



wwPDB X-ray Structure Validation Summary Report

Nov 7, 2023 – 02:01 am GMT

PDB ID : 7O1O
Title : Complex-B bound [FeFe]-hydrogenase maturase HydE from *T. Maritima* (Auxiliary cluster deleted variant)
Authors : Rohac, R.; Martin, L.; Liu, L.; Basu, D.; Tao, L.; Britt, R.D.; Rauchfuss, T.; Nicolet, Y.
Deposited on : 2021-03-30
Resolution : 1.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  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](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

PERCENTILES INFOmissingINFO

1 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 6537 atoms, of which 3045 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.

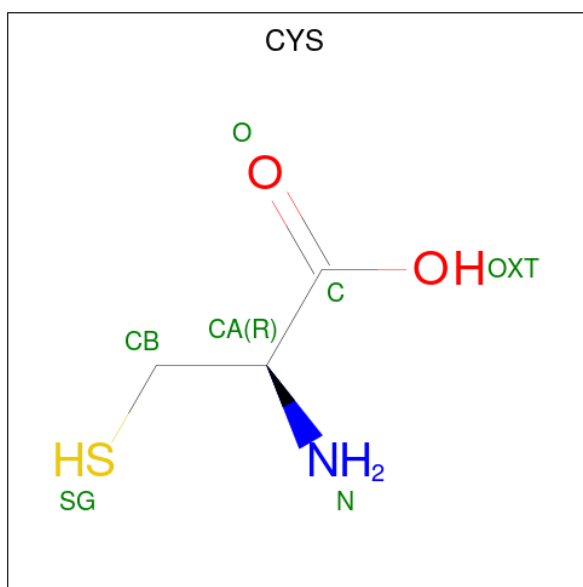
- Molecule 1 is a protein called [FeFe] hydrogenase maturase subunit HydE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	356	5981	1893	3014	515	539	20	1	29	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q9X0Z6
A	-8	TRP	-	expression tag	UNP Q9X0Z6
A	-7	SER	-	expression tag	UNP Q9X0Z6
A	-6	HIS	-	expression tag	UNP Q9X0Z6
A	-5	PRO	-	expression tag	UNP Q9X0Z6
A	-4	GLN	-	expression tag	UNP Q9X0Z6
A	-3	PHE	-	expression tag	UNP Q9X0Z6
A	-2	GLU	-	expression tag	UNP Q9X0Z6
A	-1	LYS	-	expression tag	UNP Q9X0Z6
A	0	ALA	-	expression tag	UNP Q9X0Z6
A	1	SER	-	expression tag	UNP Q9X0Z6
A	311	SER	CYS	engineered mutation	UNP Q9X0Z6
A	319	SER	CYS	engineered mutation	UNP Q9X0Z6
A	322	SER	CYS	engineered mutation	UNP Q9X0Z6
A	346	THR	-	expression tag	UNP Q9X0Z6
A	347	VAL	-	expression tag	UNP Q9X0Z6

- Molecule 2 is CYSTEINE (three-letter code: CYS) (formula: C₃H₇NO₂S) (labeled as "Ligand of Interest" by depositor).

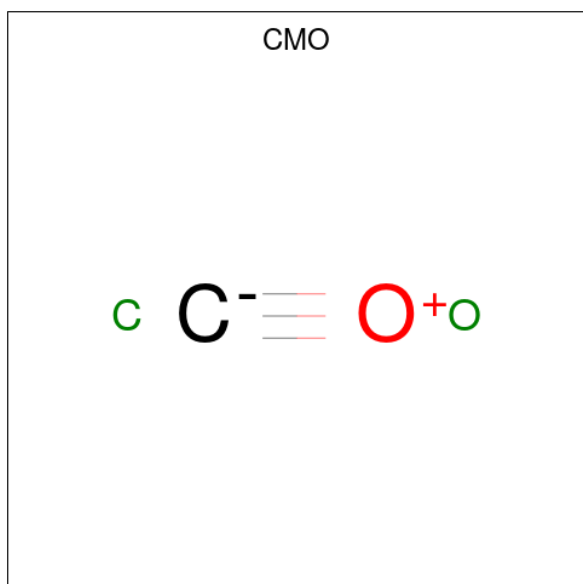


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
2	A	1	10	3	3	1	2	1	0	0

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

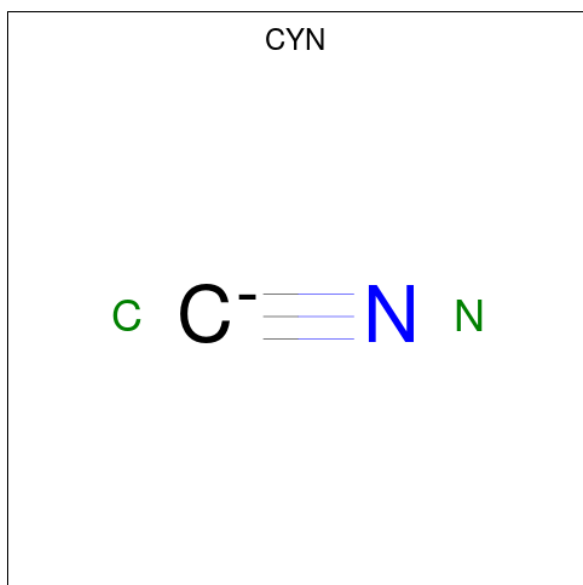
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0

- Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



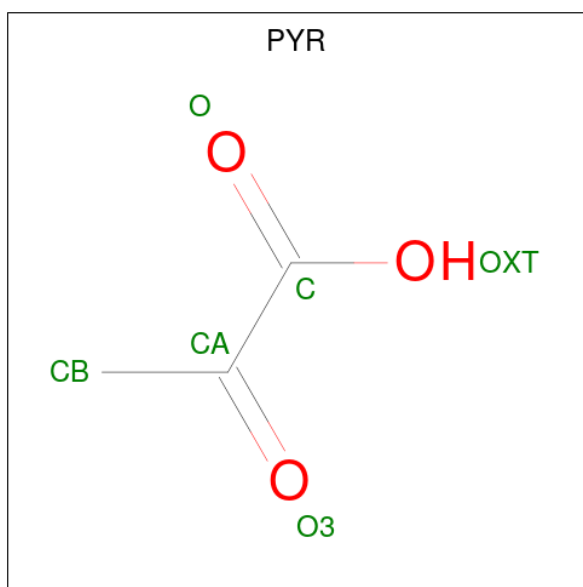
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			2	1	1		
4	A	1	Total	C	O	0	1
			2	1	1		

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN) (labeled as "Ligand of Interest" by depositor).



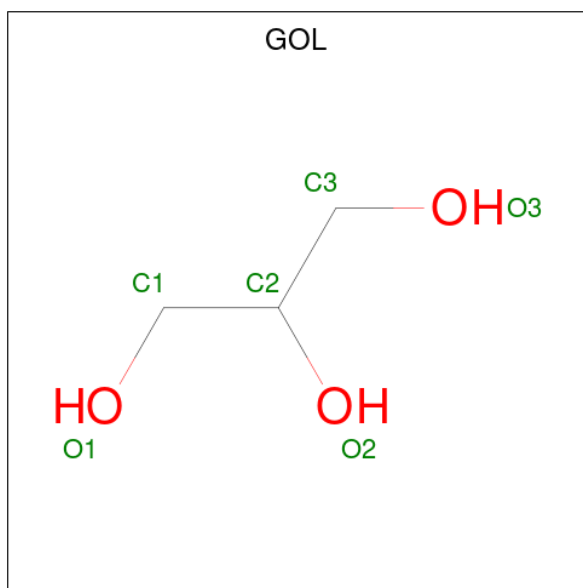
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			2	1	1		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



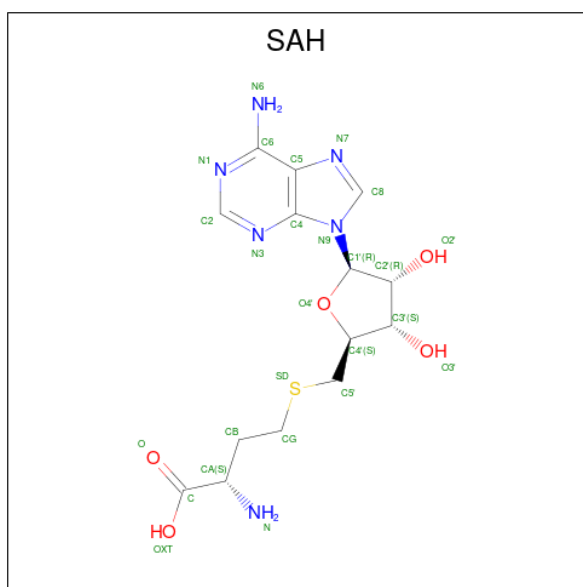
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	9	3	3	3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



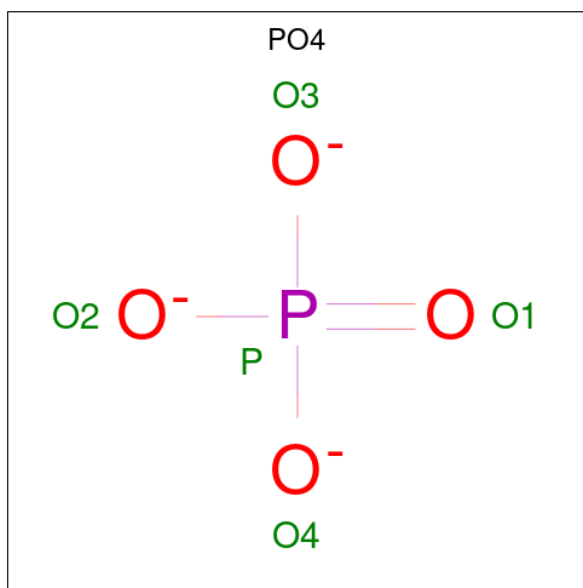
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	12	3	6	3	0	1

