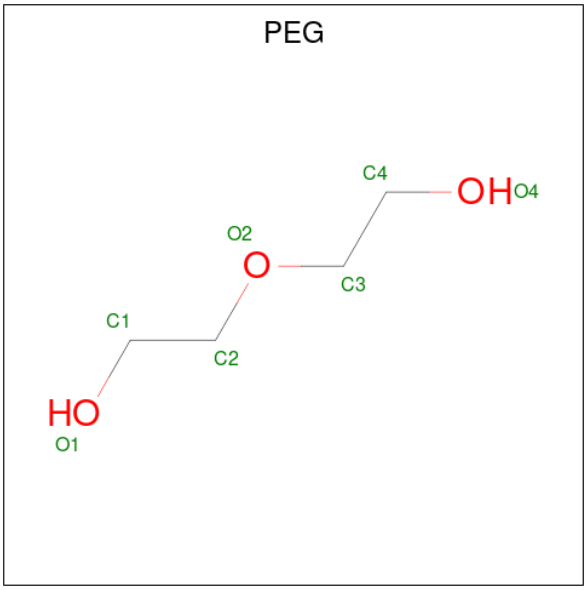
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C H O 8 2 4 2	0	0
6	H	1	Total C H O 8 2 4 2	0	0

- 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 H O 15 4 8 3	0	0
7	A	1	Total C H O 15 4 8 3	0	0
7	C	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0
7	E	1	Total C H O 15 4 8 3	0	0

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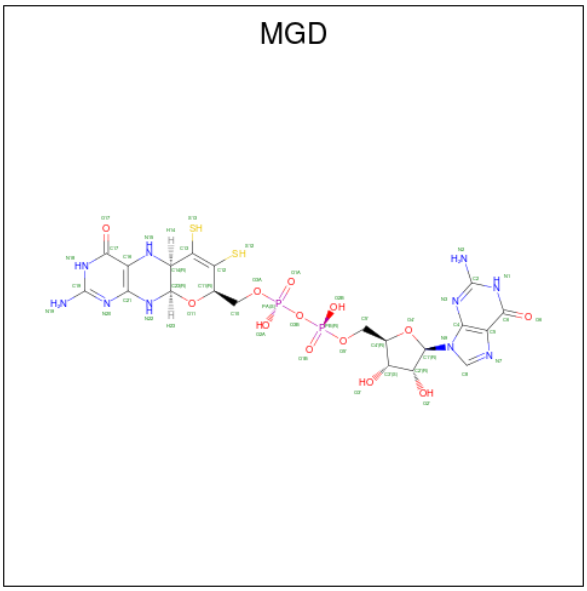
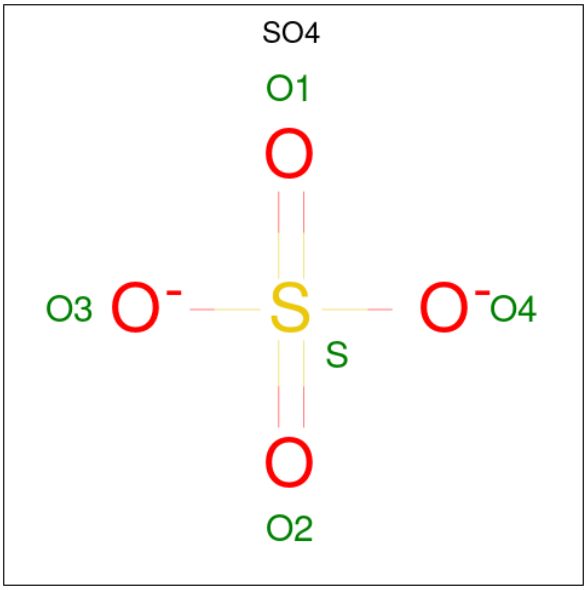
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	H	O	0	0
			15	4	8	3		
7	G	1	Total	C	H	O	0	0
			15	4	8	3		

- Molecule 8 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).



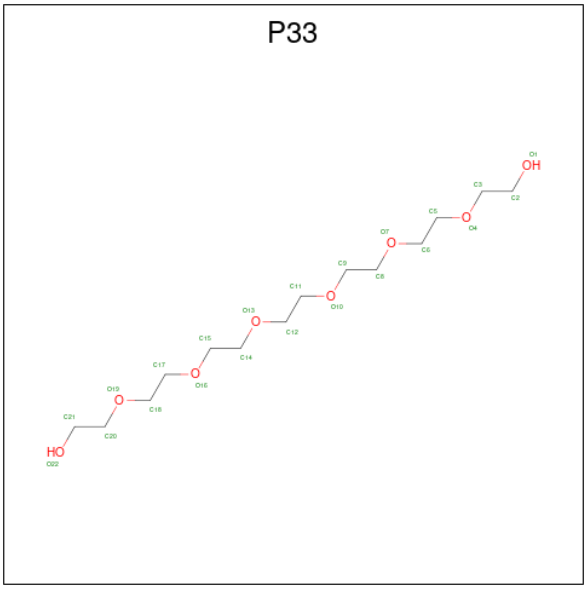
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	A	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	C	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	C	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	E	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	E	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	G	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
8	G	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



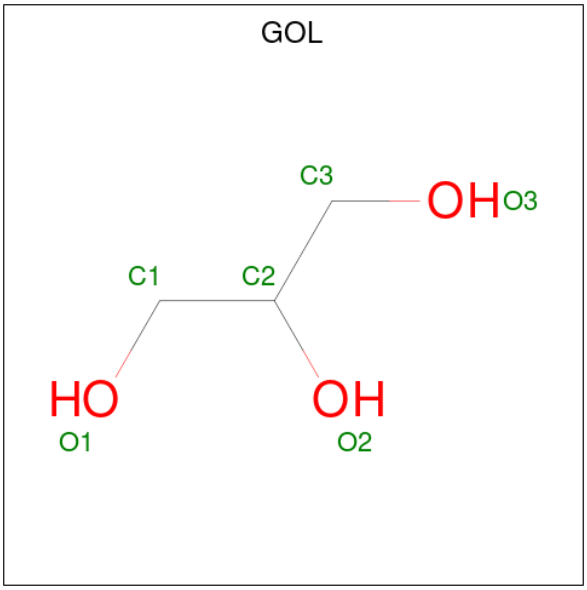
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0

- Molecule 10 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
10	A	1	Total	C	H	O	0	0
			50	14	28	8		
10	C	1	Total	C	H	O	0	0
			50	14	28	8		
10	C	1	Total	C	H	O	0	0
			50	14	28	8		
10	E	1	Total	C	H	O	0	0
			50	14	28	8		
10	G	1	Total	C	H	O	0	0
			50	14	28	8		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

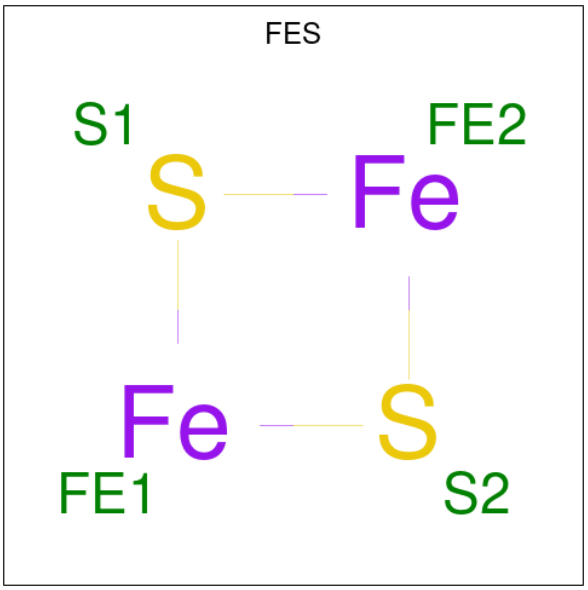


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			11	3	5	3		
11	A	1	Total	C	H	O	0	0
			11	3	5	3		
11	E	1	Total	C	H	O	0	0
			11	3	5	3		
11	G	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 12 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

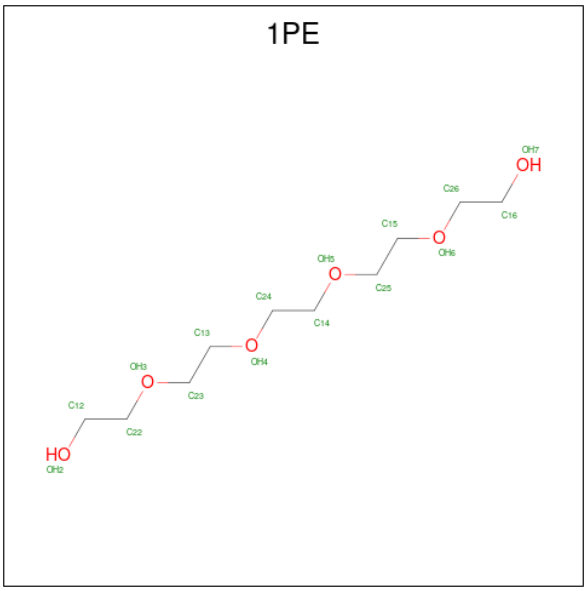
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O 1 1	0	0
12	C	1	Total O 1 1	0	0
12	E	1	Total O 1 1	0	0
12	G	1	Total O 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	E	1	Total C H O 36 10 20 6	0	0

- Molecule 15 is water.

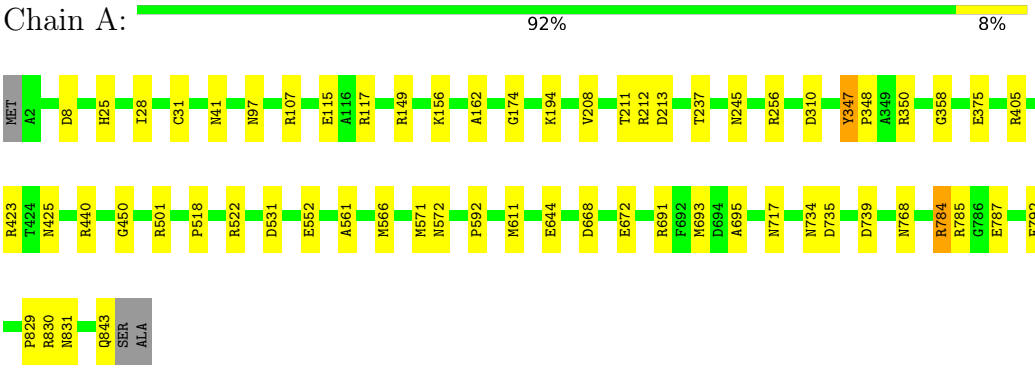
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	632	Total O 632 632	0	0
15	B	69	Total O 69 69	0	0
15	C	543	Total O 543 543	0	0
15	D	69	Total O 69 69	0	0
15	E	541	Total O 541 541	0	0
15	F	50	Total O 50 50	0	0
15	G	596	Total O 596 596	0	0
15	H	69	Total O 69 69	0	0

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.

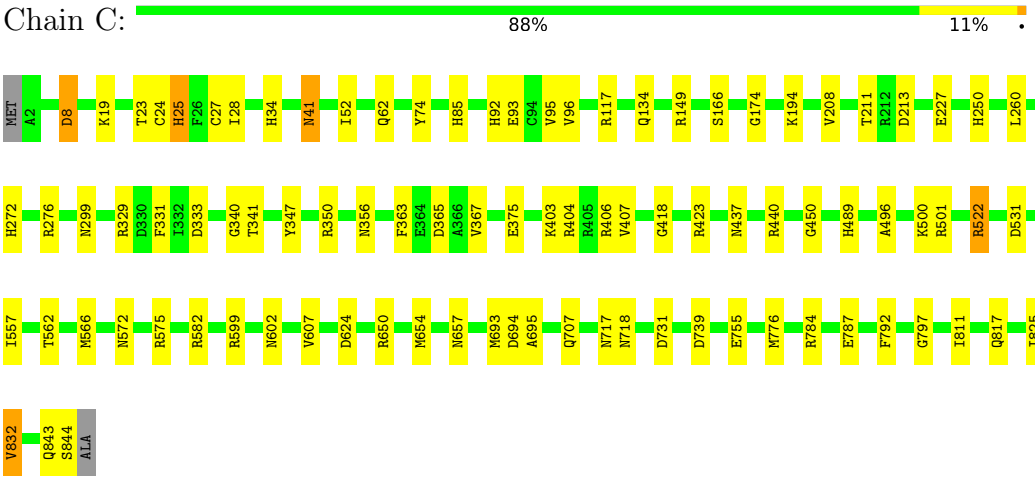
- Molecule 1: AroA

Chain A:



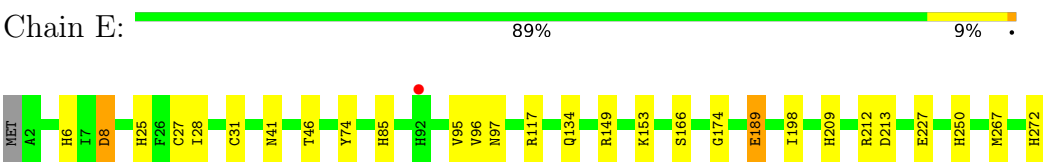
- Molecule 1: AroA

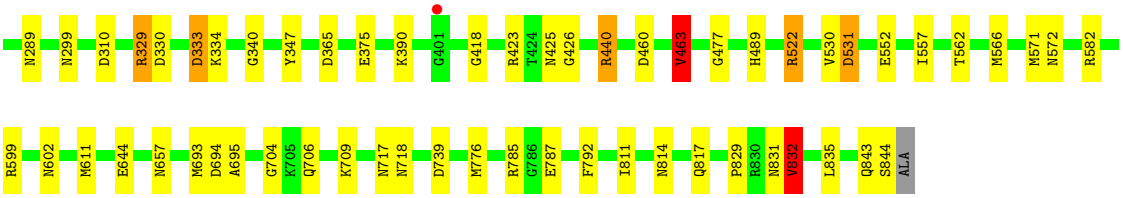
Chain C:



- Molecule 1: AroA

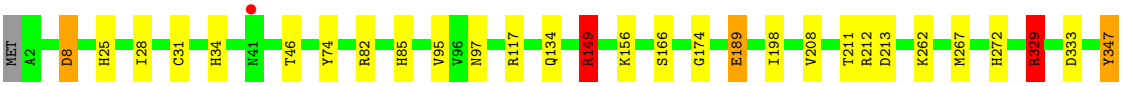
Chain E:





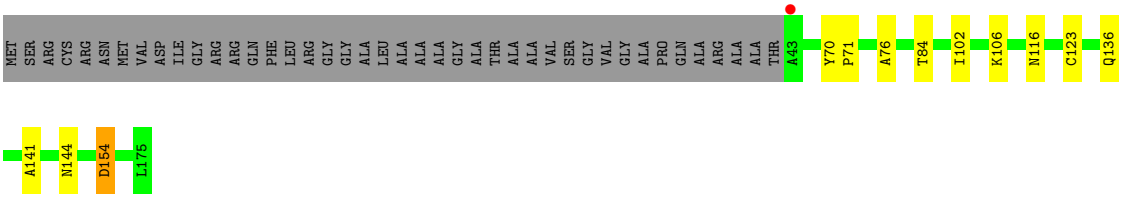
• Molecule 1: AroA

Chain G:



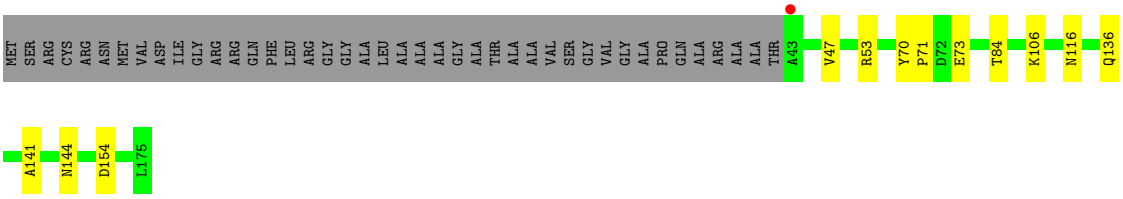
• Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain B:



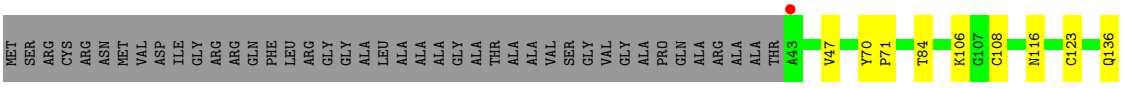
• Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

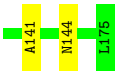
Chain D:



• Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

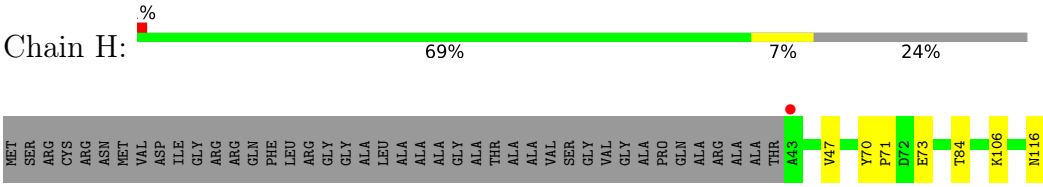
Chain F:





• Molecule 2: Arsenite oxidase small subunit AioB Rieske [2Fe-2S] cluster

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.61Å 148.93Å 231.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 1.89 49.32 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.32-1.89) 99.4 (49.32-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.152 , 0.185 0.152 , 0.185	Depositor DCC
R_{free} test set	19231 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	63455	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P33, SO4, 1PE, PEG, FES, EDO, GOL, MGD, O, 4MO, F3S

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	5/6883 (0.1%)	1.19	15/9318 (0.2%)
1	C	0.92	5/6920 (0.1%)	1.19	21/9373 (0.2%)
1	E	0.94	5/6863 (0.1%)	1.22	24/9294 (0.3%)
1	G	0.95	4/6929 (0.1%)	1.19	20/9382 (0.2%)
2	B	0.81	0/1056	1.12	1/1441 (0.1%)
2	D	0.88	0/1042	1.11	1/1421 (0.1%)
2	F	0.86	0/1042	1.18	1/1421 (0.1%)
2	H	0.82	0/1056	1.11	2/1441 (0.1%)
All	All	0.93	19/31791 (0.1%)	1.19	85/43091 (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	6
1	C	0	6
1	E	0	4
1	G	0	11
2	D	0	1
All	All	0	28

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	739[A]	ASP	CG-OD2	8.93	1.42	1.25
1	G	739[B]	ASP	CG-OD2	8.93	1.42	1.25
1	A	739[A]	ASP	CG-OD2	8.53	1.41	1.25
1	A	739[B]	ASP	CG-OD2	8.53	1.41	1.25
1	A	787	GLU	CD-OE1	8.31	1.41	1.25

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	832	VAL	N-CA-CB	-10.54	98.26	112.28
1	E	8	ASP	CA-CB-CG	9.85	122.44	112.60
1	C	832	VAL	N-CA-CB	-9.79	99.44	112.16
1	E	644	GLU	CB-CG-CD	9.26	128.35	112.60
1	G	787	GLU	CG-CD-OE2	-9.19	97.26	118.40

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149[A]	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	440	ARG	Sidechain
1	A	691	ARG	Sidechain
1	A	784	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	6648	6279	6327	44	0
1	C	6660	6287	6311	65	0
1	E	6630	6261	6315	69	0
1	G	6670	6310	6332	60	1
2	B	1017	952	960	9	0
2	D	1009	940	951	9	0
2	F	1009	940	953	8	0
2	H	1017	952	958	10	0
3	A	6	6	4	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	7	0	0	0	0
6	A	24	24	36	3	0
6	C	16	16	24	1	0
6	E	32	32	48	2	0
6	G	24	24	36	2	0
6	H	4	4	6	0	0
7	A	14	16	20	1	0
7	C	7	8	10	0	0
7	E	42	48	60	11	0
7	G	14	16	20	2	0
8	A	94	40	44	4	0
8	C	94	40	44	5	0
8	E	94	40	44	4	0
8	G	94	40	44	5	0
9	A	5	0	0	0	0
9	C	5	0	0	0	0
10	A	22	28	30	2	0
10	C	44	56	60	0	0
10	E	22	28	30	3	0
10	G	22	28	30	7	0
11	A	12	10	16	4	0
11	E	6	5	8	0	0
11	G	6	5	8	4	0
12	A	1	0	0	0	0
12	C	1	0	0	0	0
12	E	1	0	0	1	0
12	G	1	0	0	0	0
13	B	4	0	0	1	0
13	D	4	0	0	2	0
13	F	4	0	0	2	0
13	H	4	0	0	2	0
14	E	16	20	22	5	0
15	A	632	0	0	7	0
15	B	69	0	0	0	0
15	C	543	0	0	12	0
15	D	69	0	0	1	0
15	E	541	0	0	10	0
15	F	50	0	0	1	0
15	G	596	0	0	13	0
15	H	69	0	0	1	0
All	All	34000	29455	29751	280	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:GLN:C	3:A:901:SER:N	1.68	1.51
1:C:423:ARG:HA	1:C:693[A]:MET:HE1	1.34	1.10
1:G:843:GLN:HG3	2:H:116:ASN:HD21	1.31	0.95
1:G:423:ARG:HA	1:G:693[A]:MET:HE1	1.50	0.92
1:A:405:ARG:HH12	11:A:916:GOL:H31	1.38	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:686:ASP:O	1:G:686:ASP:O[2_545]	1.52	0.68

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	864/845 (102%)	835 (97%)	28 (3%)	1 (0%)	48	41
1	C	869/845 (103%)	839 (96%)	29 (3%)	1 (0%)	48	41
1	E	861/845 (102%)	829 (96%)	31 (4%)	1 (0%)	48	41
1	G	869/845 (103%)	837 (96%)	32 (4%)	0	100	100
2	B	136/175 (78%)	131 (96%)	5 (4%)	0	100	100
2	D	134/175 (77%)	130 (97%)	4 (3%)	0	100	100
2	F	134/175 (77%)	126 (94%)	8 (6%)	0	100	100
2	H	136/175 (78%)	130 (96%)	6 (4%)	0	100	100
All	All	4003/4080 (98%)	3857 (96%)	143 (4%)	3 (0%)	48	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	811	ILE
1	A	811	ILE
1	C	811	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	698/678 (103%)	692 (99%)	6 (1%)	75	77
1	C	703/678 (104%)	692 (98%)	11 (2%)	58	56
1	E	696/678 (103%)	688 (99%)	8 (1%)	70	71
1	G	703/678 (104%)	694 (99%)	9 (1%)	65	65
2	B	111/131 (85%)	110 (99%)	1 (1%)	75	77
2	D	109/131 (83%)	108 (99%)	1 (1%)	75	77
2	F	109/131 (83%)	109 (100%)	0	100	100
2	H	111/131 (85%)	111 (100%)	0	100	100
All	All	3240/3236 (100%)	3204 (99%)	36 (1%)	70	71

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	189	GLU
1	G	792	PHE
1	G	329	ARG
1	G	522[A]	ARG
1	C	341	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	542	ASN
1	G	21	ASN

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Mol	Chain	Res	Type
1	E	619	GLN
1	E	814	ASN
1	G	85	HIS