- Molecule 8 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
8	A	1	45	14	19	6	5	1	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
9	A	1	5	4	1	0	0
9	A	1	5	4	1	0	0
9	A	1	10	8	2	0	1

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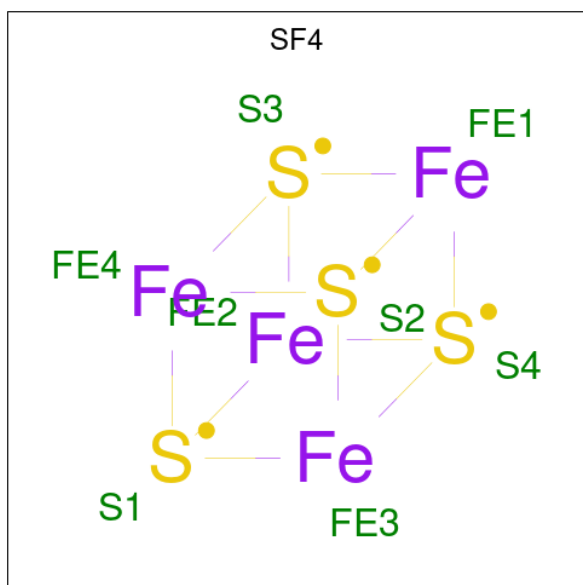
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O P 5 4 1	0	0
9	A	1	Total O P 5 4 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Fe S 8 4 4	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	433	Total O 434 434	0	6

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.42Å 81.76Å 70.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.35 – 1.25 47.13 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.35-1.25) 99.4 (47.13-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.25Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.128 , 0.152 0.128 , 0.152	Depositor DCC
R_{free} test set	5104 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtrriage
Anisotropy	0.353	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	6537	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CMO, CYN, CL, PO4, FE2, SF4, PYR, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	0/3112	0.89	9/4204 (0.2%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	279[A]	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	279[B]	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	155	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	13	ARG	NE-CZ-NH2	-5.80	117.40	120.30

There are no chirality outliers.

There are no planarity outliers.

3.2 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	2967	3014	2969	13	0
2	A	7	3	3	0	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	2	0	0	0	0
6	A	6	3	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	6	8	3	0
8	A	26	19	19	0	0
9	A	30	0	0	1	2
10	A	1	0	0	0	0
11	A	8	0	0	0	0
12	A	434	0	0	7	11
All	All	3492	3045	2999	14	11

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 2.

The worst 5 of 14 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:194[A]:THR:HG21	12:A:539:HOH:O	1.83	0.77
1:A:338:TRP:H	7:A:407[A]:GOL:H12	1.51	0.74
9:A:412:PO4:O3	12:A:501:HOH:O	2.07	0.71
1:A:304[A]:GLN:OE1	12:A:502:HOH:O	2.11	0.67
1:A:49[B]:ASP:OD2	12:A:503:HOH:O	2.12	0.67

The worst 5 of 11 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)
12:A:603:HOH:O	12:A:820:HOH:O[2_555]	1.65	0.55
12:A:863:HOH:O	12:A:891:HOH:O[4_455]	1.75	0.45
12:A:787:HOH:O	12:A:831:HOH:O[4_454]	1.79	0.41
12:A:924:HOH:O	12:A:924:HOH:O[2_555]	1.93	0.27
12:A:820:HOH:O	12:A:896:HOH:O[2_555]	1.99	0.21

3.3 Torsion angles [i](#)

3.3.1 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	379/357 (106%)	368 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

3.3.2 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	327/312 (105%)	323 (99%)	4 (1%)	71	35

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49[A]	ASP
1	A	49[B]	ASP
1	A	313	PHE
1	A	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

3.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

3.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
11	SF4	A	415	8,1	0,12,12	-	-	-		
9	PO4	A	413	-	4,4,4	0.81	0	6,6,6	0.61	0
4	CMO	A	403[C]	-	0,1,1	-	-	-		
7	GOL	A	407[A]	-	5,5,5	0.61	0	5,5,5	0.92	0
2	CYS	A	401	3	5,6,6	0.88	0	5,7,7	0.97	0
9	PO4	A	412	-	4,4,4	1.09	0	6,6,6	0.51	0
9	PO4	A	410	-	4,4,4	2.05	1 (25%)	6,6,6	1.15	0
9	PO4	A	409	-	4,4,4	0.88	0	6,6,6	0.38	0
4	CMO	A	404[C]	-	0,1,1	-	-	-		
6	PYR	A	406	-	5,5,5	2.89	3 (60%)	3,6,6	2.13	2 (66%)
9	PO4	A	411[B]	-	4,4,4	0.77	0	6,6,6	0.81	0
5	CYN	A	405	-	0,1,1	-	-	-		
9	PO4	A	411[A]	-	4,4,4	0.93	0	6,6,6	0.42	0
8	SAH	A	408	11	24,28,28	0.87	1 (4%)	25,40,40	1.22	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	A	415	8,1	-	-	0/6/5/5
7	GOL	A	407[A]	-	-	2/4/4/4	-
2	CYS	A	401	3	-	0/6/6/6	-
6	PYR	A	406	-	-	0/4/4/4	-
8	SAH	A	408	11	-	2/11/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	406	PYR	O3-CA	3.99	1.32	1.23
6	A	406	PYR	CA-C	-3.74	1.40	1.54
9	A	410	PO4	P-O4	-3.56	1.43	1.54
6	A	406	PYR	O-C	3.41	1.31	1.22
8	A	408	SAH	O4'-C4'	-2.17	1.40	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	408	SAH	N3-C2-N1	-3.61	123.04	128.68
6	A	406	PYR	OXT-C-O	-2.66	117.53	123.61
6	A	406	PYR	OXT-C-CA	2.41	120.57	113.97
8	A	408	SAH	C4-C5-N7	-2.05	107.27	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	407[A]	GOL	C1-C2-C3-O3
8	A	408	SAH	N-CA-CB-CG
8	A	408	SAH	C-CA-CB-CG
7	A	407[A]	GOL	O2-C2-C3-O3

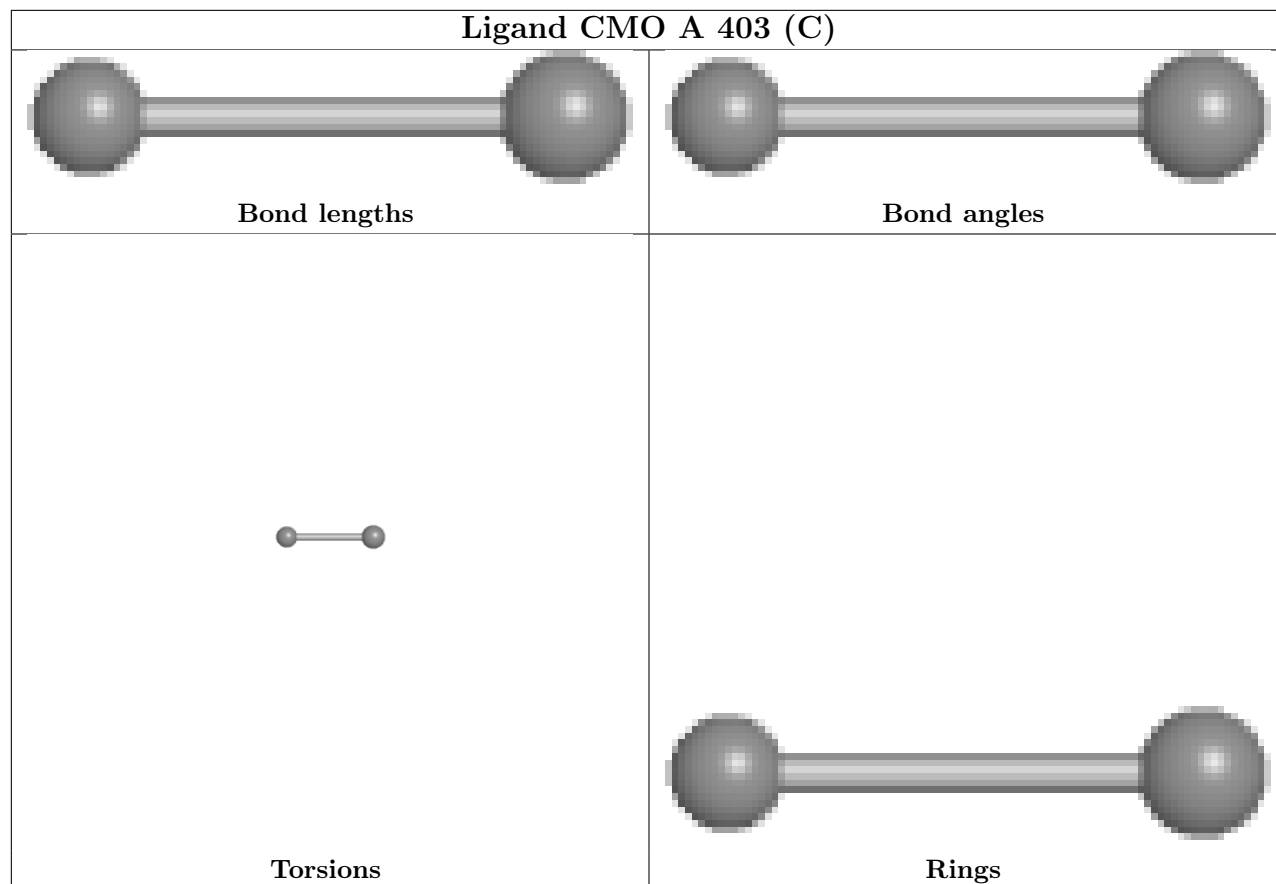
There are no ring outliers.