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 73 ligands modelled in this entry, 8 are monoatomic - leaving 65 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	$\#\|Z\| > 2$
6	EDO	H	202	-	3,3,3	0.35	0	2,2,2	0.38	0
6	EDO	A	906	-	3,3,3	0.12	0	2,2,2	0.32	0
7	PEG	G	904	-	6,6,6	0.31	0	5,5,5	0.35	0
5	F3S	E	902	1	0,9,9	-	-	-		
6	EDO	G	909	-	3,3,3	0.22	0	2,2,2	0.18	0
8	MGD	C	908	4	41,52,52	1.04	4 (9%)	40,81,81	1.45	6 (15%)
5	F3S	A	903	1	0,9,9	-	-	-		
7	PEG	E	909	-	6,6,6	0.53	0	5,5,5	0.46	0
6	EDO	E	907	-	3,3,3	0.33	0	2,2,2	0.56	0
6	EDO	C	904	-	3,3,3	0.66	0	2,2,2	0.80	0
10	P33	E	920	-	21,21,21	0.51	0	20,20,20	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MGD	C	909	4	41,52,52	1.55	5 (12%)	40,81,81	1.02	2 (5%)
7	PEG	A	910	-	6,6,6	0.35	0	5,5,5	0.24	0
8	MGD	E	919	4	41,52,52	1.03	4 (9%)	40,81,81	1.29	7 (17%)
8	MGD	G	912	4	41,52,52	1.12	4 (9%)	40,81,81	1.22	3 (7%)
7	PEG	E	908	-	6,6,6	0.34	0	5,5,5	0.24	0
6	EDO	A	904	-	3,3,3	1.15	0	2,2,2	0.94	0
8	MGD	A	911	4	41,52,52	1.36	3 (7%)	40,81,81	1.16	3 (7%)
6	EDO	C	903	-	3,3,3	0.18	0	2,2,2	0.66	0
6	EDO	C	906	-	3,3,3	0.20	0	2,2,2	0.14	0
7	PEG	E	915	-	6,6,6	0.64	0	5,5,5	0.50	0
6	EDO	A	907	-	3,3,3	1.97	2 (66%)	2,2,2	1.67	1 (50%)
7	PEG	E	916	-	6,6,6	0.60	0	5,5,5	0.61	0
13	FES	D	201	2	0,4,4	-	-	-		
6	EDO	E	903	-	3,3,3	0.87	0	2,2,2	0.61	0
8	MGD	A	912	4	41,52,52	1.10	5 (12%)	40,81,81	1.06	4 (10%)
10	P33	C	912	-	21,21,21	0.80	0	20,20,20	0.73	0
6	EDO	E	913	-	3,3,3	0.13	0	2,2,2	0.56	0
11	GOL	A	915	-	5,5,5	0.31	0	5,5,5	0.54	0
11	GOL	E	921	-	5,5,5	0.18	0	5,5,5	0.86	0
9	SO4	A	913	-	4,4,4	0.68	0	6,6,6	0.90	0
10	P33	A	914	-	21,21,21	0.92	0	20,20,20	0.76	0
8	MGD	G	911	4	41,52,52	1.35	2 (4%)	40,81,81	1.38	4 (10%)
6	EDO	G	910	-	3,3,3	0.60	0	2,2,2	1.10	0
7	PEG	E	904	-	6,6,6	0.51	0	5,5,5	0.87	0
6	EDO	G	907	-	3,3,3	0.10	0	2,2,2	0.48	0
6	EDO	E	911	-	3,3,3	0.39	0	2,2,2	1.02	0
5	F3S	C	902	1	0,9,9	-	-	-		
10	P33	C	911	-	21,21,21	0.36	0	20,20,20	0.57	0
6	EDO	A	908[A]	-	3,3,3	0.28	0	2,2,2	0.61	0
13	FES	H	201	2	0,4,4	-	-	-		
6	EDO	E	914	-	3,3,3	0.32	0	2,2,2	0.68	0
14	1PE	E	917	-	15,15,15	0.57	0	14,14,14	0.58	0
7	PEG	E	905	-	6,6,6	0.34	0	5,5,5	0.37	0
11	GOL	A	916	-	5,5,5	0.32	0	5,5,5	0.71	0
13	FES	B	201	2	0,4,4	-	-	-		
6	EDO	G	908	-	3,3,3	0.37	0	2,2,2	1.06	0
6	EDO	C	907	-	3,3,3	0.96	0	2,2,2	0.98	0
6	EDO	E	912	-	3,3,3	0.17	0	2,2,2	0.34	0
7	PEG	C	905	-	6,6,6	0.36	0	5,5,5	0.41	0
6	EDO	A	909	-	3,3,3	0.20	0	2,2,2	0.22	0
3	SER	A	901	-	4,5,6	1.09	0	0,5,7	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	G	905	-	3,3,3	1.05	0	2,2,2	0.37	0
13	FES	F	201	2	0,4,4	-	-	-		
11	GOL	G	914	-	5,5,5	0.49	0	5,5,5	0.81	0
6	EDO	G	903	-	3,3,3	0.20	0	2,2,2	0.03	0
6	EDO	A	908[B]	-	3,3,3	0.19	0	2,2,2	0.49	0
7	PEG	G	906	-	6,6,6	0.49	0	5,5,5	0.43	0
10	P33	G	913	-	21,21,21	0.69	0	20,20,20	0.62	0
6	EDO	E	906	-	3,3,3	0.66	0	2,2,2	0.67	0
6	EDO	E	910	-	3,3,3	0.43	0	2,2,2	0.43	0
9	SO4	C	910	-	4,4,4	0.57	0	6,6,6	0.71	0
7	PEG	A	905	-	6,6,6	0.43	0	5,5,5	0.27	0
5	F3S	G	902	1	0,9,9	-	-	-		
8	MGD	E	918	4	41,52,52	1.12	4 (9%)	40,81,81	1.14	2 (5%)

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
6	EDO	H	202	-	-	0/1/1/1	-
6	EDO	A	906	-	-	1/1/1/1	-
7	PEG	G	904	-	-	0/4/4/4	-
6	EDO	G	909	-	-	1/1/1/1	-
8	MGD	C	908	4	-	3/18/66/66	0/6/6/6
5	F3S	E	902	1	-	-	0/3/3/3
5	F3S	A	903	1	-	-	0/3/3/3
7	PEG	E	909	-	-	2/4/4/4	-
6	EDO	E	907	-	-	1/1/1/1	-
6	EDO	C	904	-	-	1/1/1/1	-
10	P33	E	920	-	-	10/19/19/19	-
8	MGD	C	909	4	-	4/18/66/66	0/6/6/6
7	PEG	A	910	-	-	2/4/4/4	-
8	MGD	E	919	4	-	5/18/66/66	0/6/6/6
5	F3S	G	902	1	-	-	0/3/3/3
8	MGD	G	912	4	-	3/18/66/66	0/6/6/6
7	PEG	E	908	-	-	3/4/4/4	-
6	EDO	A	904	-	-	0/1/1/1	-
8	MGD	A	911	4	-	4/18/66/66	0/6/6/6
6	EDO	C	903	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	906	-	-	1/1/1/1	-
7	PEG	E	915	-	-	2/4/4/4	-
6	EDO	A	907	-	-	0/1/1/1	-
7	PEG	E	916	-	-	2/4/4/4	-
13	FES	D	201	2	-	-	0/1/1/1
6	EDO	E	903	-	-	0/1/1/1	-
8	MGD	A	912	4	-	5/18/66/66	0/6/6/6
10	P33	C	912	-	-	12/19/19/19	-
6	EDO	E	913	-	-	1/1/1/1	-
11	GOL	A	915	-	-	0/4/4/4	-
11	GOL	E	921	-	-	0/4/4/4	-
10	P33	A	914	-	-	7/19/19/19	-
8	MGD	G	911	4	-	4/18/66/66	0/6/6/6
6	EDO	G	910	-	-	0/1/1/1	-
7	PEG	E	904	-	-	2/4/4/4	-
6	EDO	G	907	-	-	1/1/1/1	-
6	EDO	E	911	-	-	0/1/1/1	-
5	F3S	C	902	1	-	-	0/3/3/3
10	P33	C	911	-	-	9/19/19/19	-
6	EDO	A	908[A]	-	-	1/1/1/1	-
13	FES	H	201	2	-	-	0/1/1/1
6	EDO	E	914	-	-	0/1/1/1	-
14	1PE	E	917	-	-	11/13/13/13	-
7	PEG	E	905	-	-	2/4/4/4	-
11	GOL	A	916	-	-	2/4/4/4	-
13	FES	B	201	2	-	-	0/1/1/1
6	EDO	G	908	-	-	0/1/1/1	-
6	EDO	C	907	-	-	1/1/1/1	-
6	EDO	E	912	-	-	1/1/1/1	-
7	PEG	C	905	-	-	3/4/4/4	-
6	EDO	A	909	-	-	1/1/1/1	-
3	SER	A	901	-	-	0/2/4/6	-
6	EDO	G	905	-	-	0/1/1/1	-
13	FES	F	201	2	-	-	0/1/1/1
11	GOL	G	914	-	-	4/4/4/4	-
6	EDO	G	903	-	-	1/1/1/1	-
6	EDO	A	908[B]	-	-	1/1/1/1	-
7	PEG	G	906	-	-	3/4/4/4	-
6	EDO	E	906	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	E	910	-	-	1/1/1/1	-
7	PEG	A	905	-	-	2/4/4/4	-
10	P33	G	913	-	-	14/19/19/19	-
8	MGD	E	918	4	-	4/18/66/66	0/6/6/6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	909	MGD	C23-C14	6.71	1.59	1.53
8	A	911	MGD	C23-C14	6.07	1.58	1.53
8	G	911	MGD	C23-C14	5.97	1.58	1.53
8	E	918	MGD	C10-C11	-3.25	1.47	1.52
8	C	909	MGD	C5-C6	-3.05	1.41	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	908	MGD	O11-C23-N22	-4.50	103.94	108.57
8	G	912	MGD	O11-C23-N22	-3.76	104.71	108.57
8	G	911	MGD	C19-N20-C21	3.64	120.00	113.43
8	C	908	MGD	O11-C23-C14	3.29	111.16	108.96
8	E	919	MGD	O6-C6-C5	3.19	130.60	124.37

There are no chirality outliers.

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	911	MGD	C5'-O5'-PB-O3B
8	A	912	MGD	C5'-O5'-PB-O1B
8	A	912	MGD	C5'-O5'-PB-O3B
8	C	908	MGD	PA-O3B-PB-O5'
8	C	908	MGD	C5'-O5'-PB-O1B

There are no ring outliers.

32 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	908	MGD	2	0
7	E	909	PEG	3	0
6	E	907	EDO	1	0

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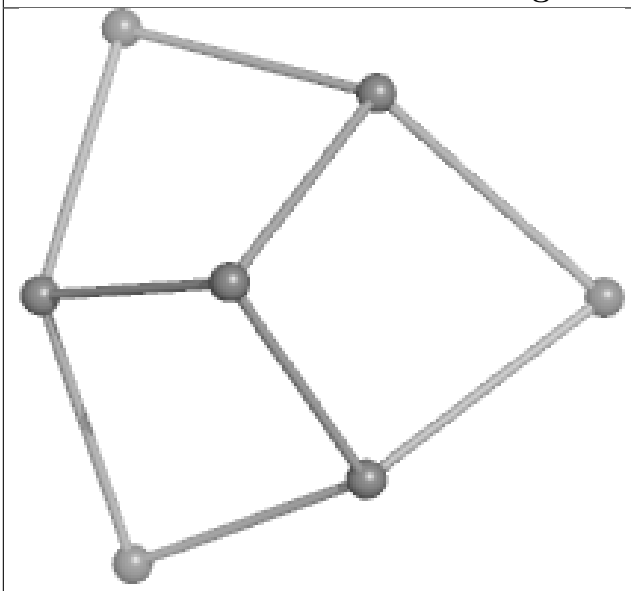
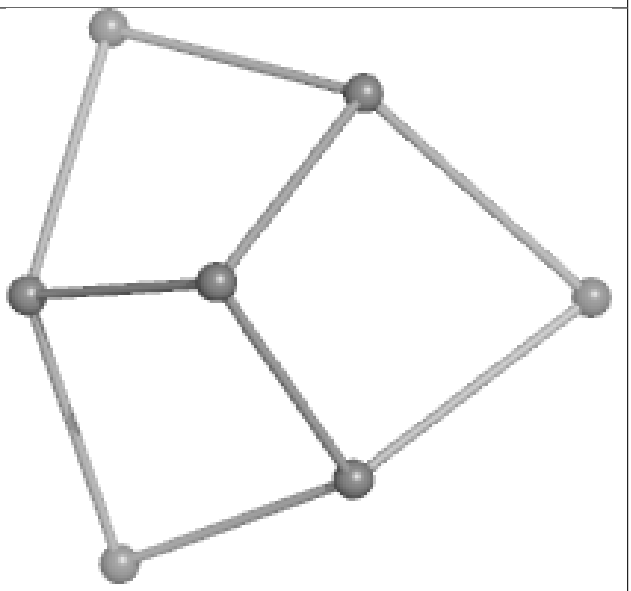
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	920	P33	3	0
8	C	909	MGD	3	0
8	E	919	MGD	3	0
8	G	912	MGD	2	0
7	E	908	PEG	4	0
6	A	904	EDO	2	0
8	A	911	MGD	2	0
13	D	201	FES	2	0
8	A	912	MGD	2	0
11	A	915	GOL	2	0
10	A	914	P33	2	0
8	G	911	MGD	3	0
7	E	904	PEG	4	0
6	G	907	EDO	1	0
6	E	911	EDO	1	0
13	H	201	FES	2	0
14	E	917	1PE	5	0
11	A	916	GOL	2	0
13	B	201	FES	1	0
6	G	908	EDO	1	0
6	C	907	EDO	1	0
6	A	909	EDO	1	0
3	A	901	SER	3	0
13	F	201	FES	2	0
11	G	914	GOL	4	0
7	G	906	PEG	2	0
10	G	913	P33	7	0
7	A	905	PEG	1	0
8	E	918	MGD	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.

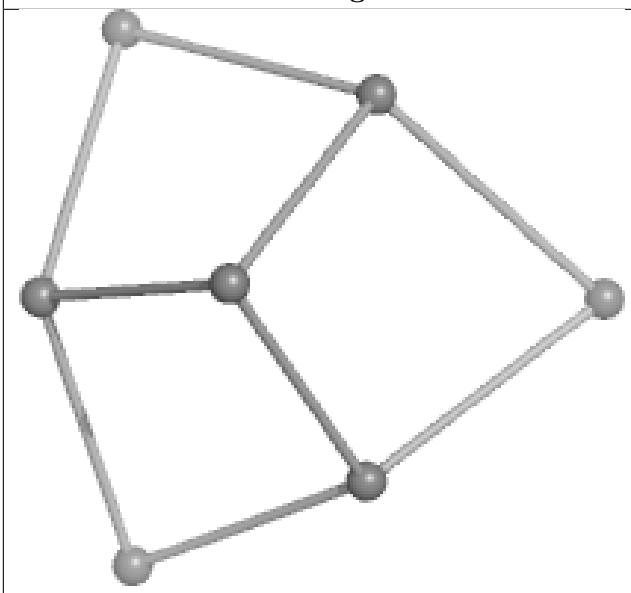
Ligand F3S E 902



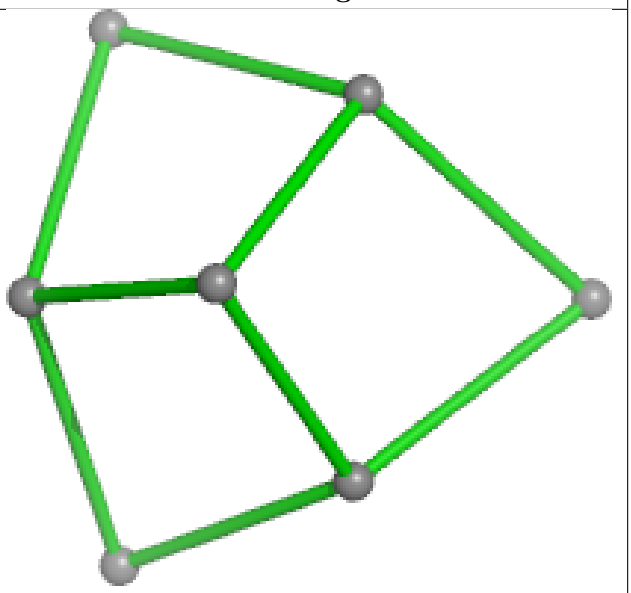
Bond lengths



Bond angles

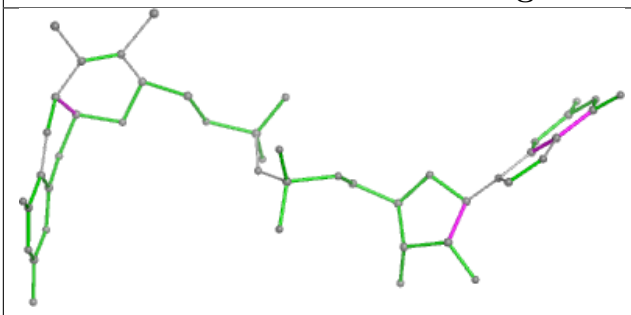


Torsions

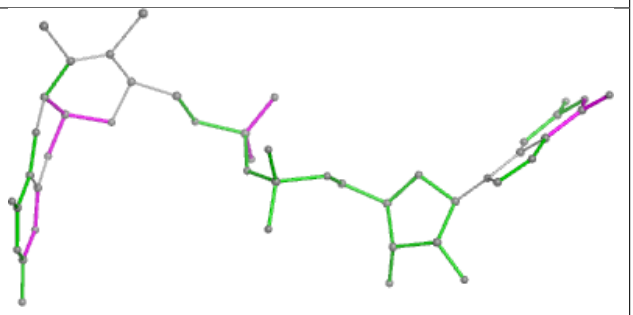


Rings

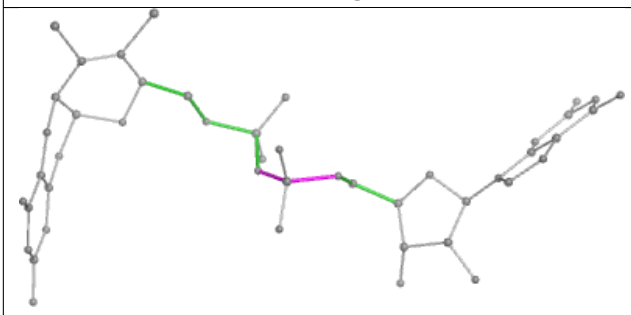
Ligand MGD C 908



Bond lengths



Bond angles



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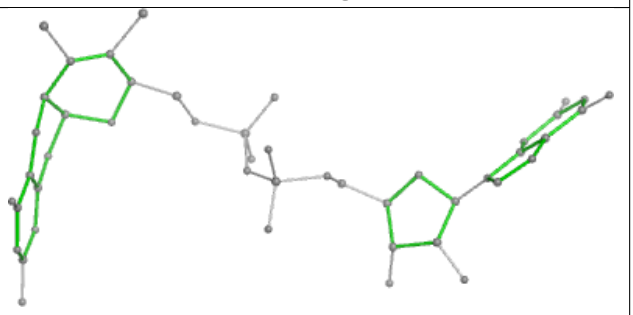
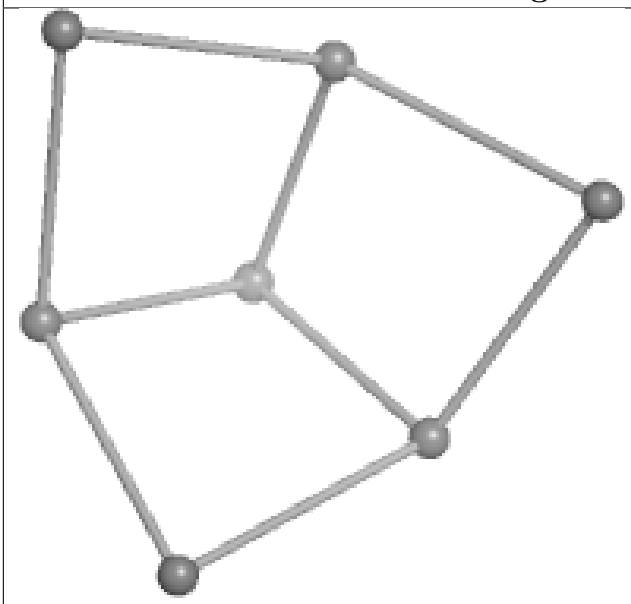
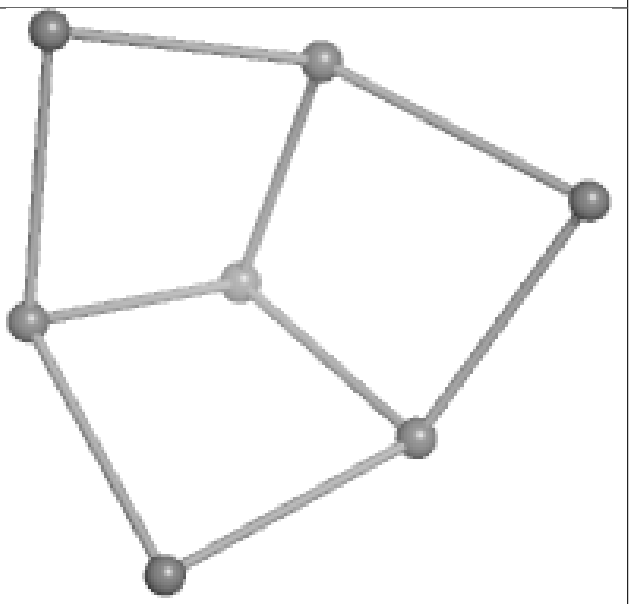


Rings

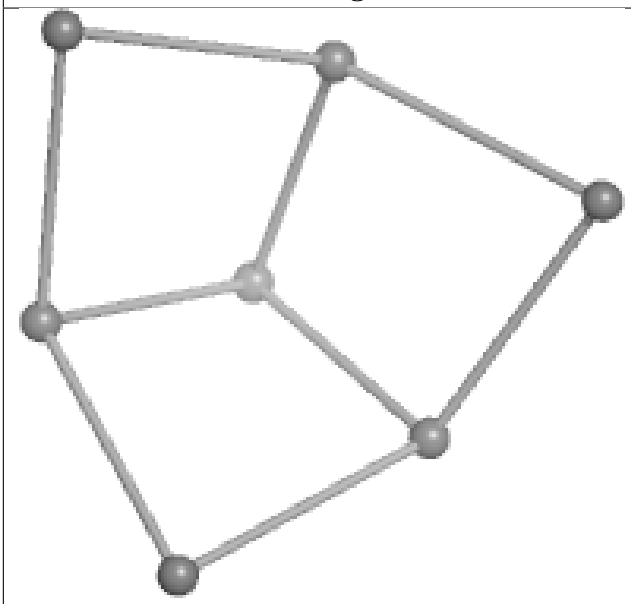
Ligand F3S A 903



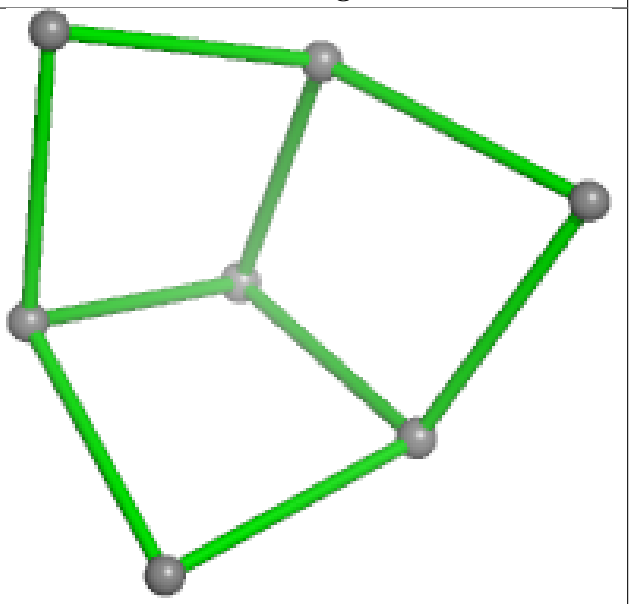
Bond lengths



Bond angles

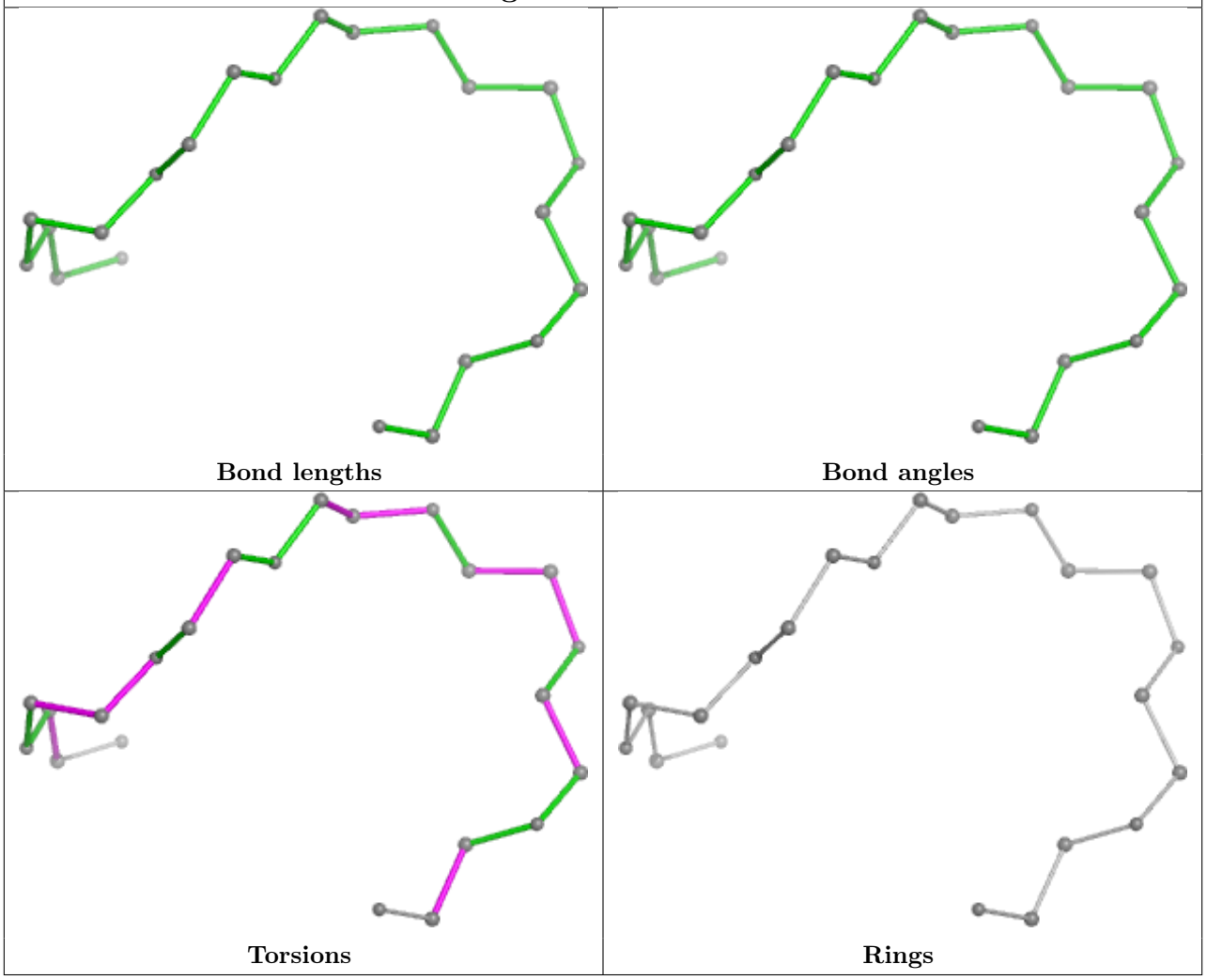


Torsions

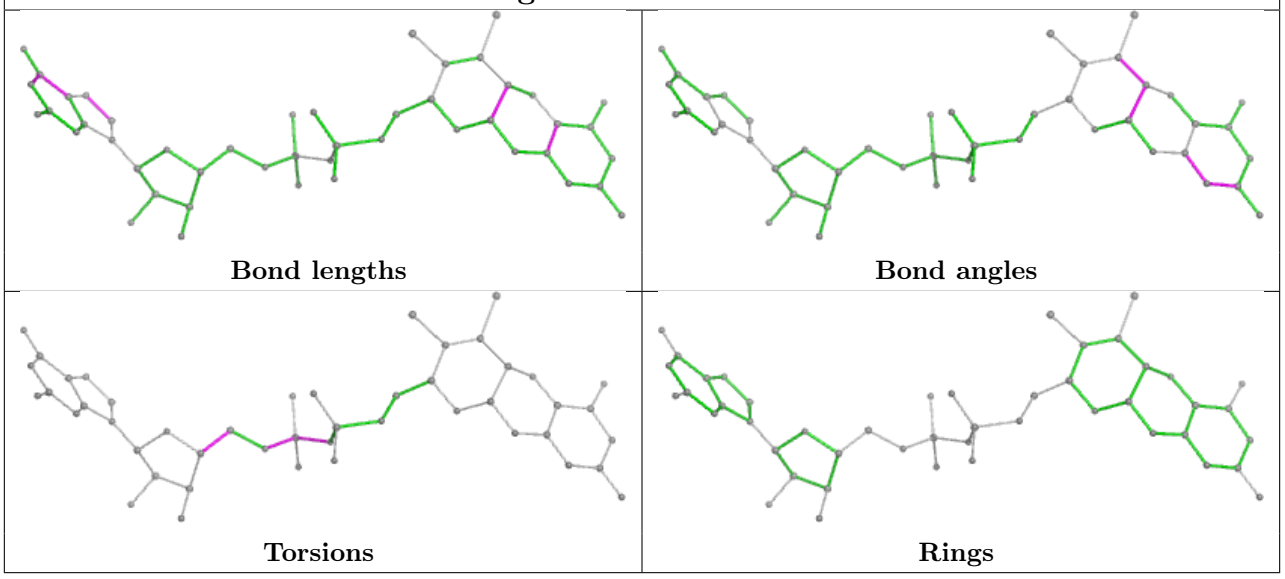


Rings

Ligand P33 E 920



Ligand MGD C 909



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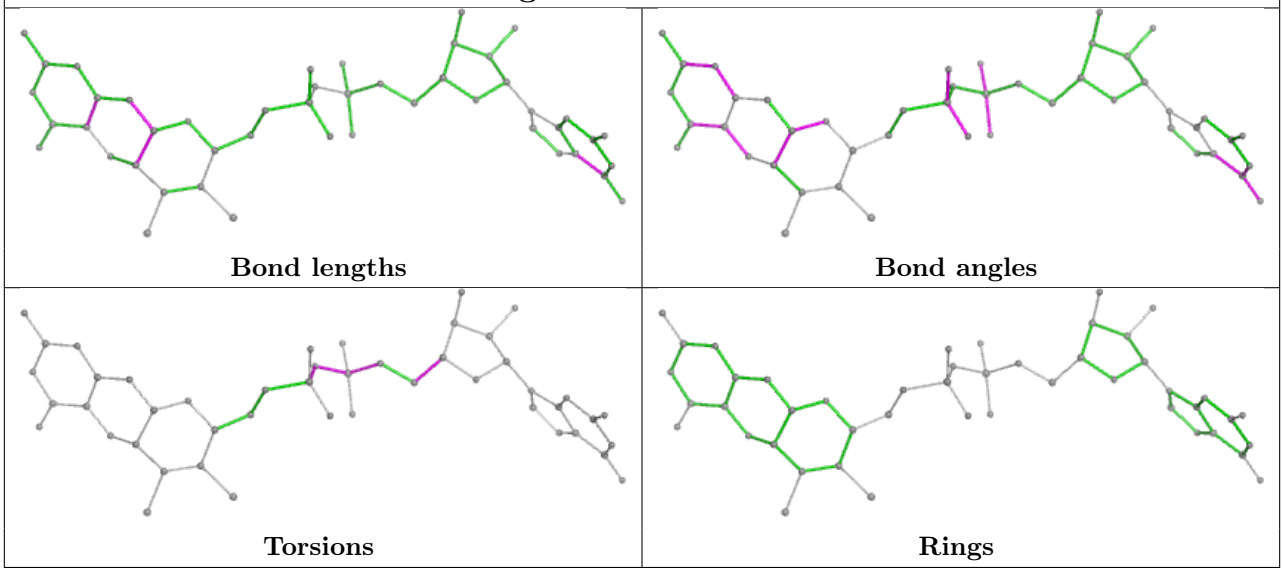
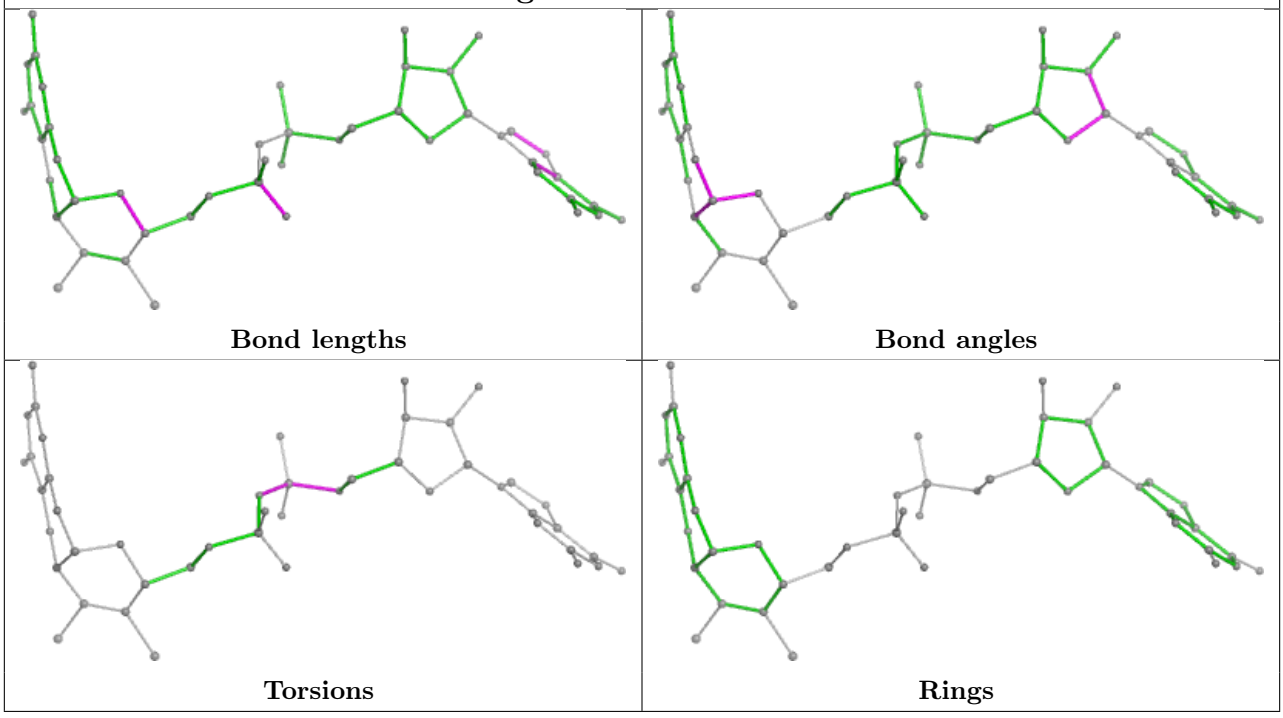
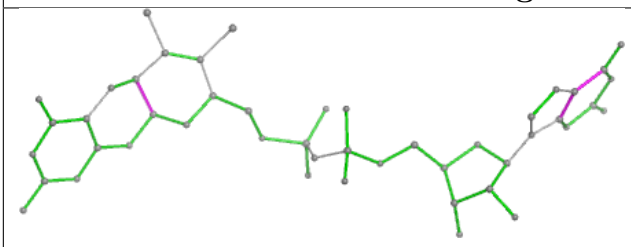


Ligand MGD G 912



Ligand MGD A 911



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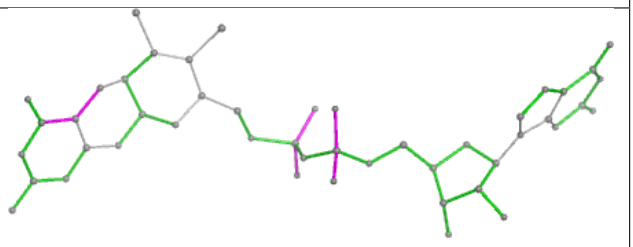

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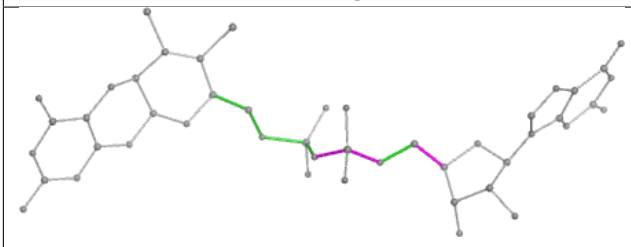
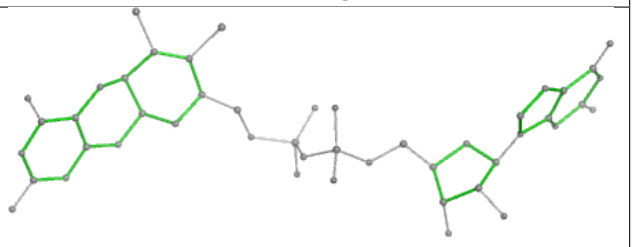
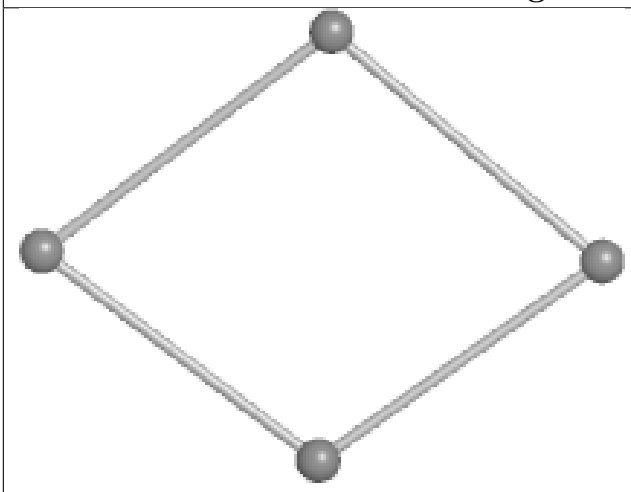


Torsions



Rings

Ligand FES D 201



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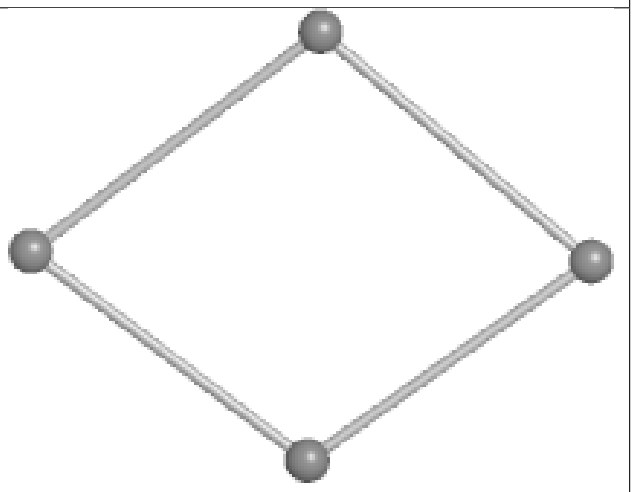
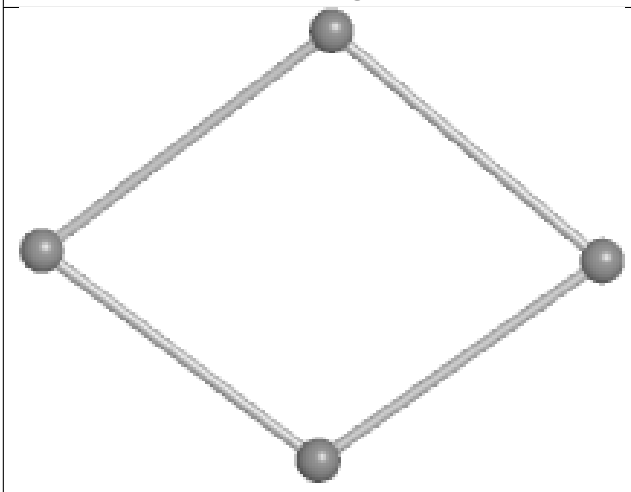


Bond angles



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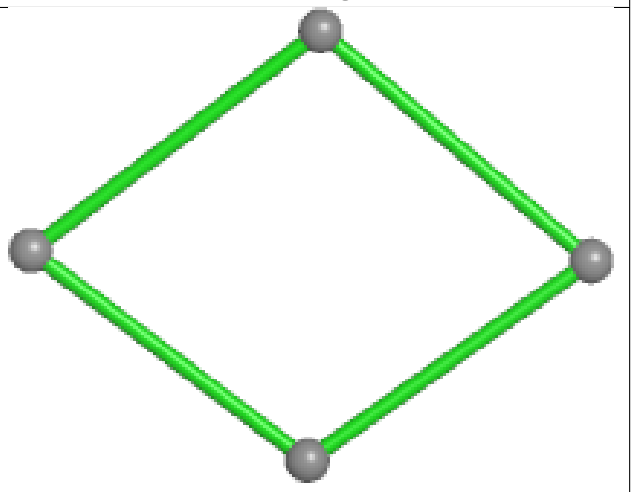
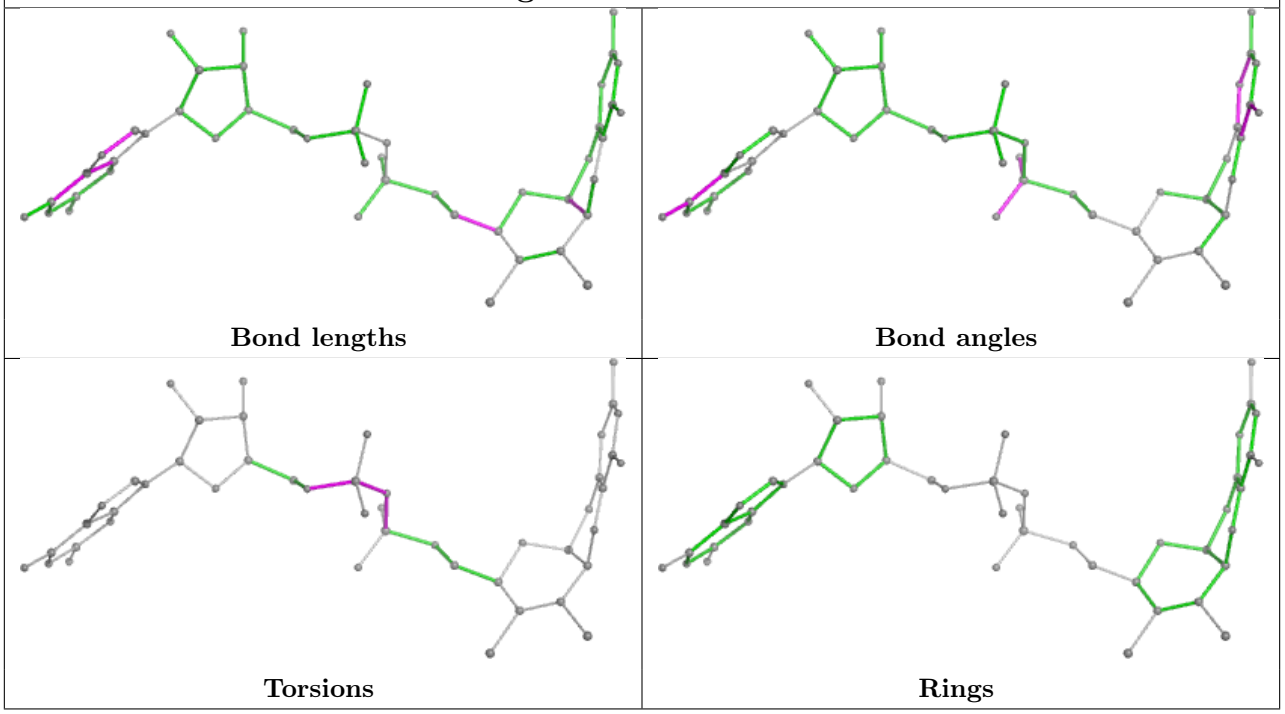
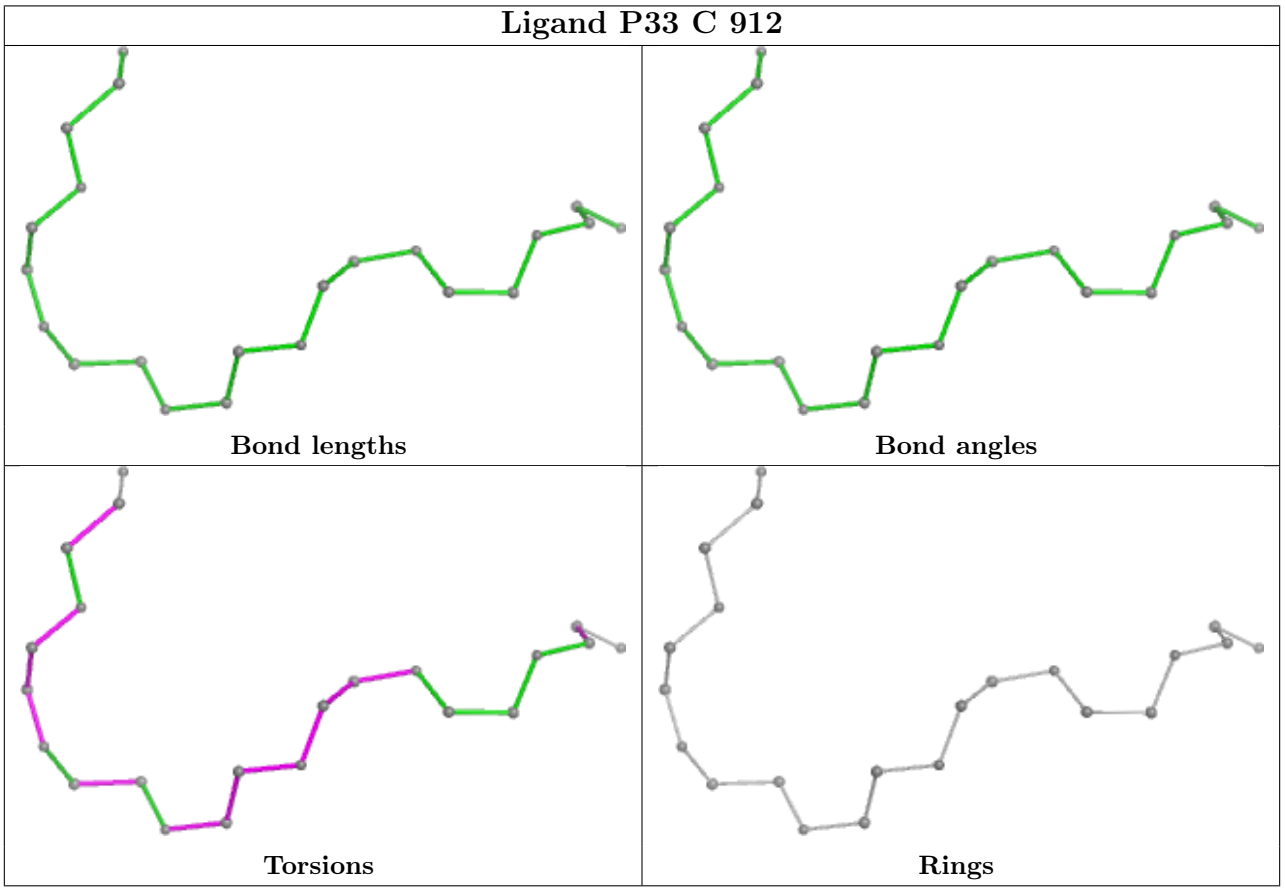