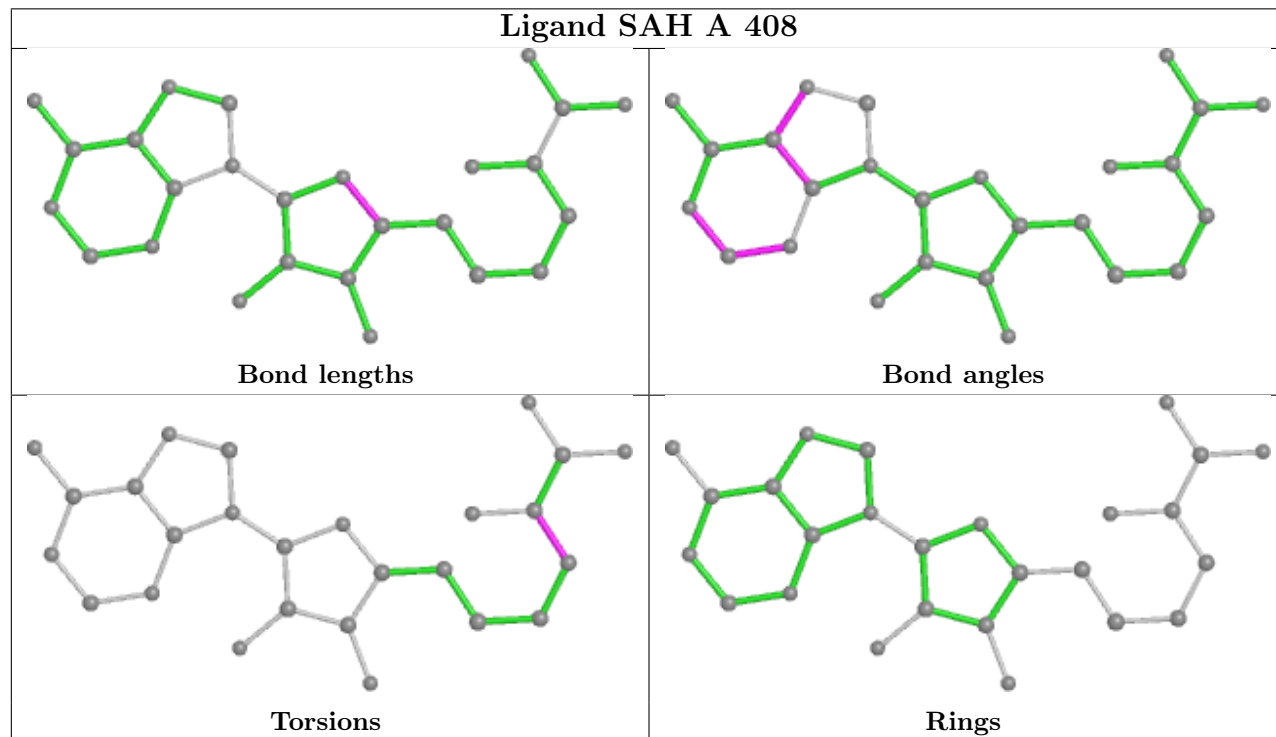
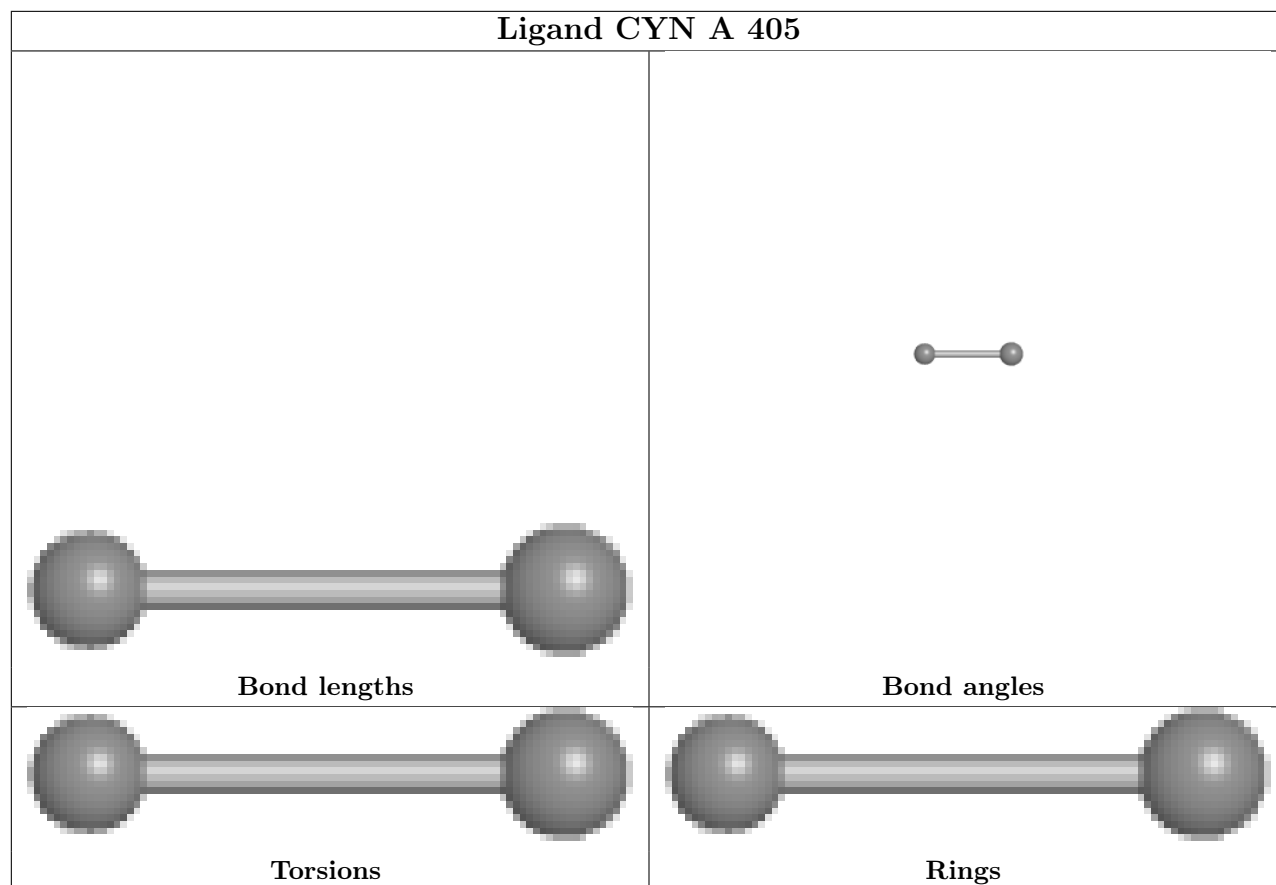
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	413	PO4	0	1
7	A	407[A]	GOL	3	0
9	A	412	PO4	1	1

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 than 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.





3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	356/357 (99%)	-0.05	6 (1%) 70 60	13, 18, 38, 65	3 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-8	TRP	3.7
1	A	-9	MET	3.0
1	A	344	VAL	2.8
1	A	334[B]	PRO	2.7
1	A	346	THR	2.3

4.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PYR	A	406	6/6	0.68	0.17	55,57,66,66	0
9	PO4	A	411[A]	5/5	0.78	0.22	36,41,42,43	5

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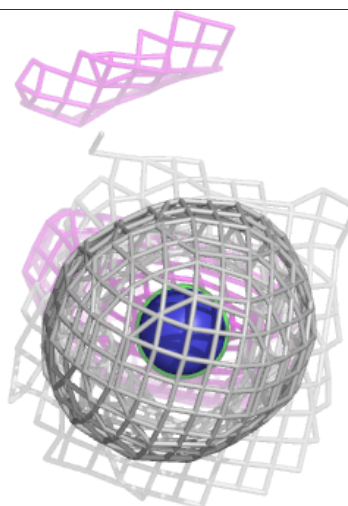
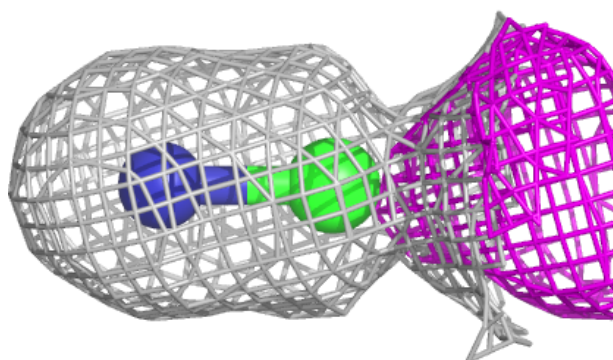
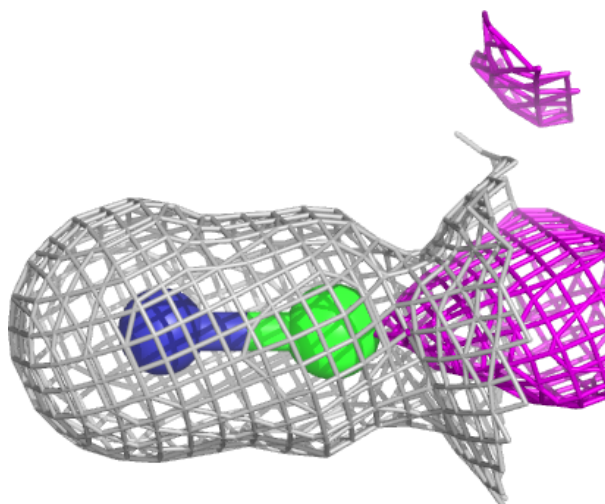
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PO4	A	411[B]	5/5	0.78	0.22	41,44,49,50	5
9	PO4	A	409	5/5	0.89	0.24	77,78,79,80	0
9	PO4	A	412	5/5	0.89	0.18	43,45,50,51	5
9	PO4	A	413	5/5	0.89	0.26	40,41,41,42	5
5	CYN	A	405	2/2	0.92	0.14	14,14,14,16	0
7	GOL	A	407[A]	6/6	0.93	0.16	38,46,50,53	12
4	CMO	A	404[C]	2/2	0.97	0.09	14,14,14,15	0
9	PO4	A	410	5/5	0.97	0.08	29,30,34,40	0
2	CYS	A	401	7/7	0.98	0.10	14,17,19,21	0
4	CMO	A	403[C]	2/2	0.98	0.09	15,15,15,17	0
8	SAH	A	408	26/26	0.98	0.07	13,16,22,23	0
11	SF4	A	415	8/8	0.99	0.07	14,14,15,16	0
10	CL	A	414	1/1	1.00	0.07	18,18,18,18	0
3	FE2	A	402	1/1	1.00	0.07	14,14,14,14	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.