Rings

Ligand MGD A 912



Ligand P33 C 912



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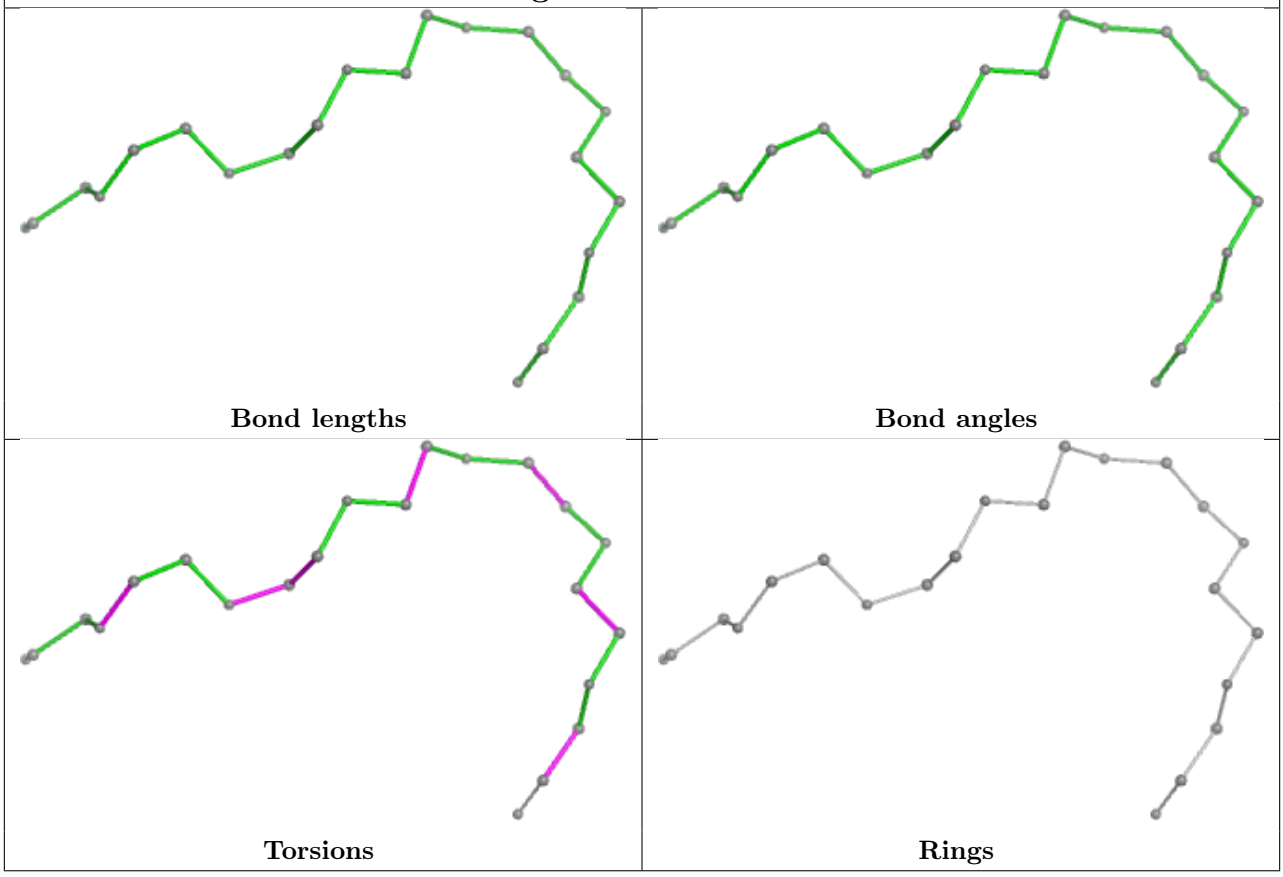
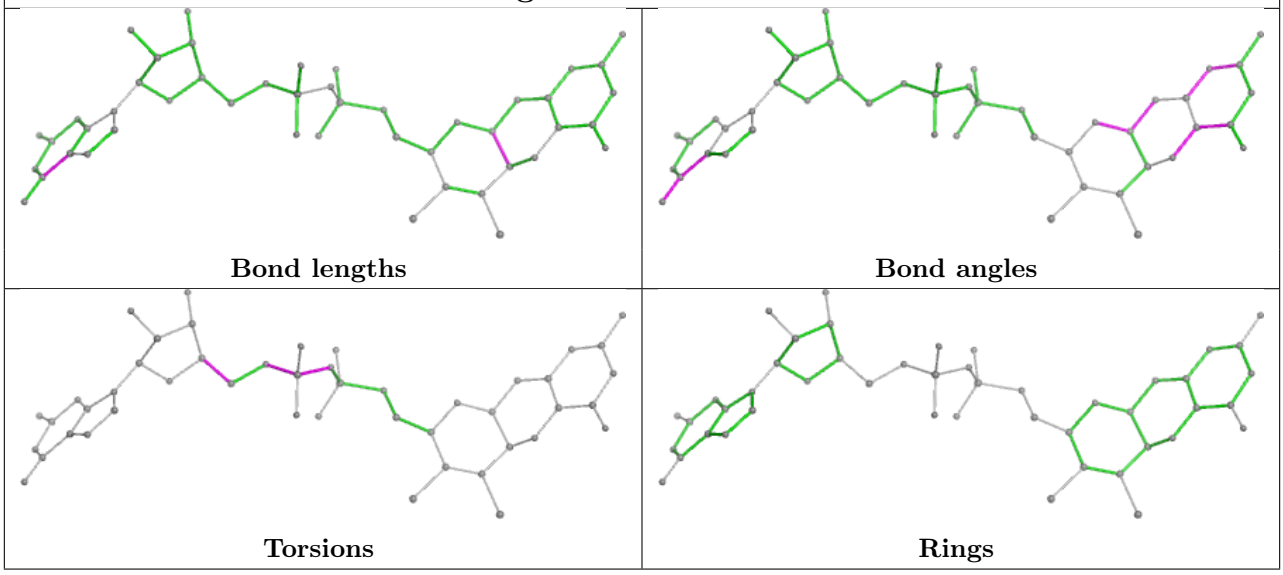
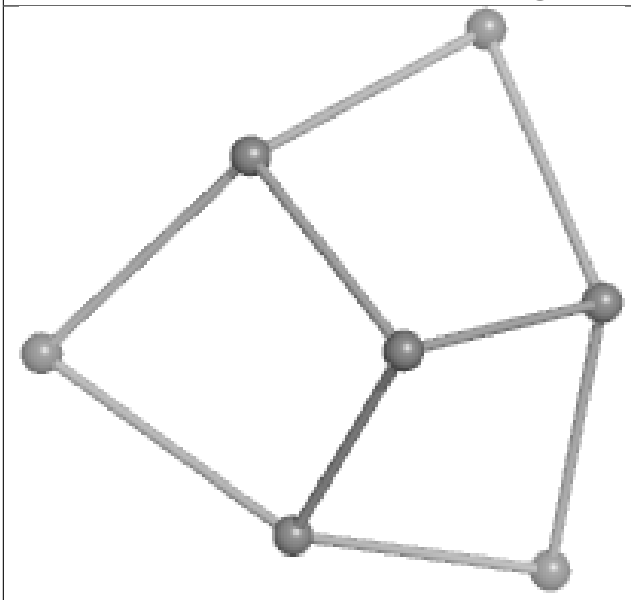


Ligand MGD G 911



Ligand F3S C 902



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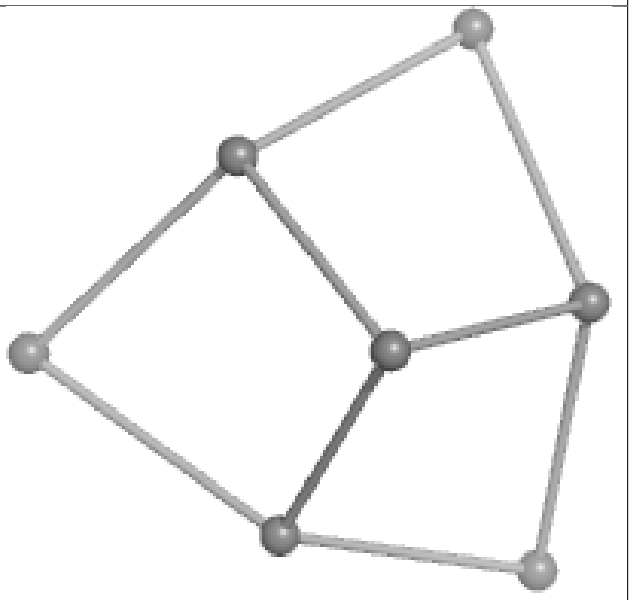
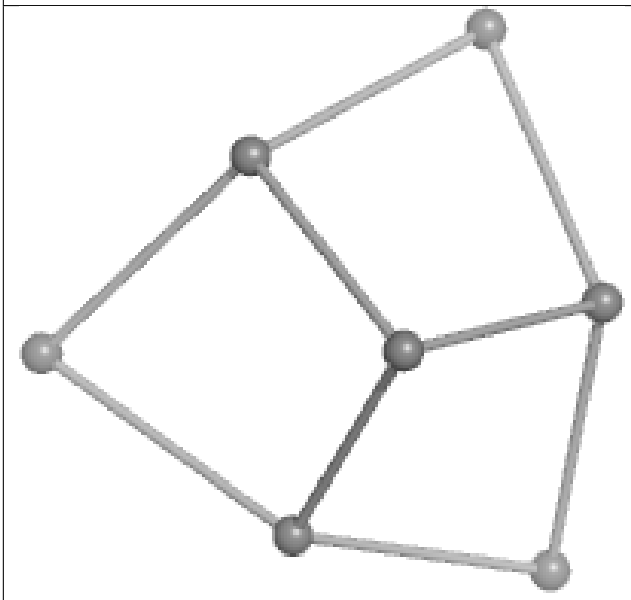
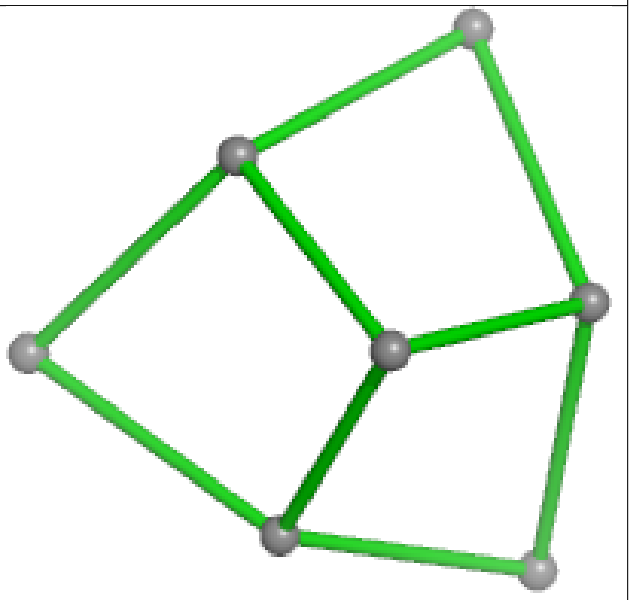


Bond angles



Torsions



Rings

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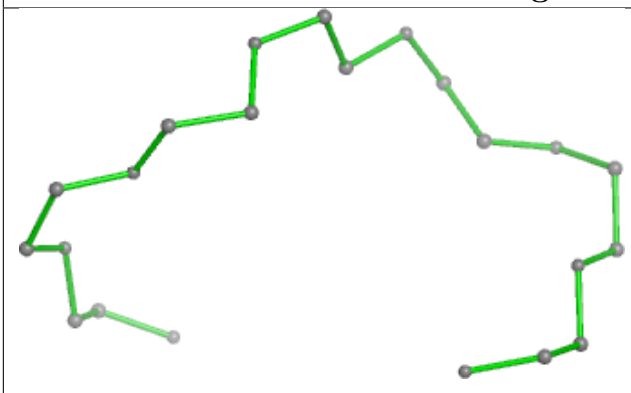

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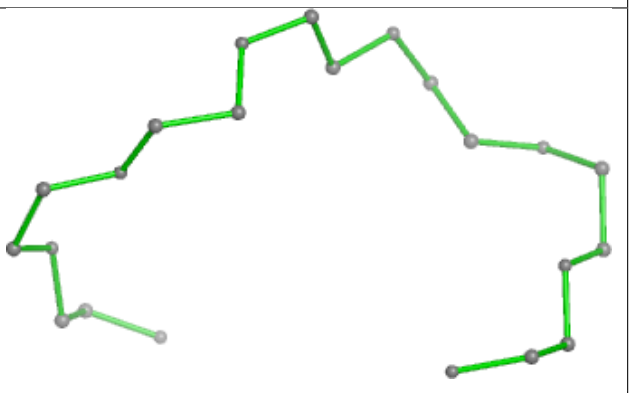
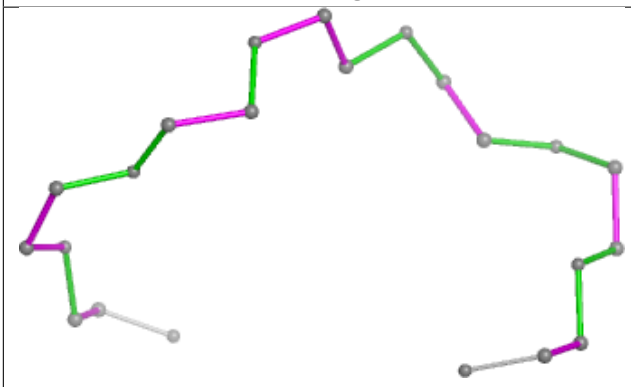


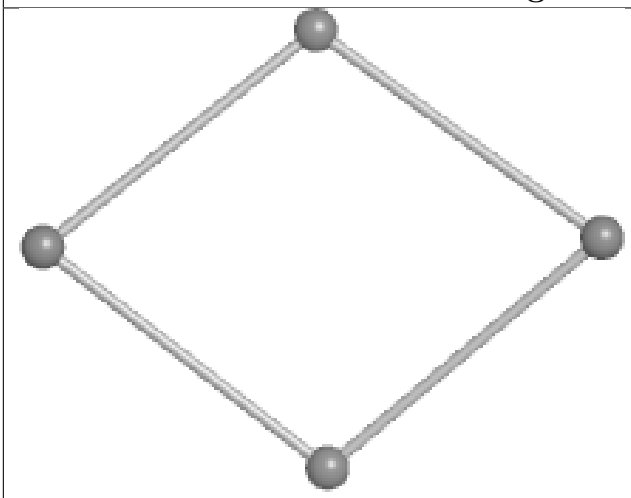
Bond angles



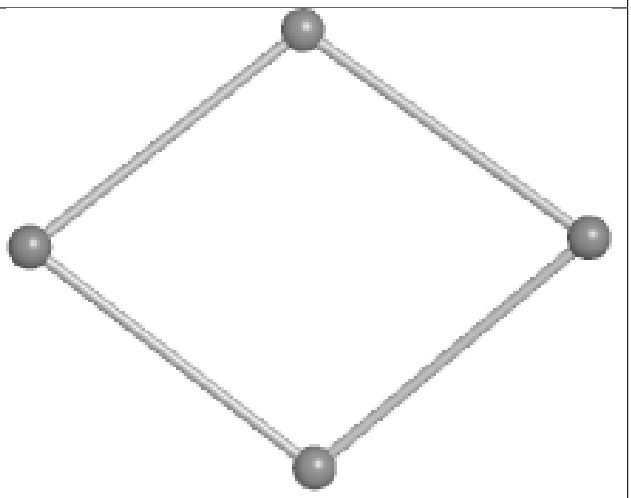
Torsions

Rings

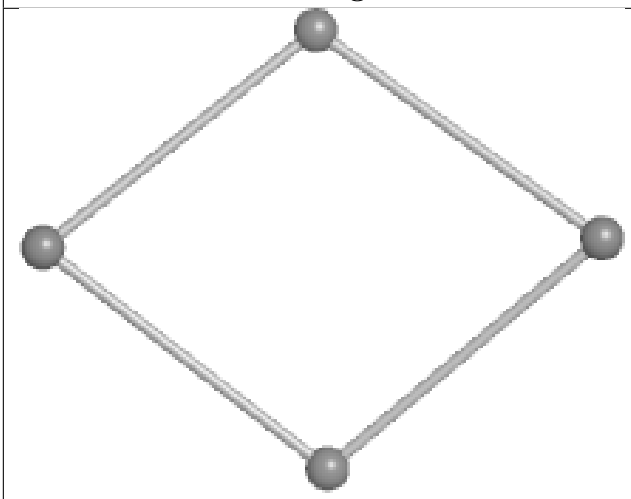
Ligand FES H 201



Bond lengths



Bond angles



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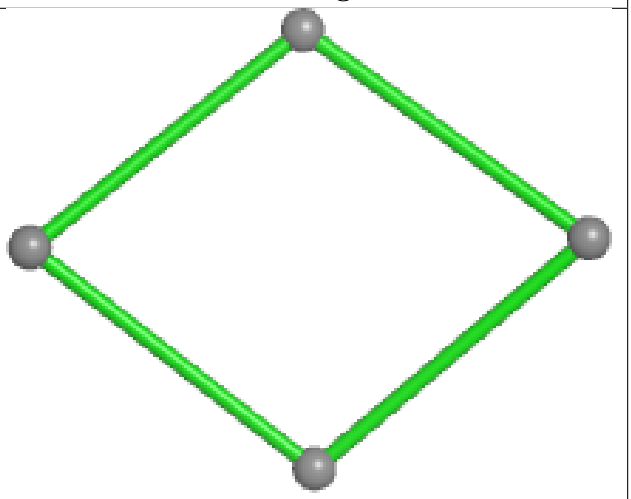
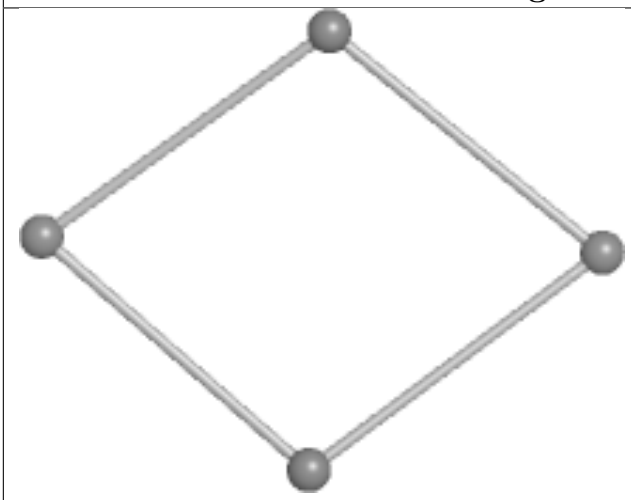
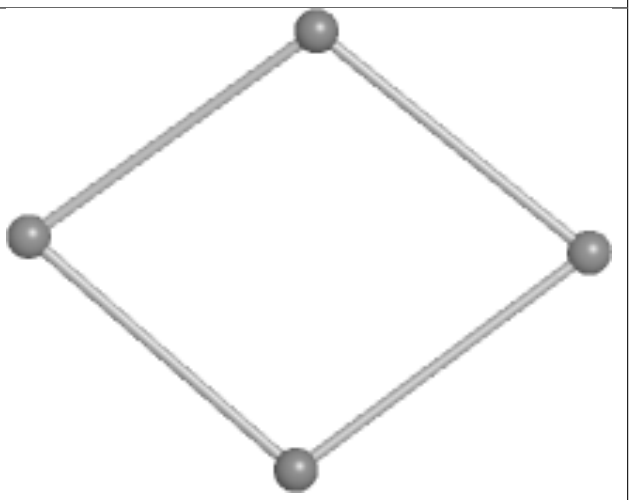