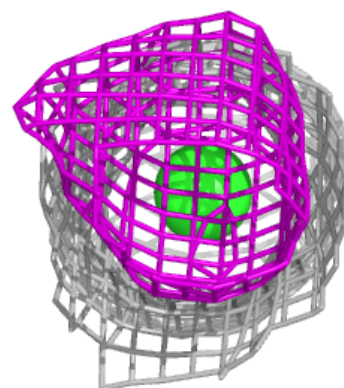
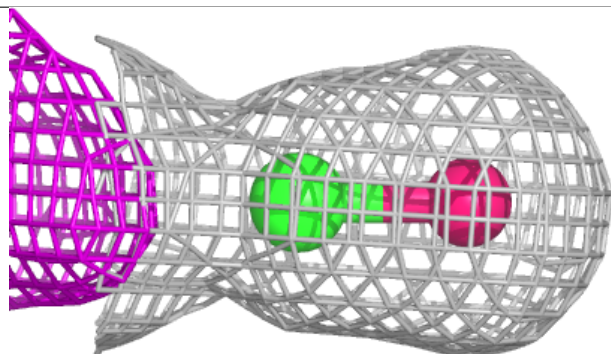
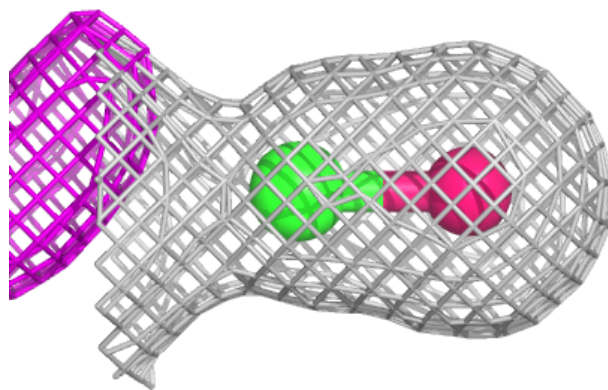
Electron density around CYN A 405:

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

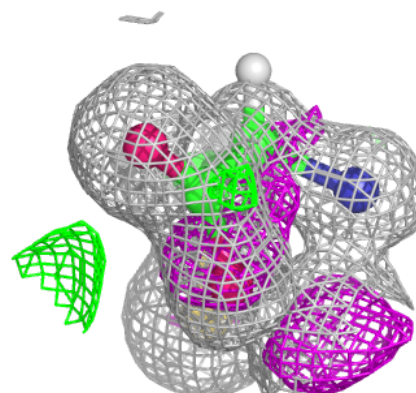
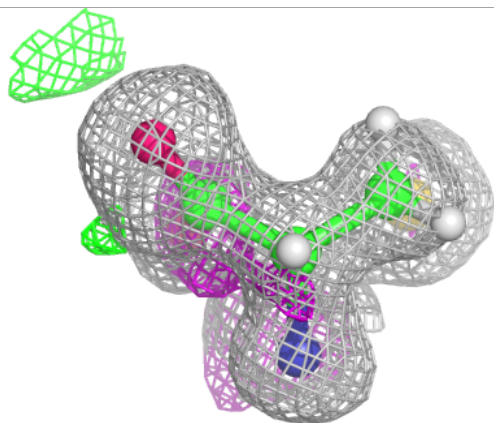
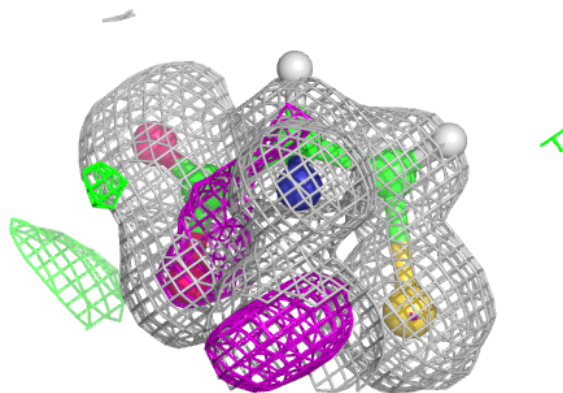