Rings

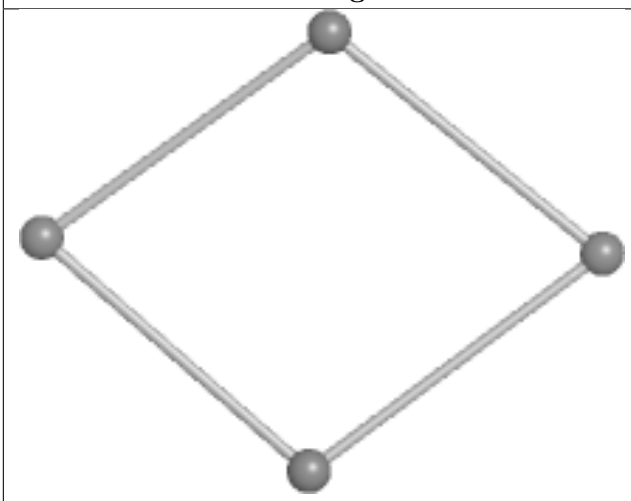
Ligand FES B 201



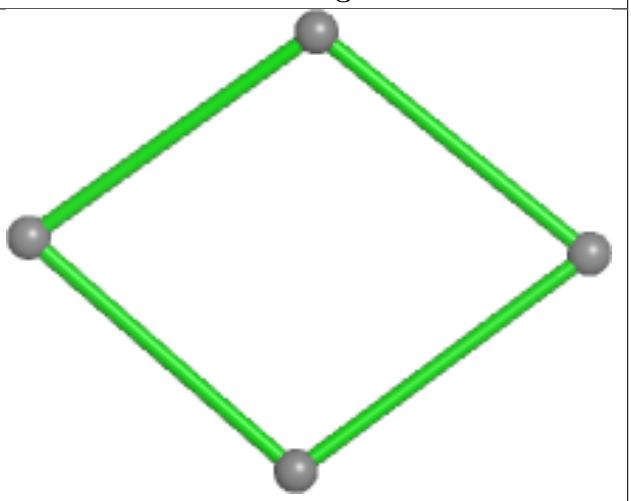
Bond lengths



Bond angles

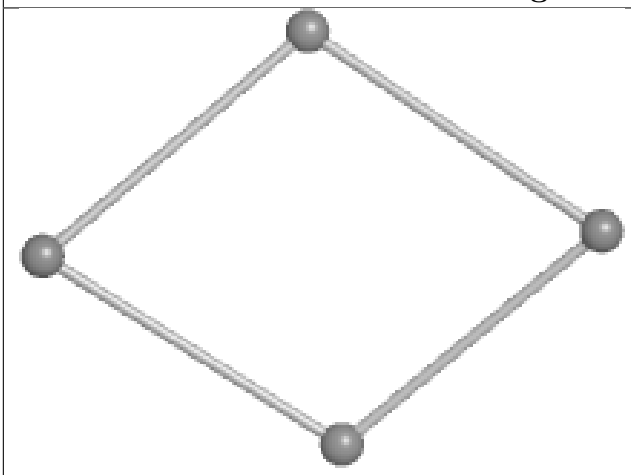


Torsions

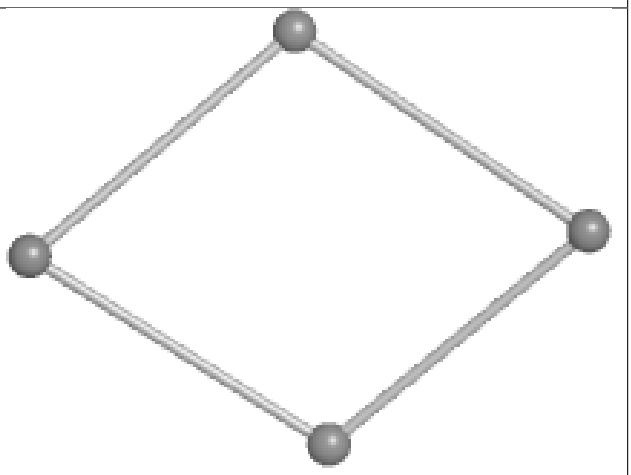


Rings

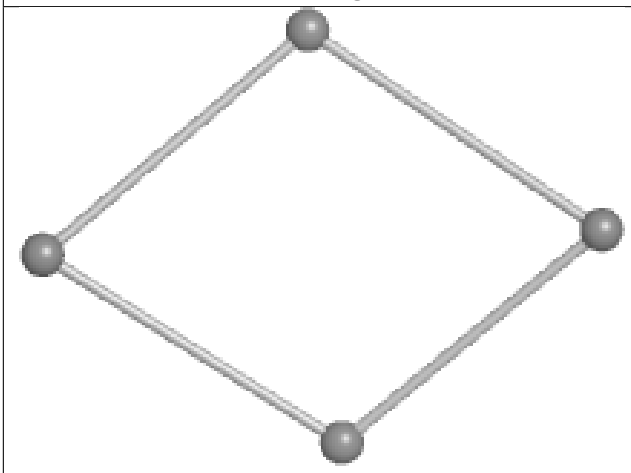
Ligand FES F 201



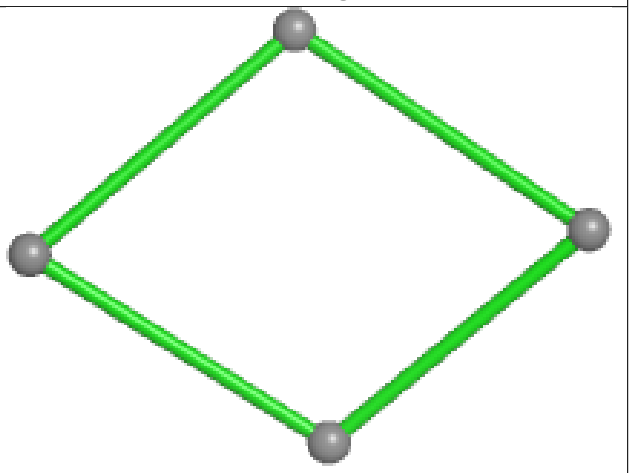
Bond lengths



Bond angles

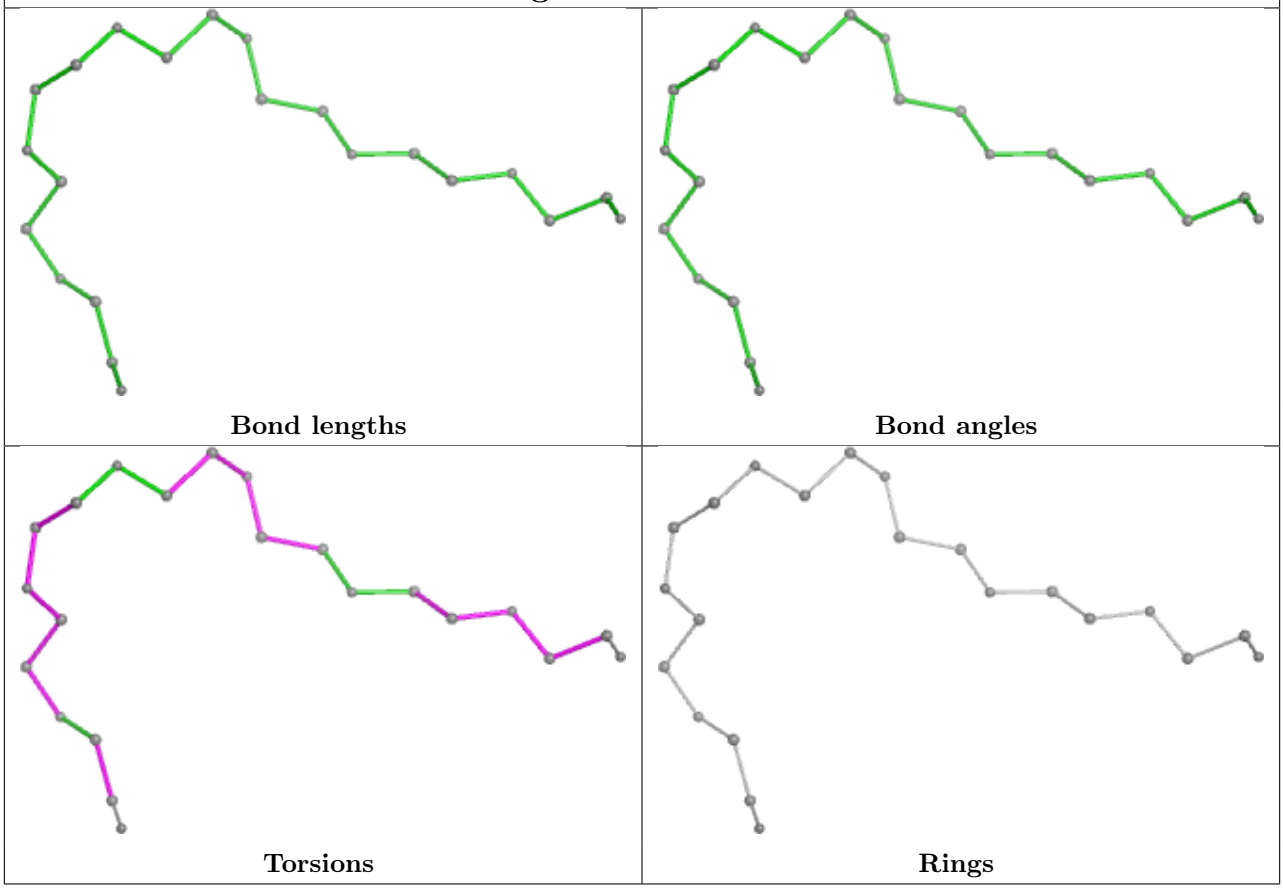


Torsions

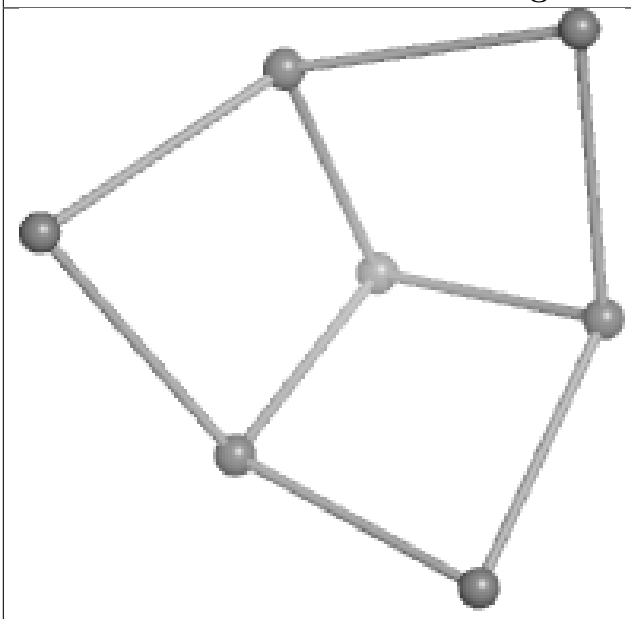


Rings

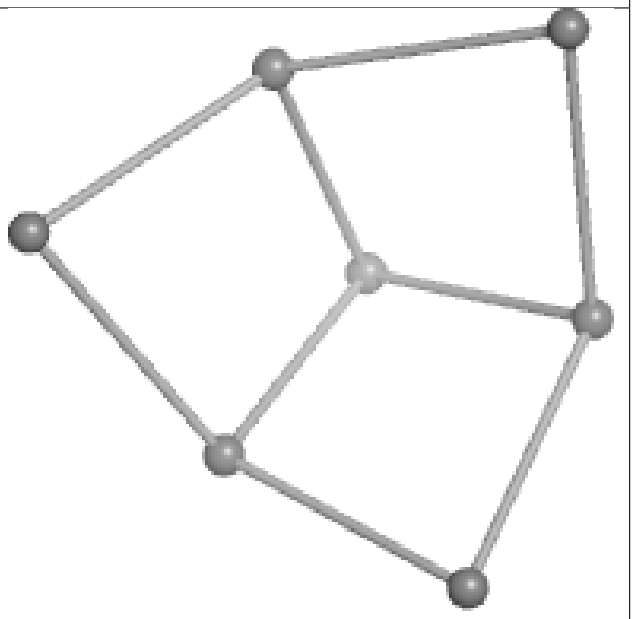
Ligand P33 G 913



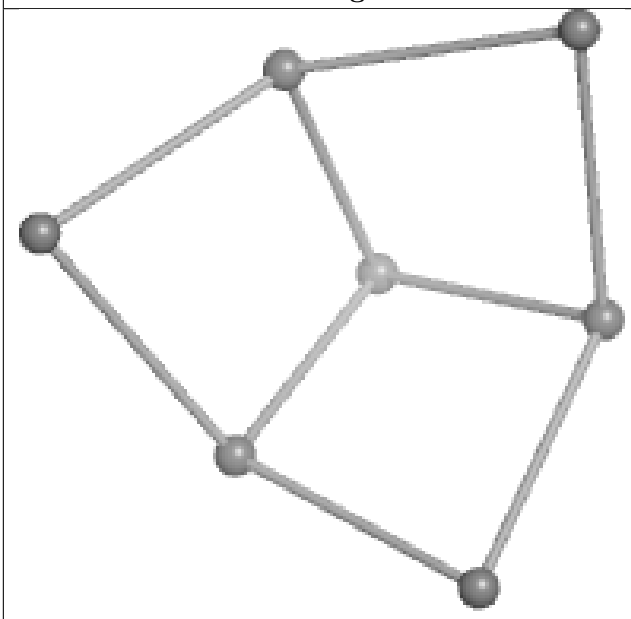
Ligand F3S G 902



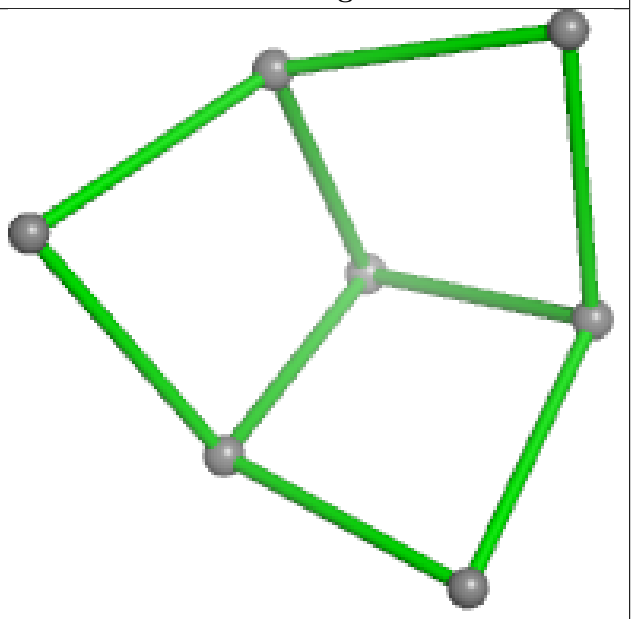
Bond lengths



Bond angles

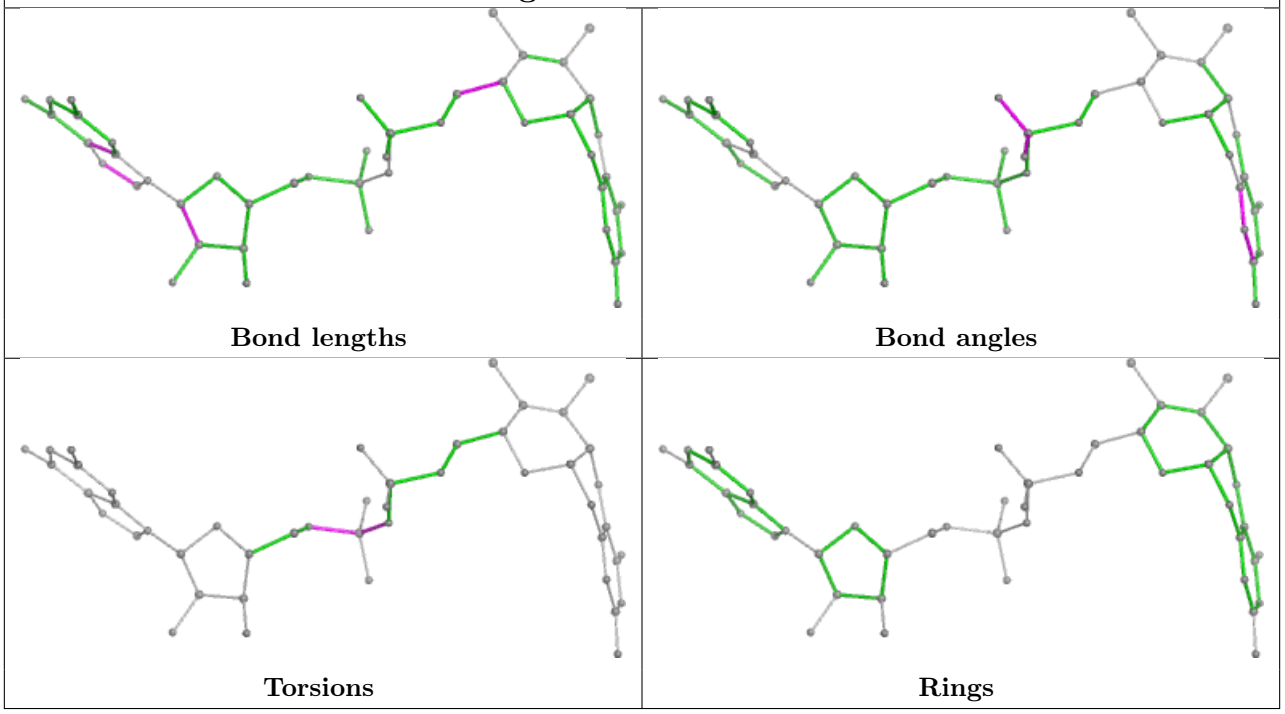


Torsions



Rings

Ligand MGD E 918



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	842/845 (99%)	-0.97	0	100	100	10, 23, 42, 67	13 (1%)
1	C	843/845 (99%)	-0.83	0	100	100	10, 26, 44, 73	14 (1%)
1	E	843/845 (99%)	-0.75	2 (0%)	92	92	10, 27, 47, 71	10 (1%)
1	G	843/845 (99%)	-0.96	2 (0%)	92	92	9, 24, 42, 73	15 (1%)
2	B	133/175 (76%)	-0.35	1 (0%)	82	84	18, 35, 53, 70	3 (2%)
2	D	133/175 (76%)	-0.38	1 (0%)	82	84	18, 35, 52, 61	2 (1%)
2	F	133/175 (76%)	0.06	1 (0%)	82	84	21, 40, 57, 68	2 (1%)
2	H	133/175 (76%)	-0.62	1 (0%)	82	84	15, 33, 50, 60	3 (2%)
All	All	3903/4080 (95%)	-0.80	8 (0%)	92	92	9, 26, 48, 73	62 (1%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	ALA	4.2
2	B	43	ALA	3.5
2	F	43	ALA	3.1
2	H	43	ALA	2.8
1	E	401	GLY	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (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
7	PEG	G	904	7/7	0.76	0.17	66,76,78,86	0
6	EDO	A	907	4/4	0.80	0.20	42,52,55,58	0
6	EDO	E	912	4/4	0.81	0.15	58,62,66,66	0
6	EDO	G	903	4/4	0.83	0.20	60,63,65,70	0
10	P33	A	914	22/22	0.83	0.18	47,56,66,72	0
6	EDO	G	907	4/4	0.84	0.16	47,64,65,72	0
7	PEG	E	916	7/7	0.85	0.16	49,56,64,66	0
6	EDO	E	903	4/4	0.85	0.13	42,49,49,52	0
3	SER	A	901	6/7	0.85	0.12	37,46,50,56	0
6	EDO	E	910	4/4	0.86	0.16	47,65,65,65	0
6	EDO	E	906	4/4	0.86	0.19	46,47,52,55	0
6	EDO	G	910	4/4	0.86	0.16	46,53,56,60	0
7	PEG	E	915	7/7	0.87	0.15	57,64,67,70	0
6	EDO	G	905	4/4	0.87	0.15	39,48,51,54	0
14	1PE	E	917	16/16	0.87	0.14	41,56,64,73	0
6	EDO	A	908[A]	4/4	0.88	0.13	26,28,30,31	8
6	EDO	A	908[B]	4/4	0.88	0.13	35,40,45,47	8
7	PEG	G	906	7/7	0.88	0.16	53,63,71,76	0
7	PEG	E	905	7/7	0.88	0.12	54,60,67,68	0
10	P33	C	912	22/22	0.88	0.16	40,53,76,80	0
11	GOL	A	916	6/6	0.88	0.14	47,59,63,70	0
6	EDO	C	904	4/4	0.88	0.14	40,47,52,71	0
6	EDO	C	907	4/4	0.89	0.13	48,50,53,62	0
6	EDO	A	909	4/4	0.89	0.14	56,58,60,60	0
6	EDO	E	913	4/4	0.89	0.14	52,59,60,64	0
6	EDO	A	904	4/4	0.89	0.14	40,51,53,56	0
6	EDO	G	909	4/4	0.90	0.13	54,60,64,64	0
6	EDO	G	908	4/4	0.90	0.14	35,44,55,71	0
7	PEG	A	905	7/7	0.90	0.12	25,47,64,66	0
6	EDO	A	906	4/4	0.91	0.13	49,51,52,52	0
7	PEG	E	908	7/7	0.91	0.11	49,59,65,69	0
6	EDO	E	914	4/4	0.91	0.13	37,42,45,47	0
10	P33	G	913	22/22	0.91	0.13	33,50,61,77	0
11	GOL	A	915	6/6	0.91	0.12	29,41,48,67	0
6	EDO	C	903	4/4	0.91	0.11	44,48,49,56	0
7	PEG	C	905	7/7	0.91	0.13	51,58,62,71	0
6	EDO	C	906	4/4	0.92	0.11	45,53,55,61	0

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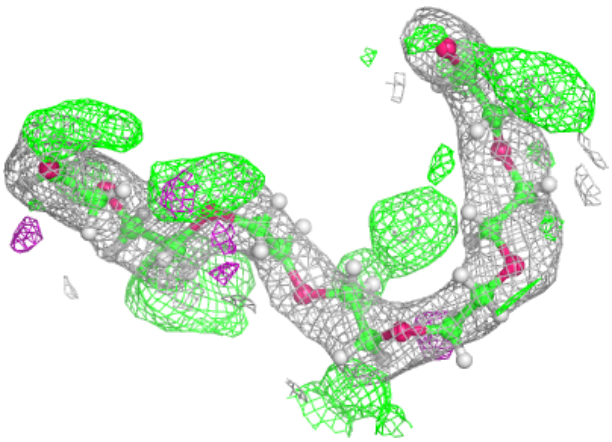
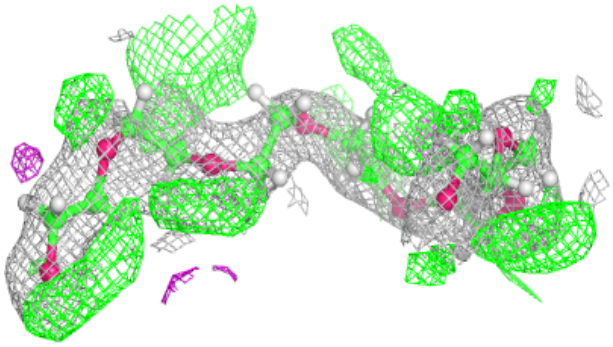
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	E	909	7/7	0.92	0.11	42,50,54,62	0
7	PEG	A	910	7/7	0.92	0.11	56,62,66,66	0
6	EDO	E	907	4/4	0.92	0.12	50,57,58,58	0
7	PEG	E	904	7/7	0.92	0.12	31,41,55,57	0
11	GOL	G	914	6/6	0.92	0.13	31,44,55,57	0
6	EDO	H	202	4/4	0.92	0.12	45,57,61,62	0
10	P33	E	920	22/22	0.93	0.11	34,45,60,64	0
11	GOL	E	921	6/6	0.93	0.10	36,47,51,55	0
6	EDO	E	911	4/4	0.94	0.10	30,45,50,52	0
10	P33	C	911	22/22	0.94	0.10	38,46,56,61	0
9	SO4	C	910	5/5	0.97	0.08	25,27,37,40	0
12	O	E	922	1/1	0.98	0.07	34,34,34,34	0
9	SO4	A	913	5/5	0.98	0.06	25,30,41,46	0
8	MGD	C	909	47/47	0.99	0.03	18,22,26,28	0
8	MGD	E	918	47/47	0.99	0.03	19,23,27,29	0
8	MGD	E	919	47/47	0.99	0.03	17,22,27,32	0
8	MGD	G	911	47/47	0.99	0.03	17,21,25,28	0
8	MGD	G	912	47/47	0.99	0.03	18,20,23,25	0
5	F3S	E	902	7/7	0.99	0.02	25,26,27,27	0
8	MGD	A	911	47/47	0.99	0.03	16,19,25,28	0
12	O	A	917	1/1	0.99	0.05	28,28,28,28	0
12	O	C	913	1/1	0.99	0.06	25,25,25,25	0
8	MGD	A	912	47/47	0.99	0.03	14,18,22,23	0
12	O	G	915	1/1	0.99	0.08	32,32,32,32	0
13	FES	B	201	4/4	0.99	0.04	35,36,37,38	0
13	FES	D	201	4/4	0.99	0.05	37,39,39,39	0
13	FES	F	201	4/4	0.99	0.05	40,41,42,45	0
13	FES	H	201	4/4	0.99	0.05	34,34,36,36	0
8	MGD	C	908	47/47	0.99	0.04	19,23,26,27	0
4	4MO	E	901	1/1	1.00	0.02	26,26,26,26	0
4	4MO	G	901	1/1	1.00	0.01	23,23,23,23	0
5	F3S	A	903	7/7	1.00	0.02	22,23,24,25	0
5	F3S	C	902	7/7	1.00	0.02	23,26,26,27	0
4	4MO	A	902	1/1	1.00	0.01	22,22,22,22	0
5	F3S	G	902	7/7	1.00	0.02	23,23,24,26	0
4	4MO	C	901	1/1	1.00	0.02	24,24,24,24	0

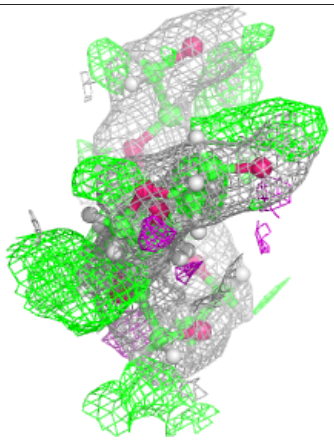
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P33 A 914:

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

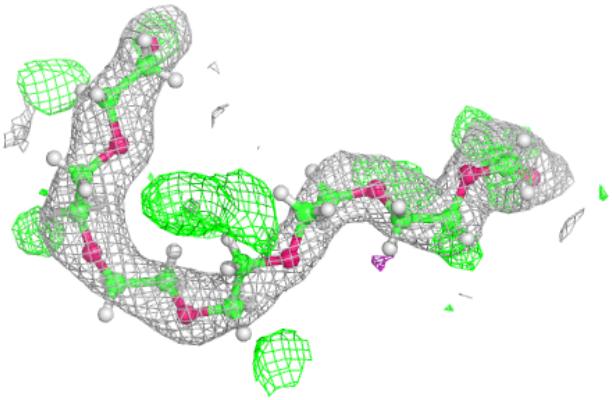


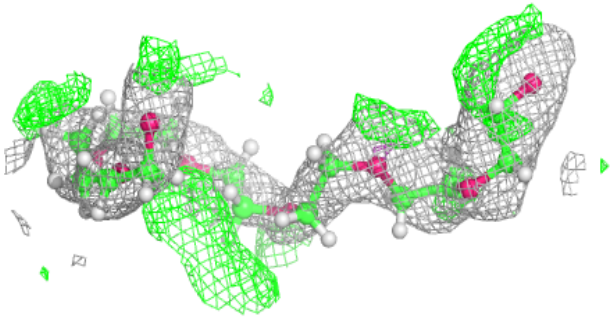


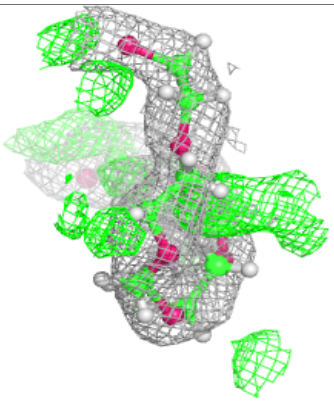


Electron density around P33 C 912:

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

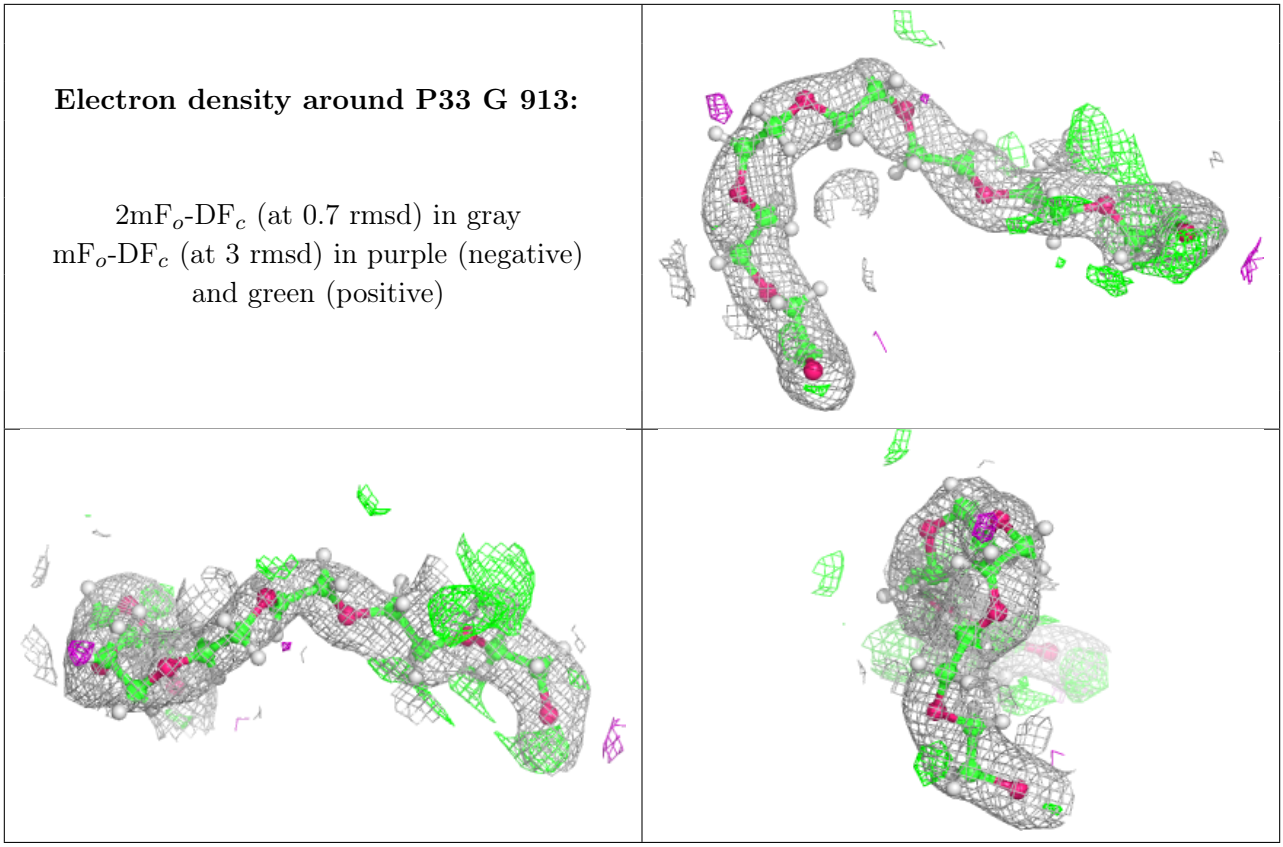






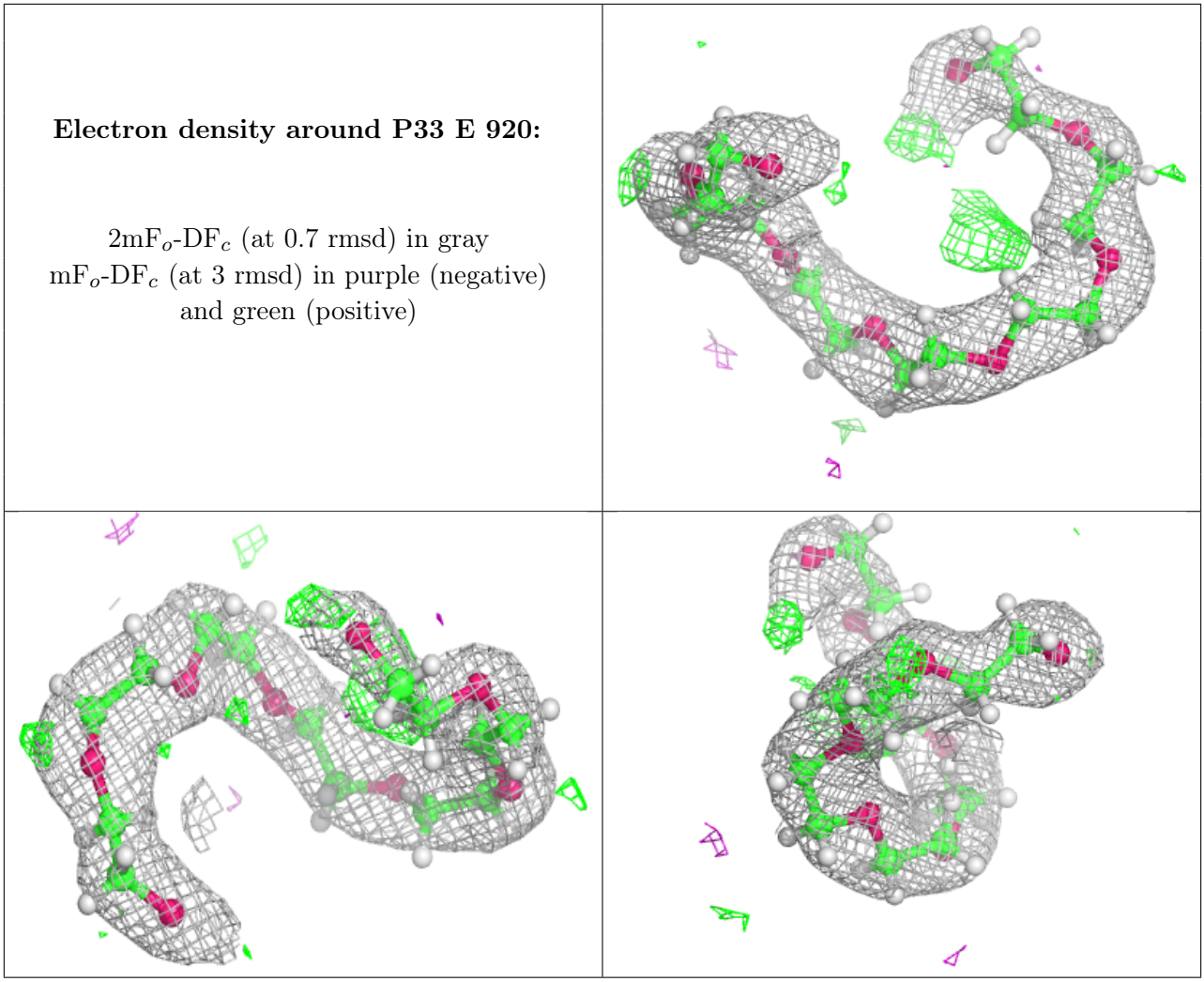
Electron density around P33 G 913:

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



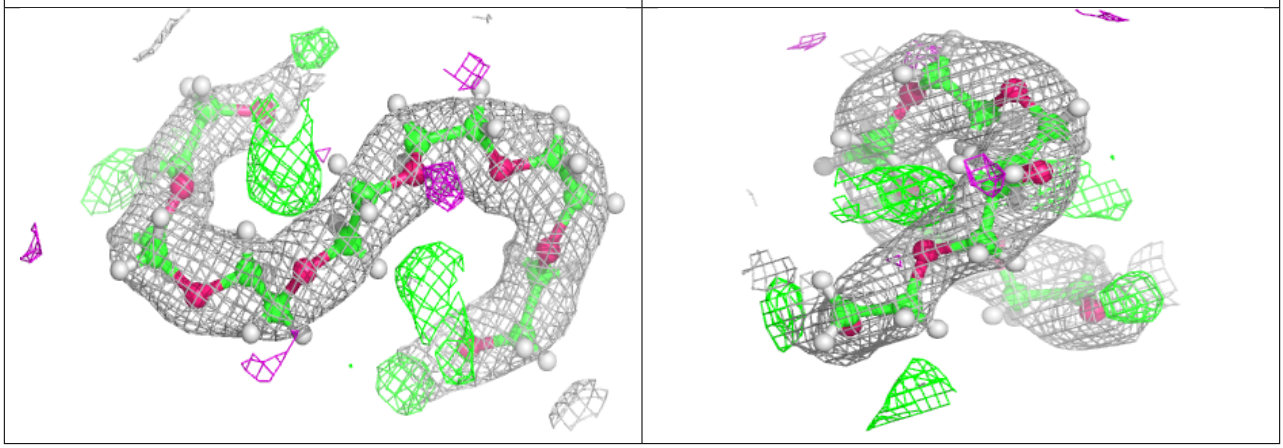
Electron density around P33 E 920:

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



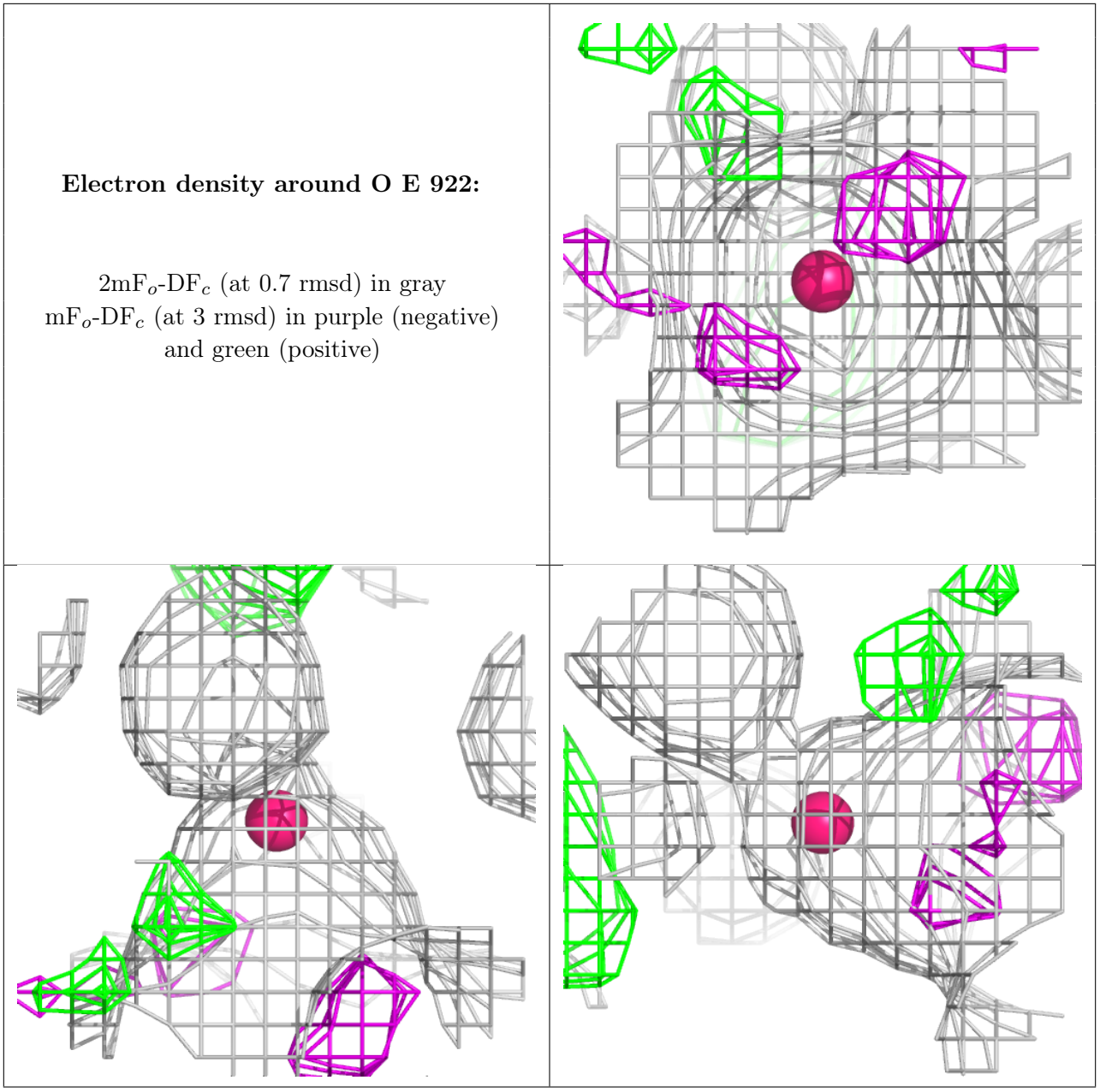
Electron density around P33 C 911:

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



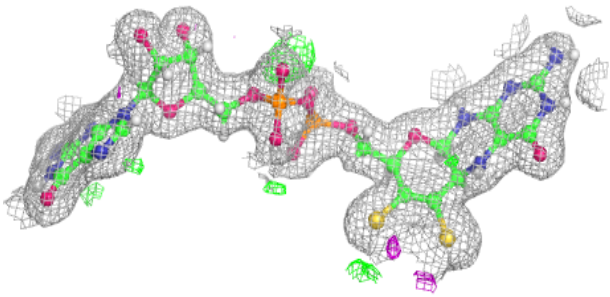
Electron density around O E 922:

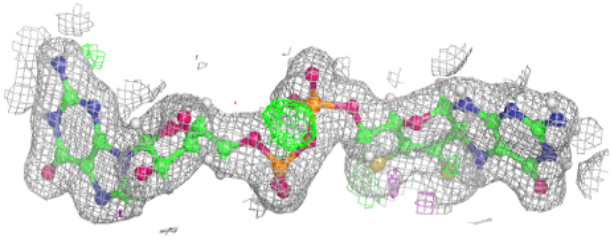
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

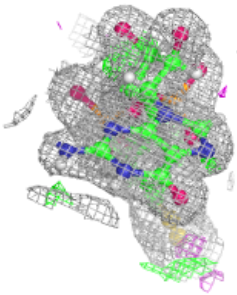


Electron density around MGD C 909:

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

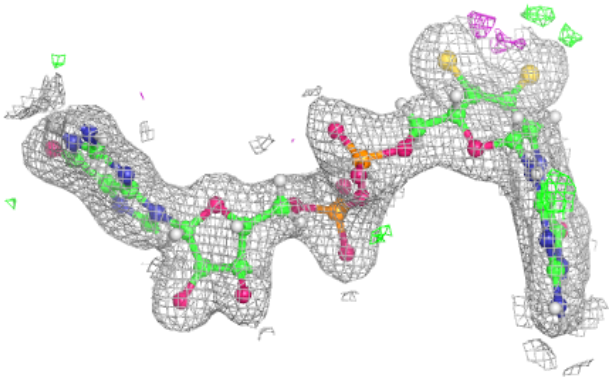


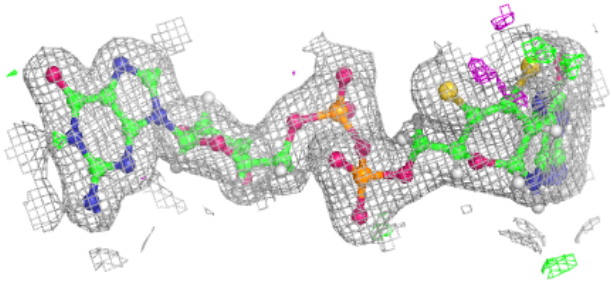


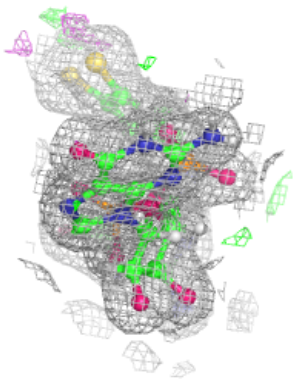


Electron density around MGD E 918:

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

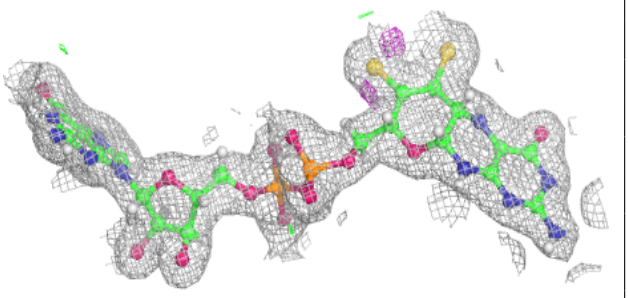


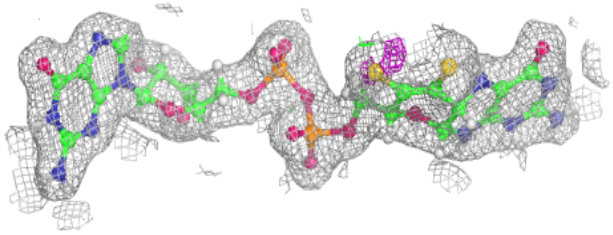


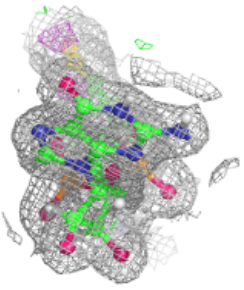


Electron density around MGD E 919:

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

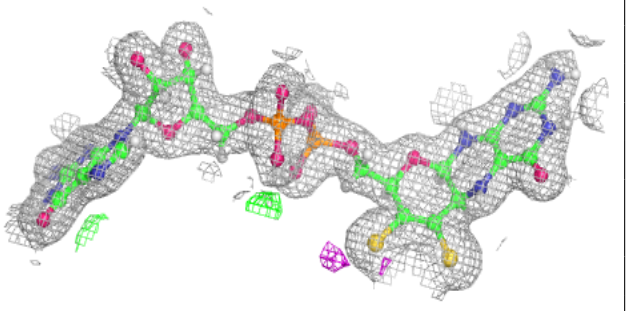


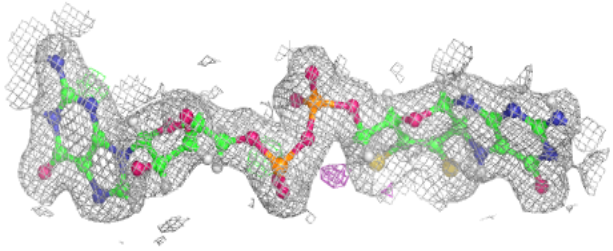


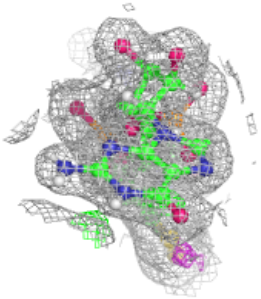


Electron density around MGD G 911:

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

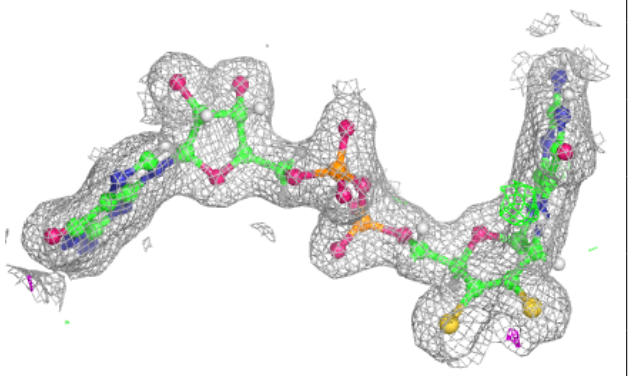


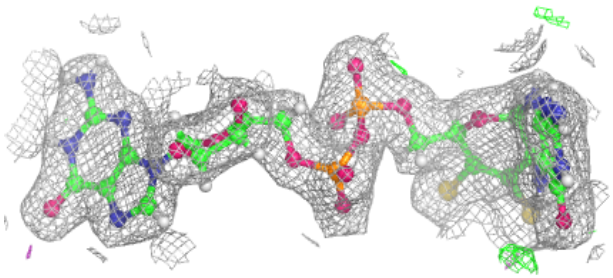


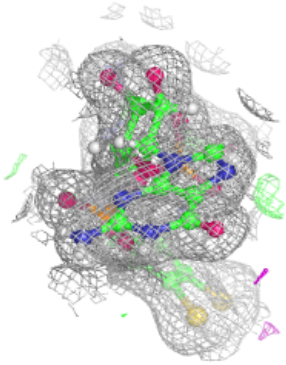


Electron density around MGD G 912:

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

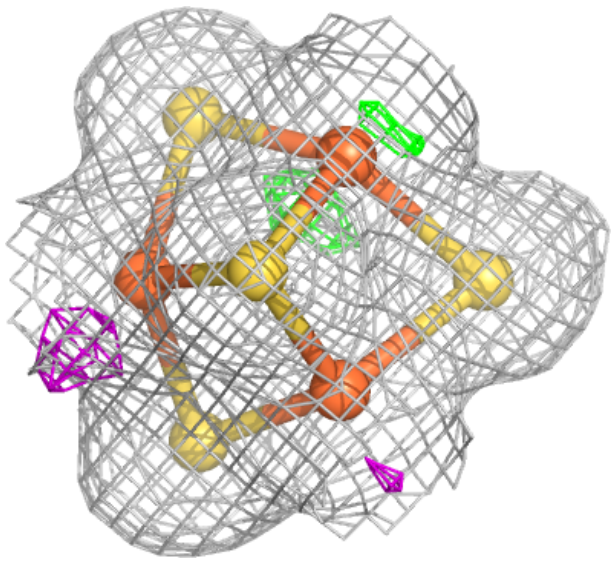


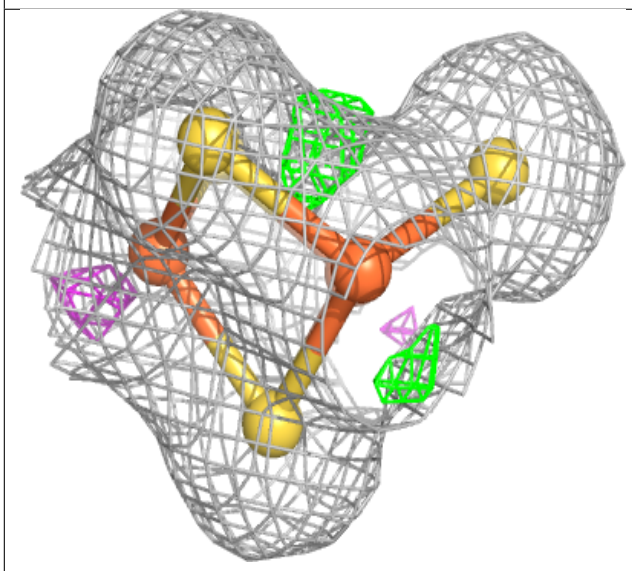


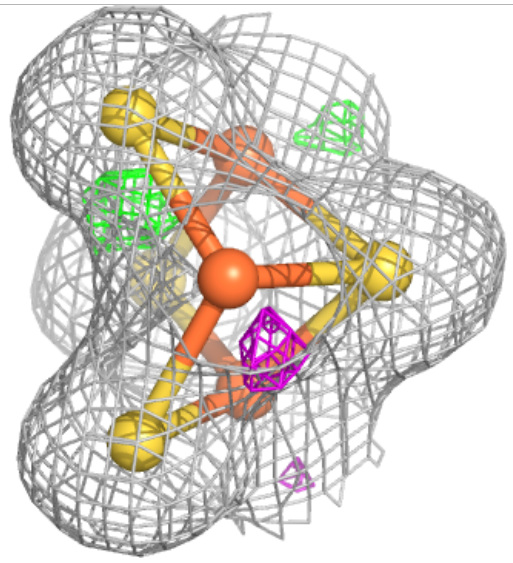


Electron density around F3S E 902:

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

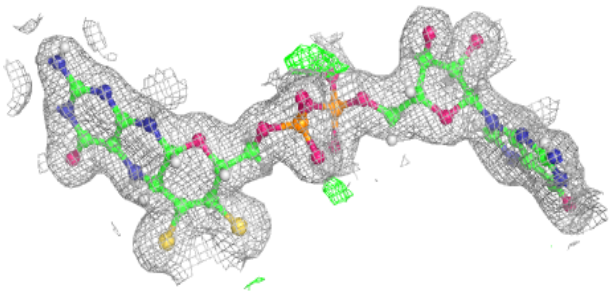


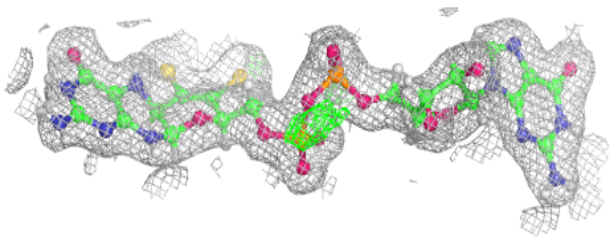


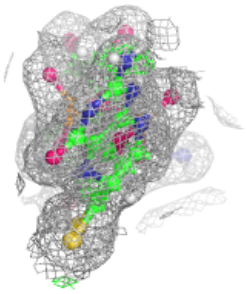


Electron density around MGD A 911:

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

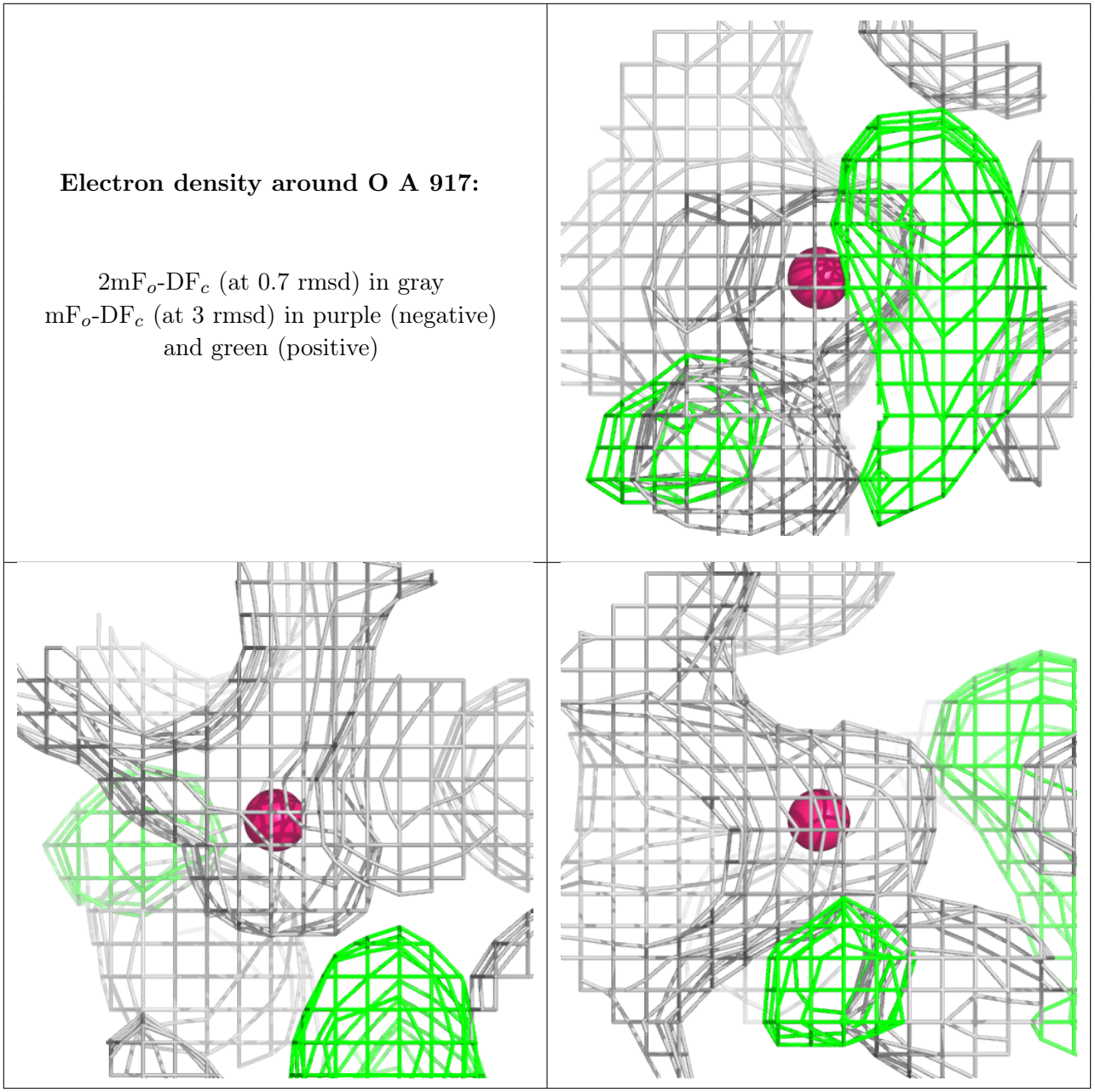






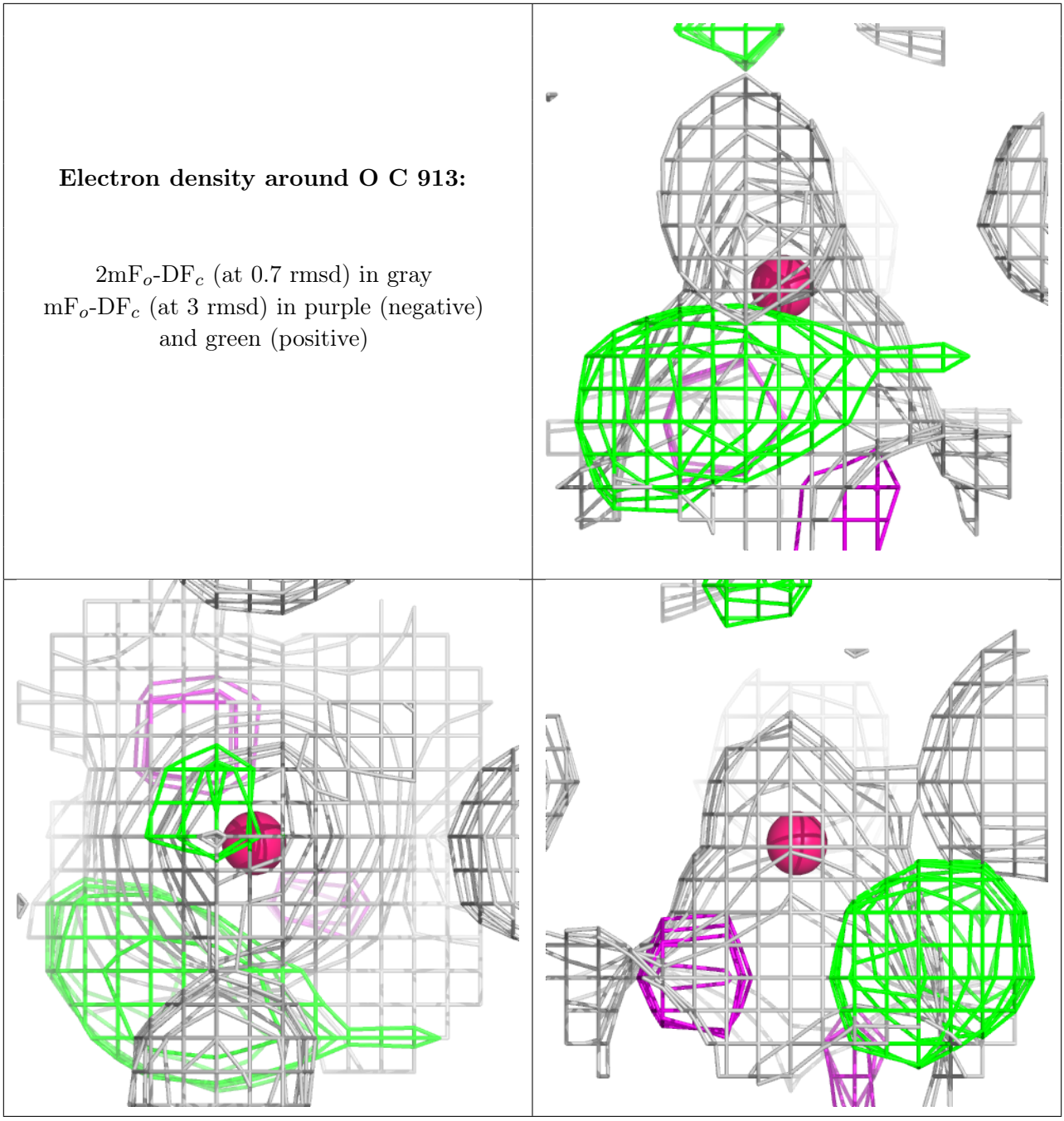
Electron density around O A 917:

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



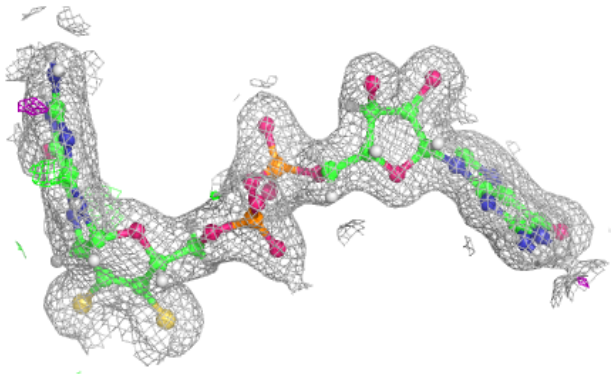
Electron density around O C 913:

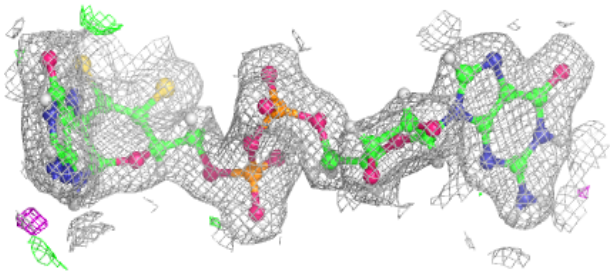
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

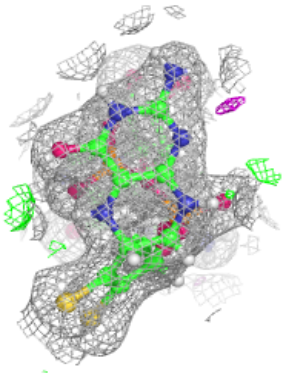


Electron density around MGD A 912:

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

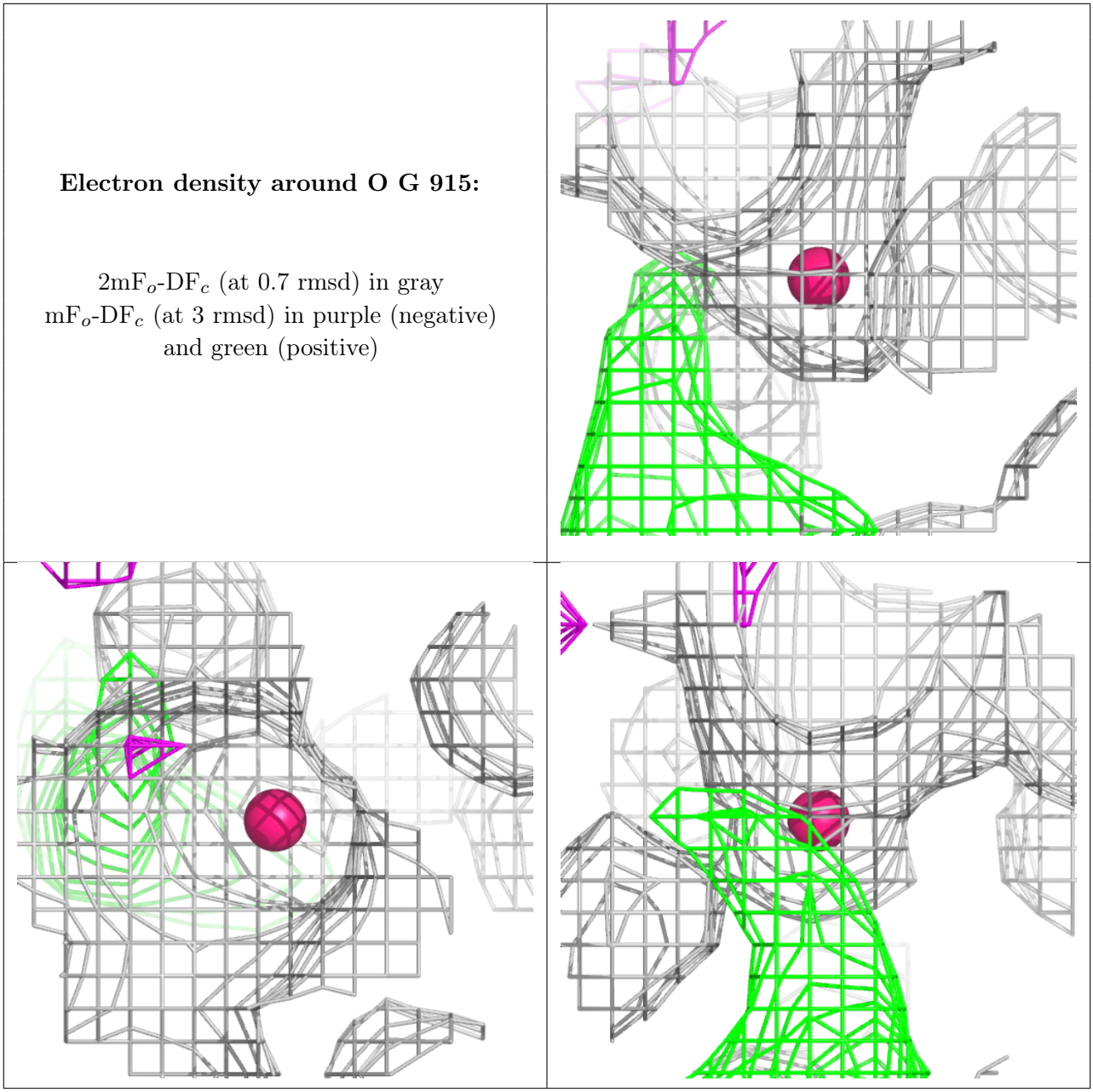






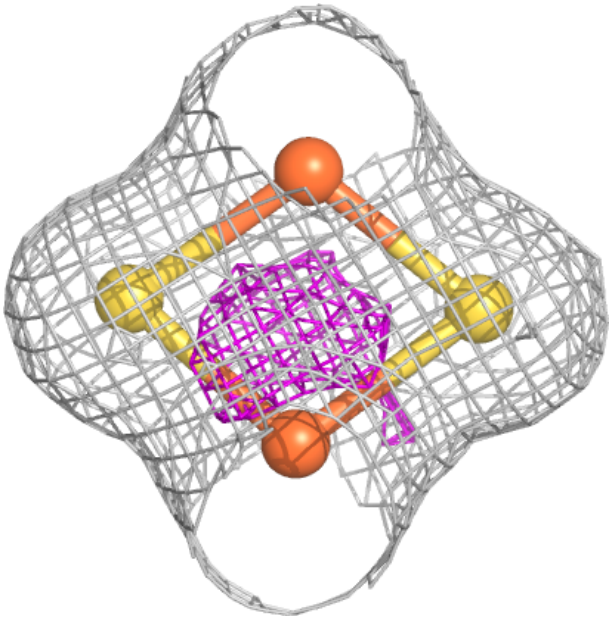
Electron density around O G 915:

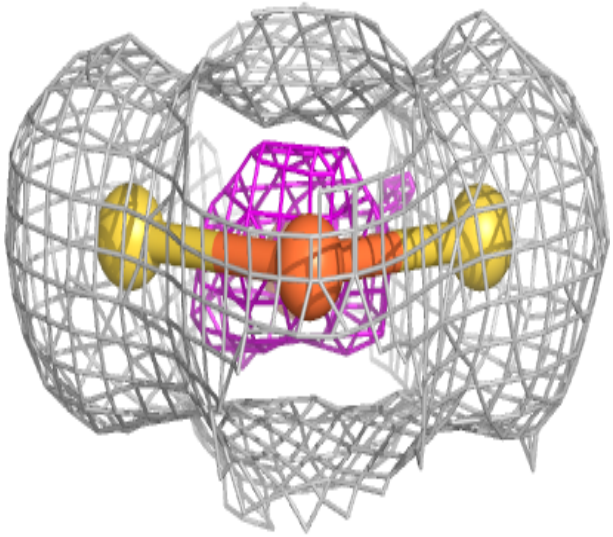
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

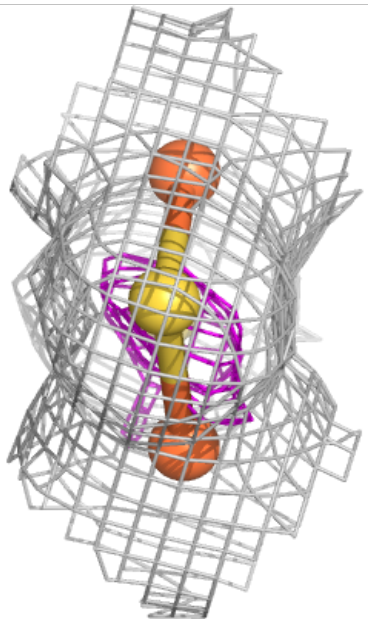


Electron density around FES B 201:

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

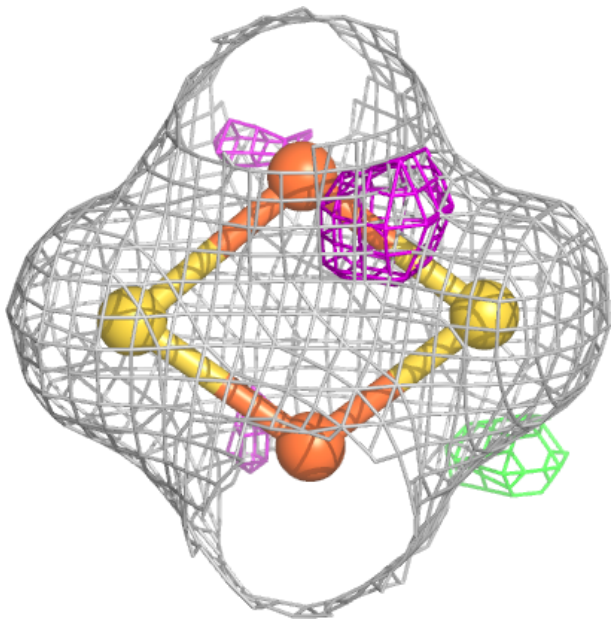


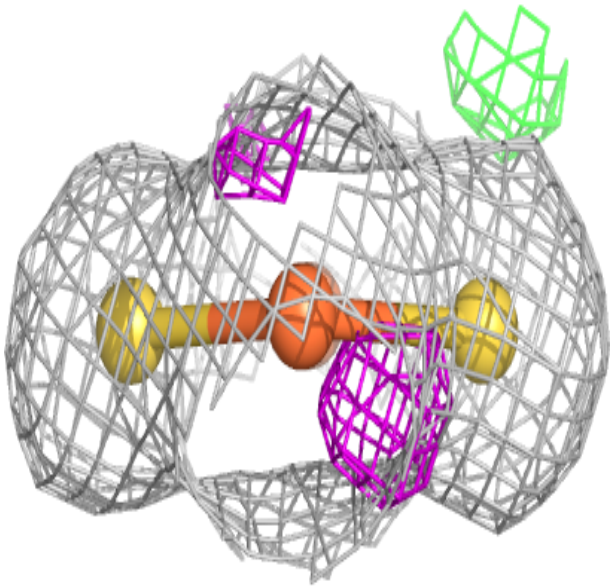


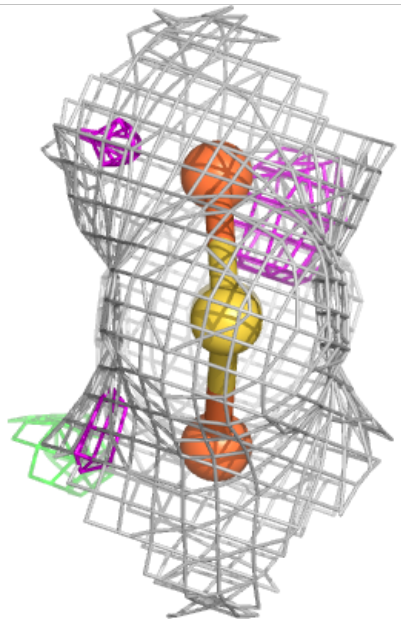


Electron density around FES D 201:

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

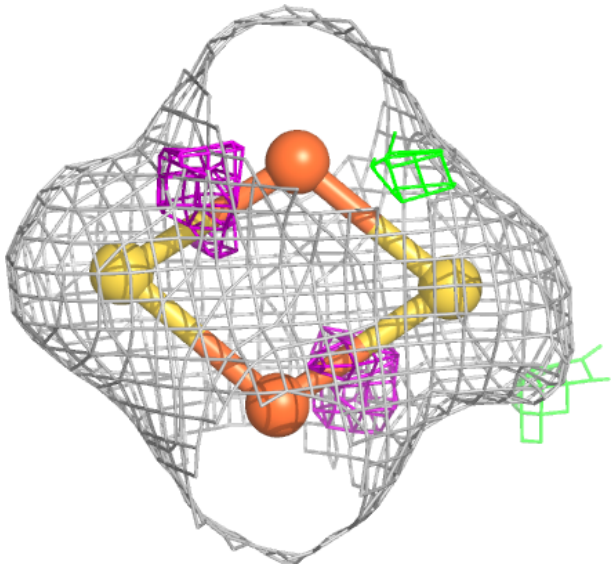


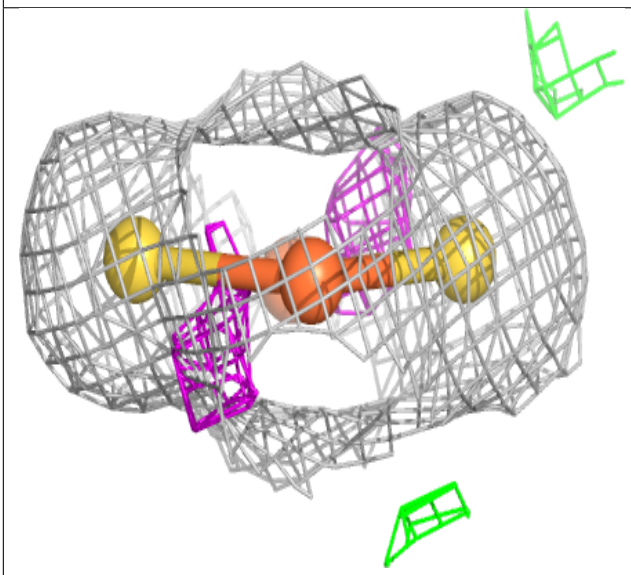


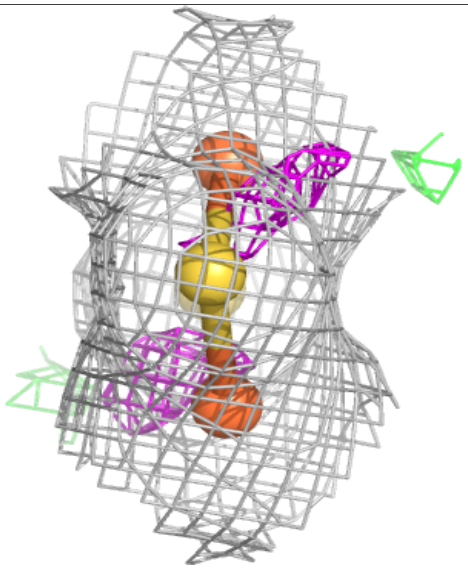


Electron density around FES F 201:

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

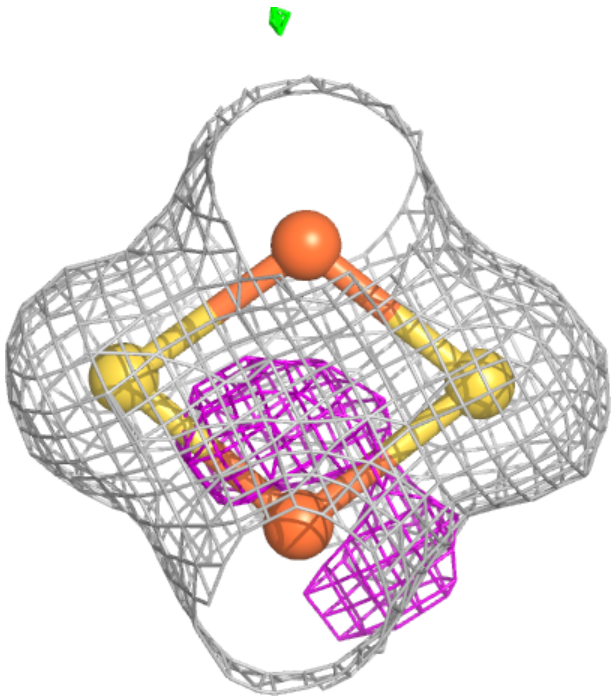


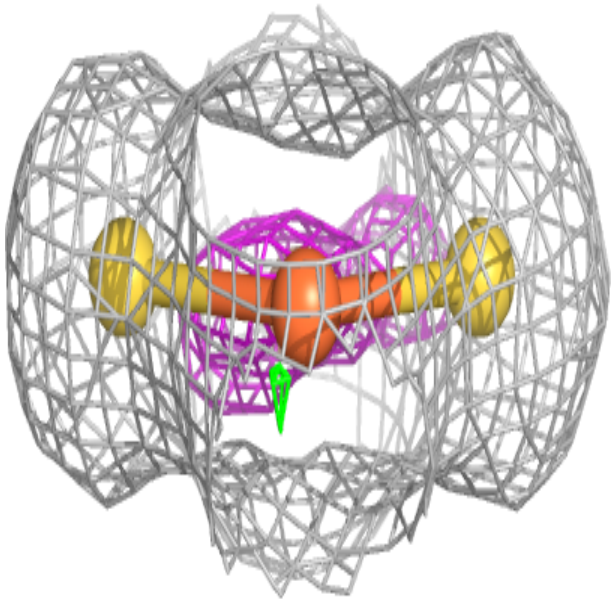


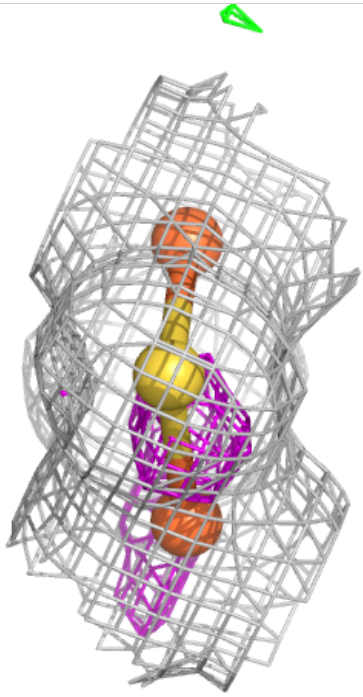


Electron density around FES H 201:

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

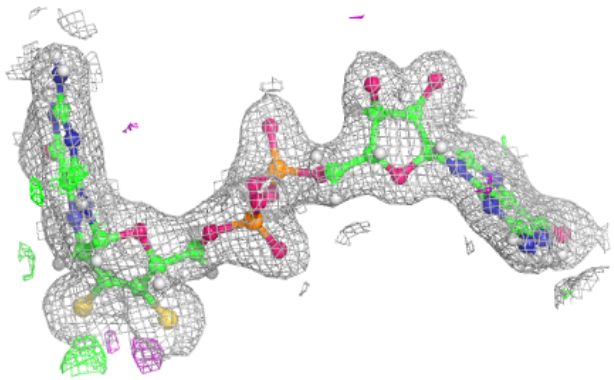


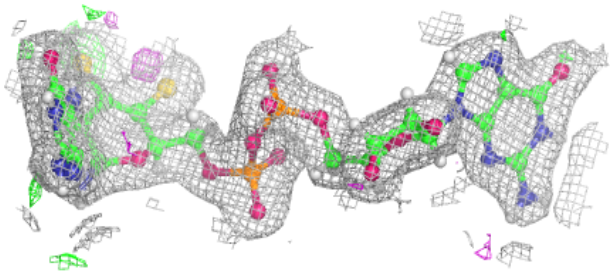


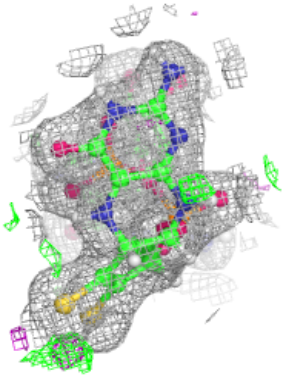


Electron density around MGD C 908:

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

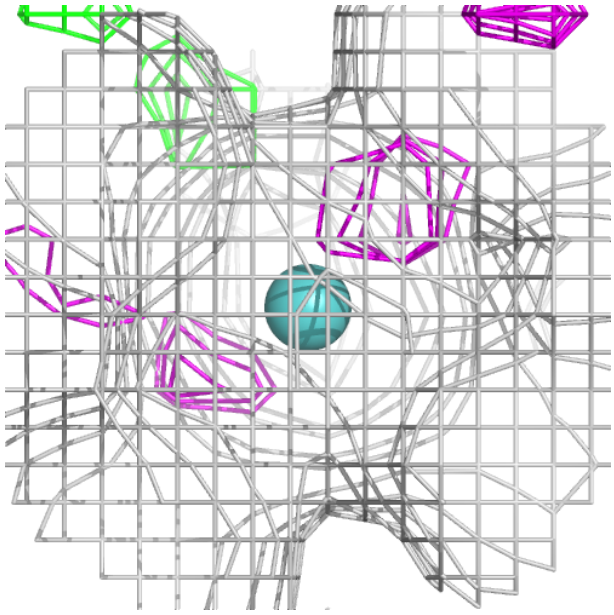


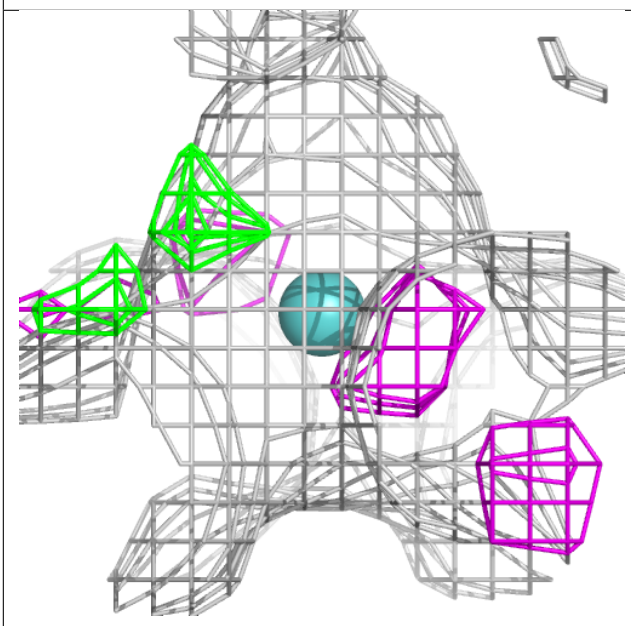


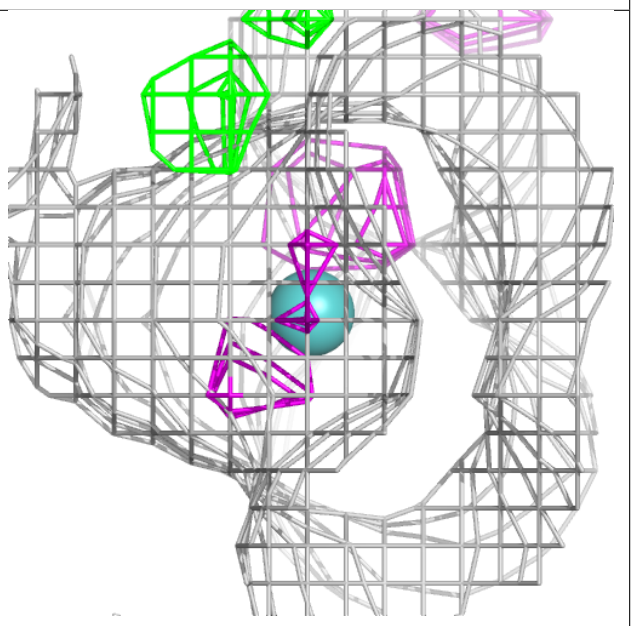


Electron density around 4MO E 901:

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

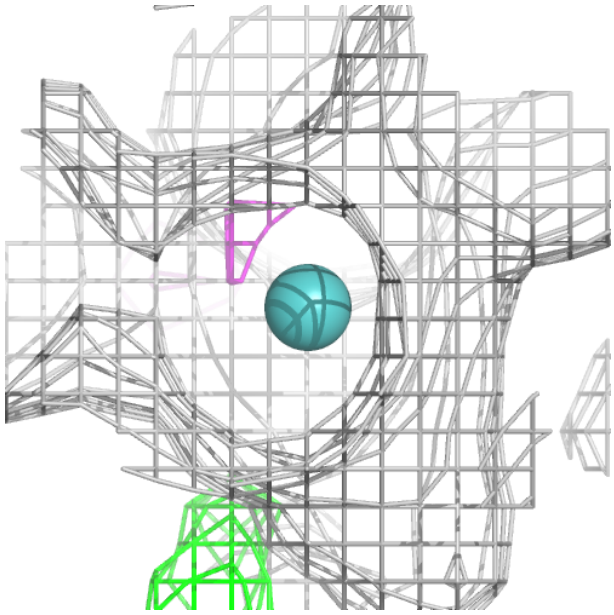


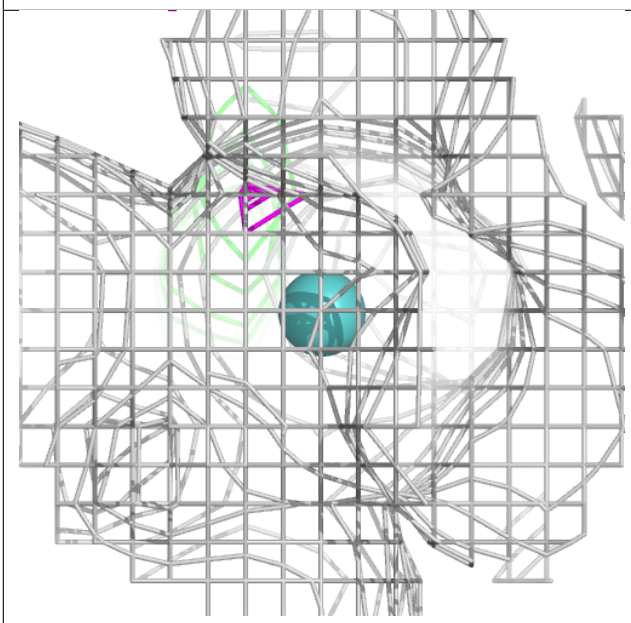


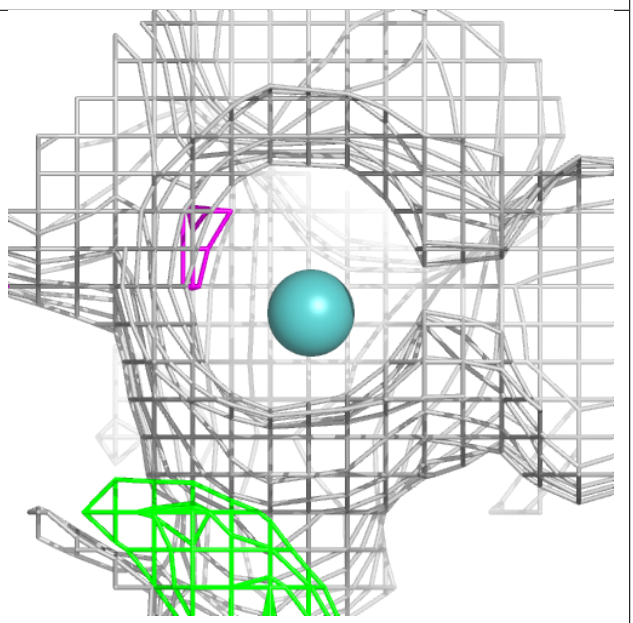


Electron density around 4MO G 901:

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

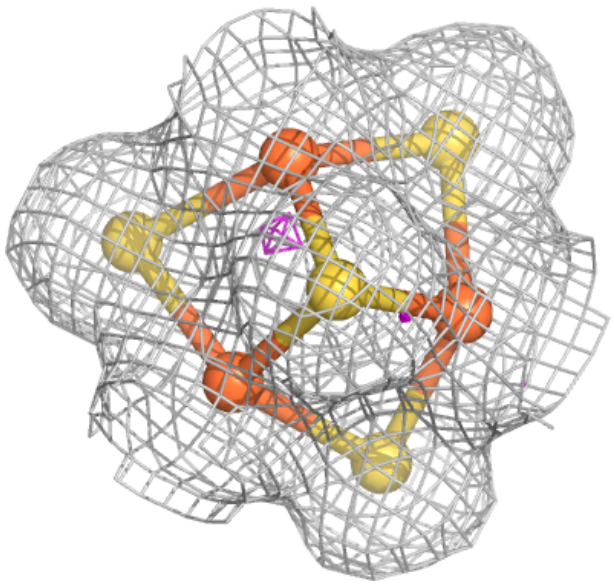


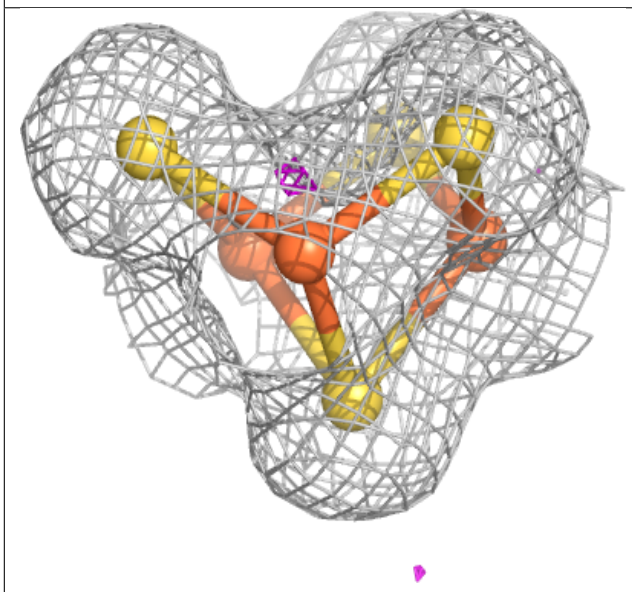


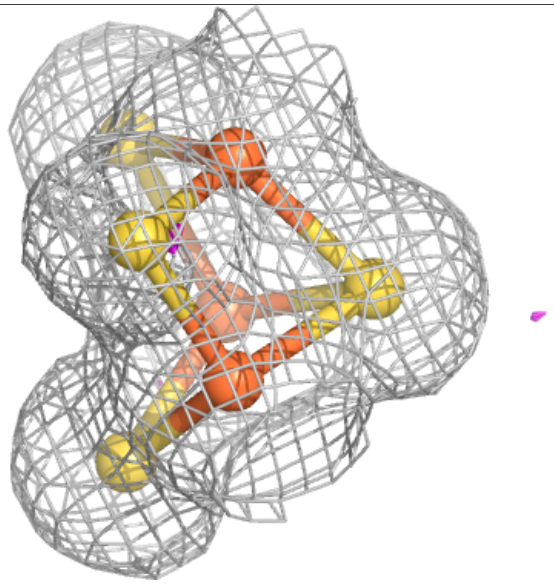


Electron density around F3S A 903:

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

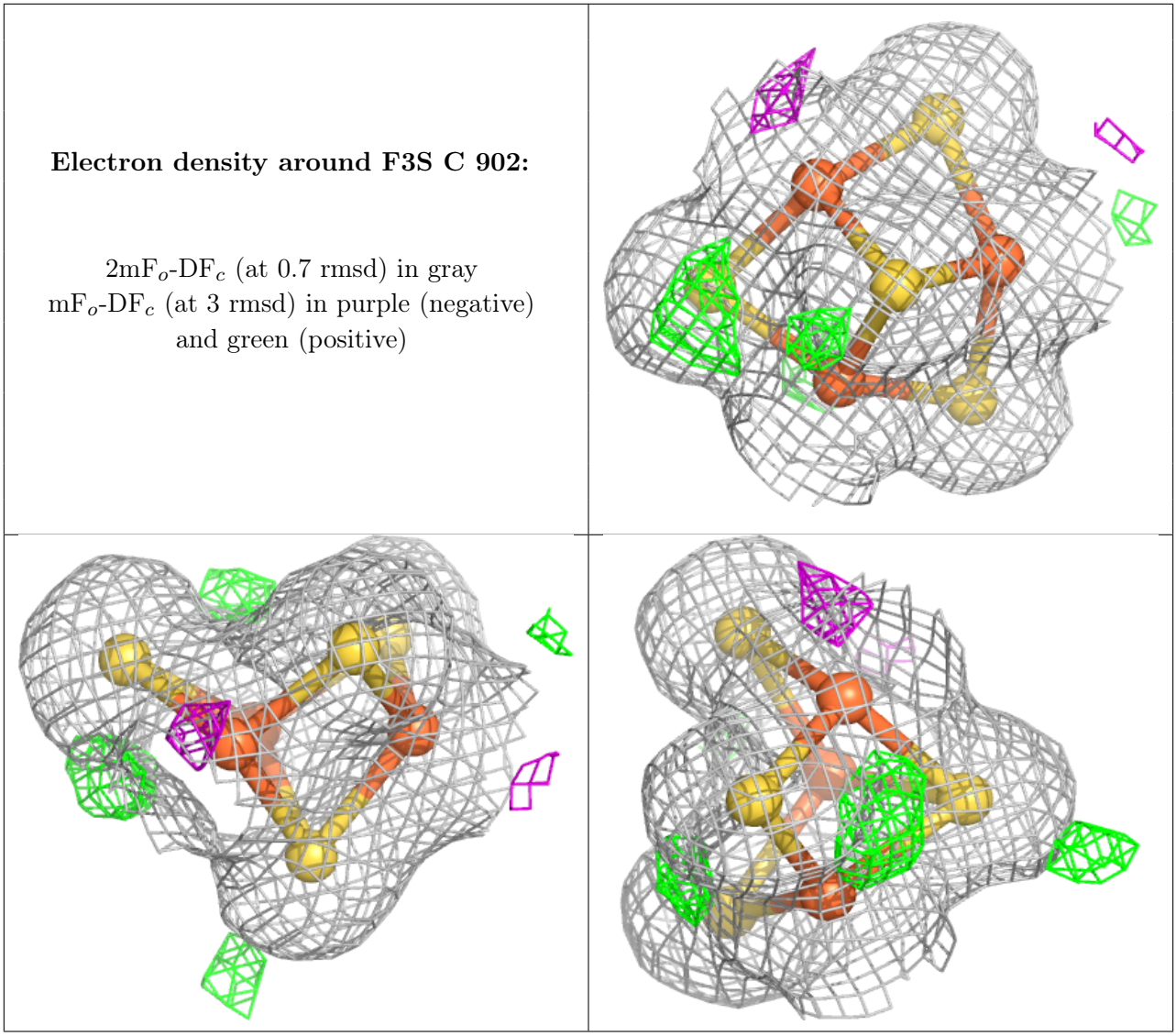






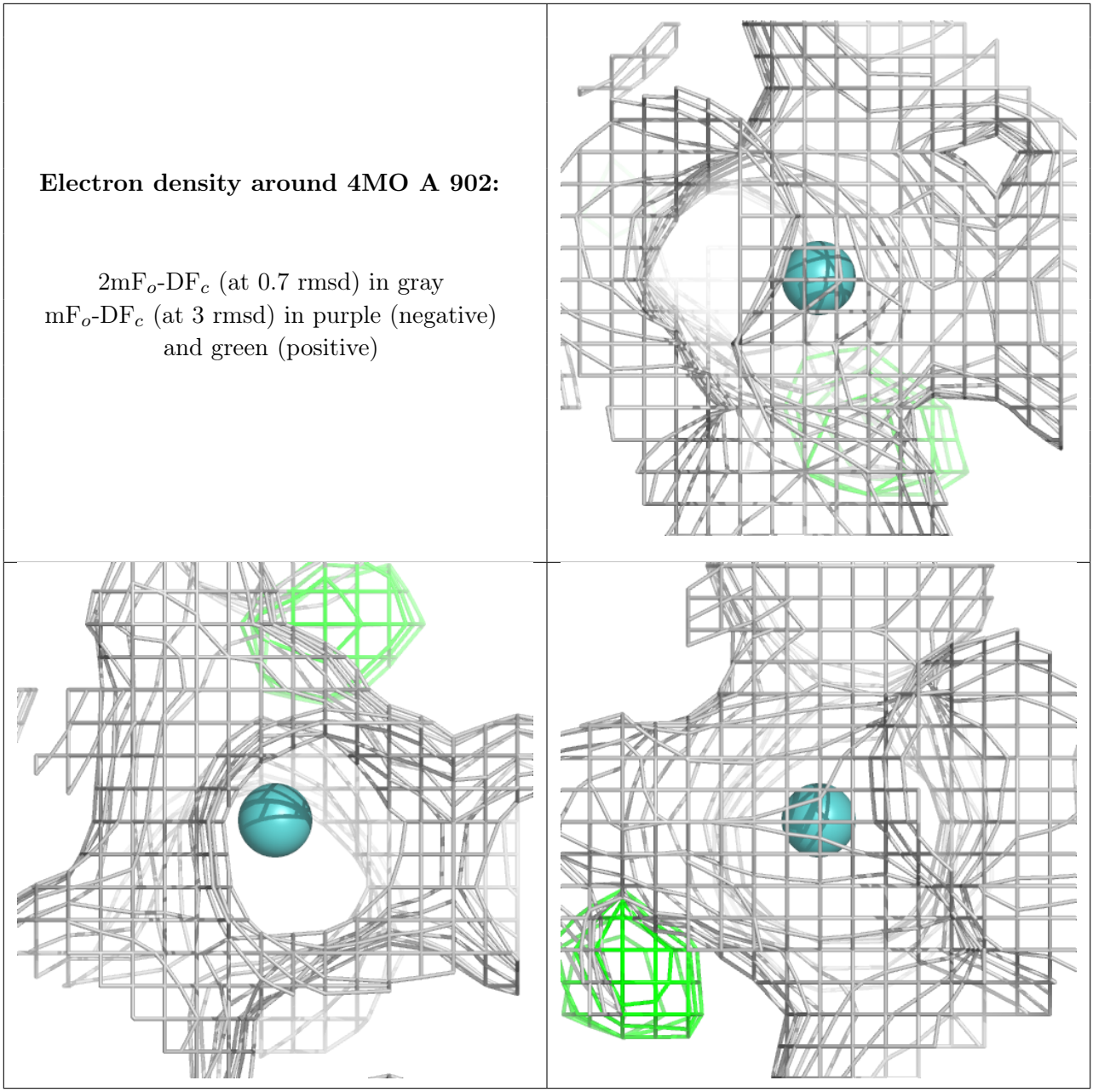
Electron density around F3S C 902:

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



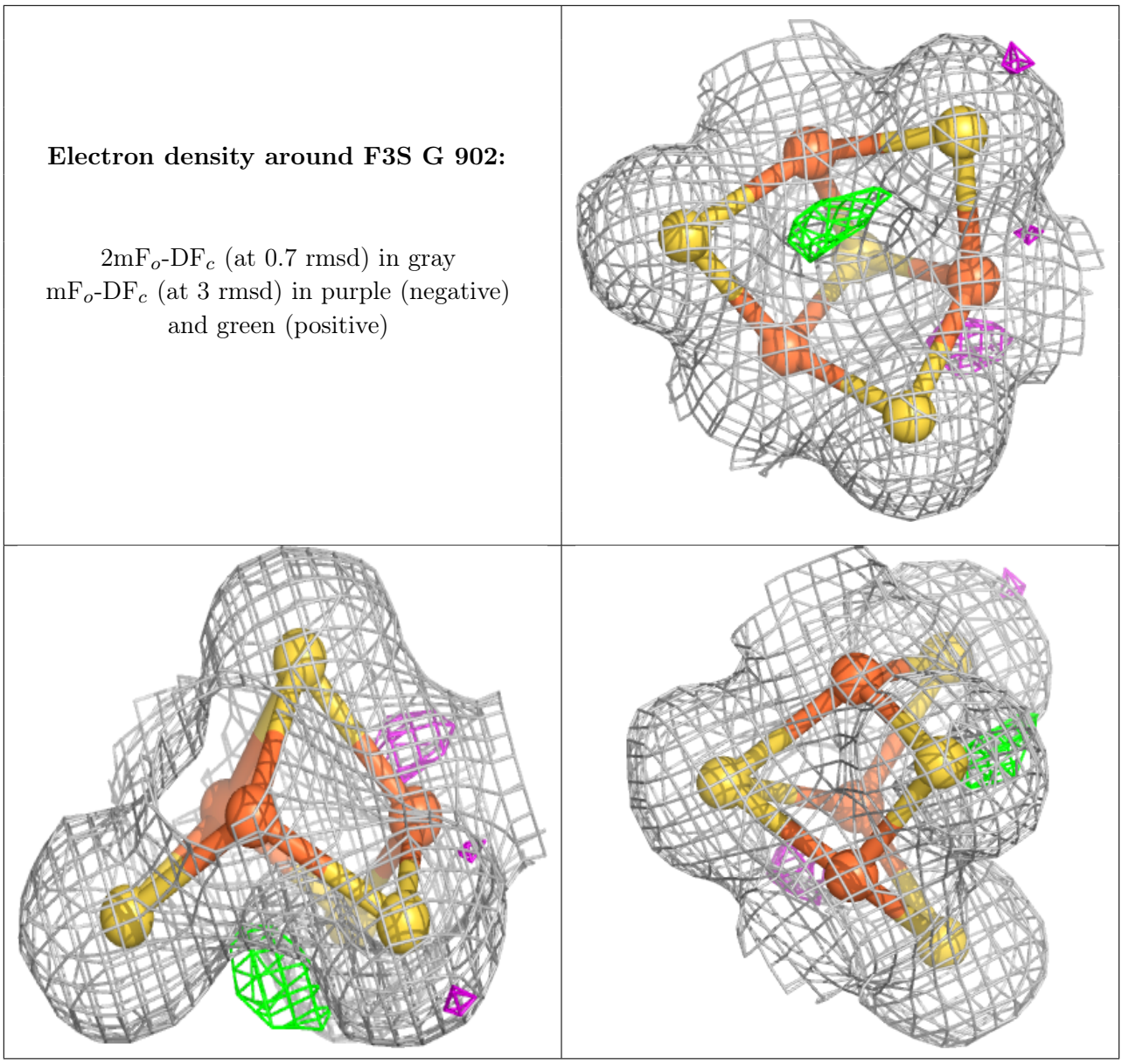
Electron density around 4MO A 902:

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



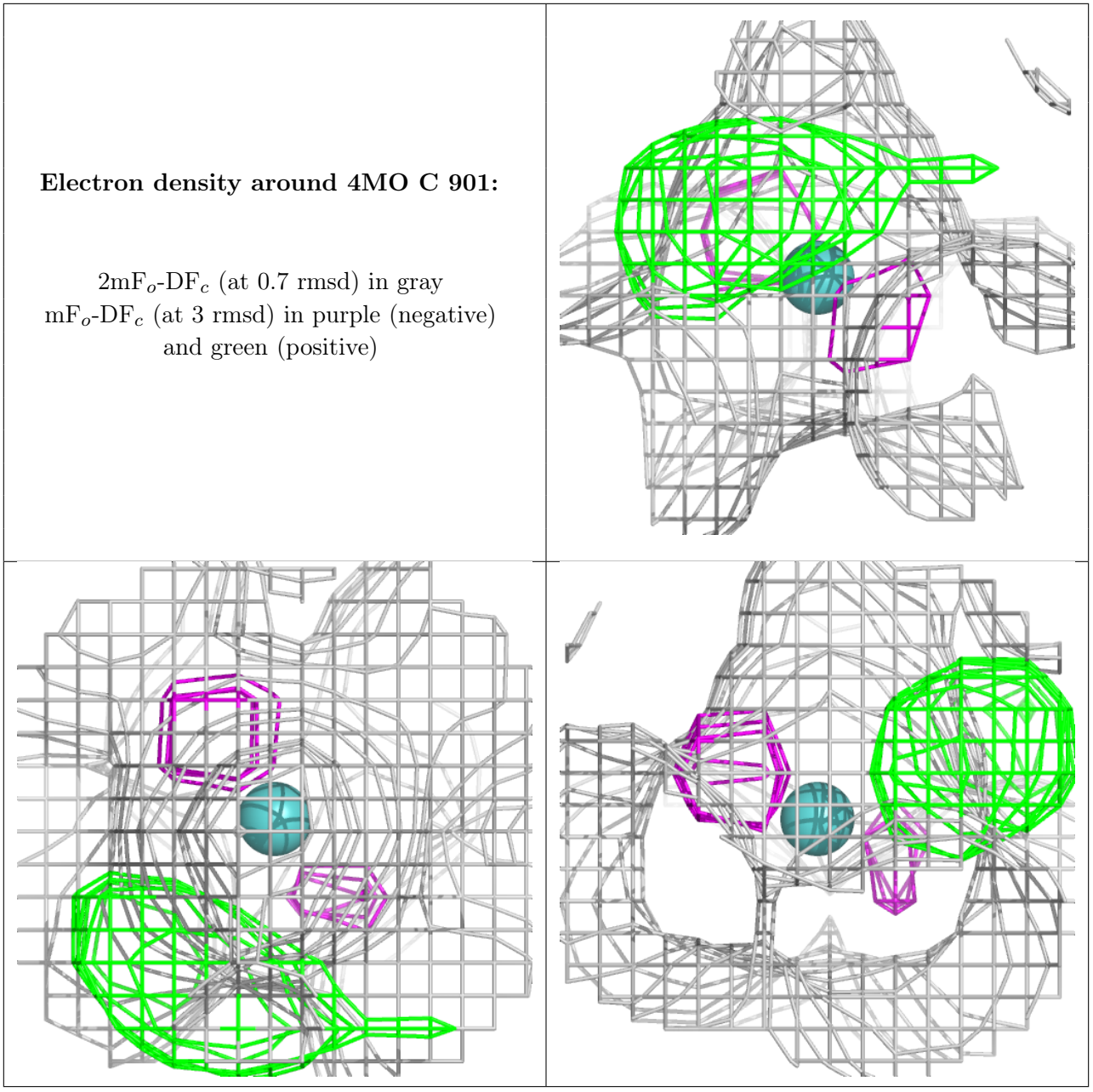
Electron density around F3S G 902:

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



Electron density around 4MO 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)



6.5 Other polymers

There are no such residues in this entry.