Electron density around CMO A 404 (C):

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

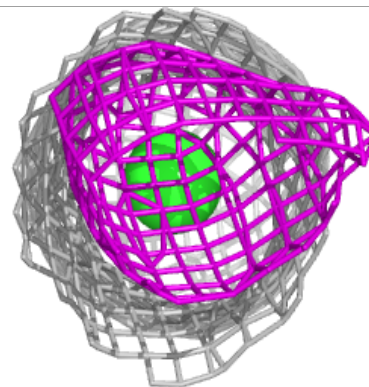
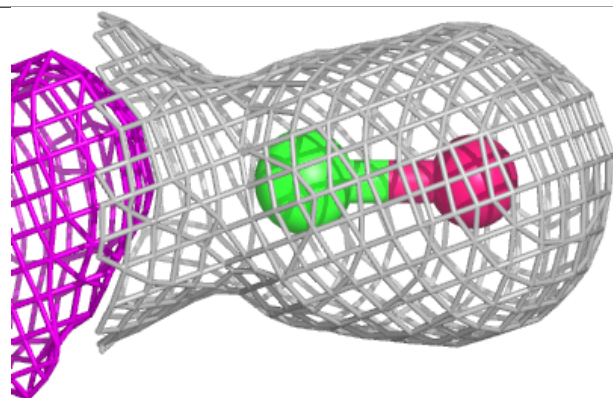
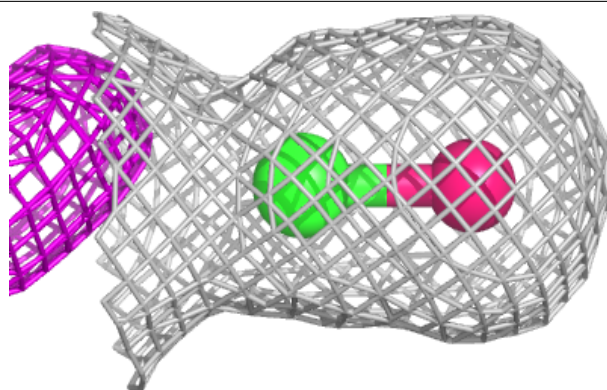
**Electron density around CYS A 401:**

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

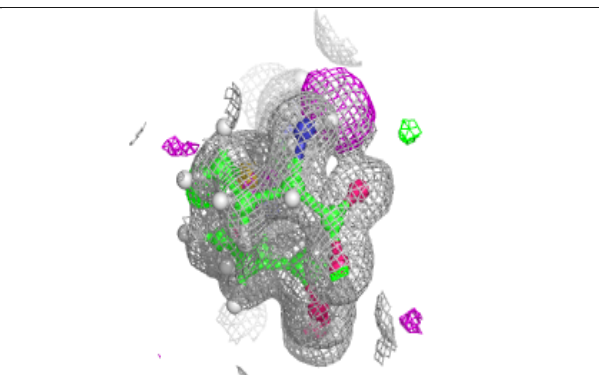
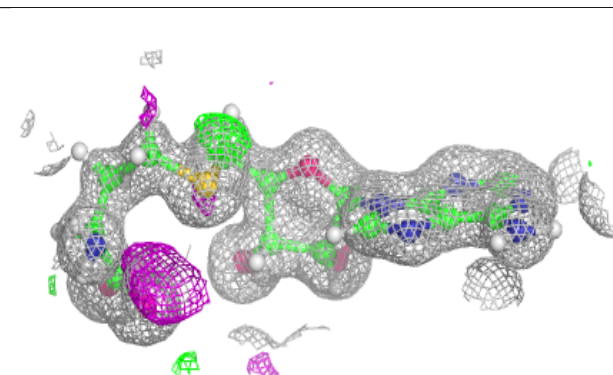
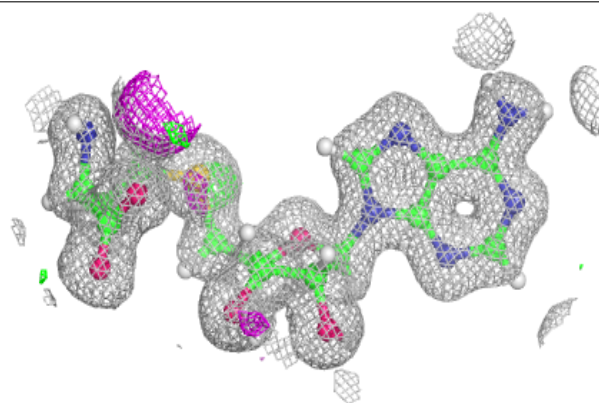


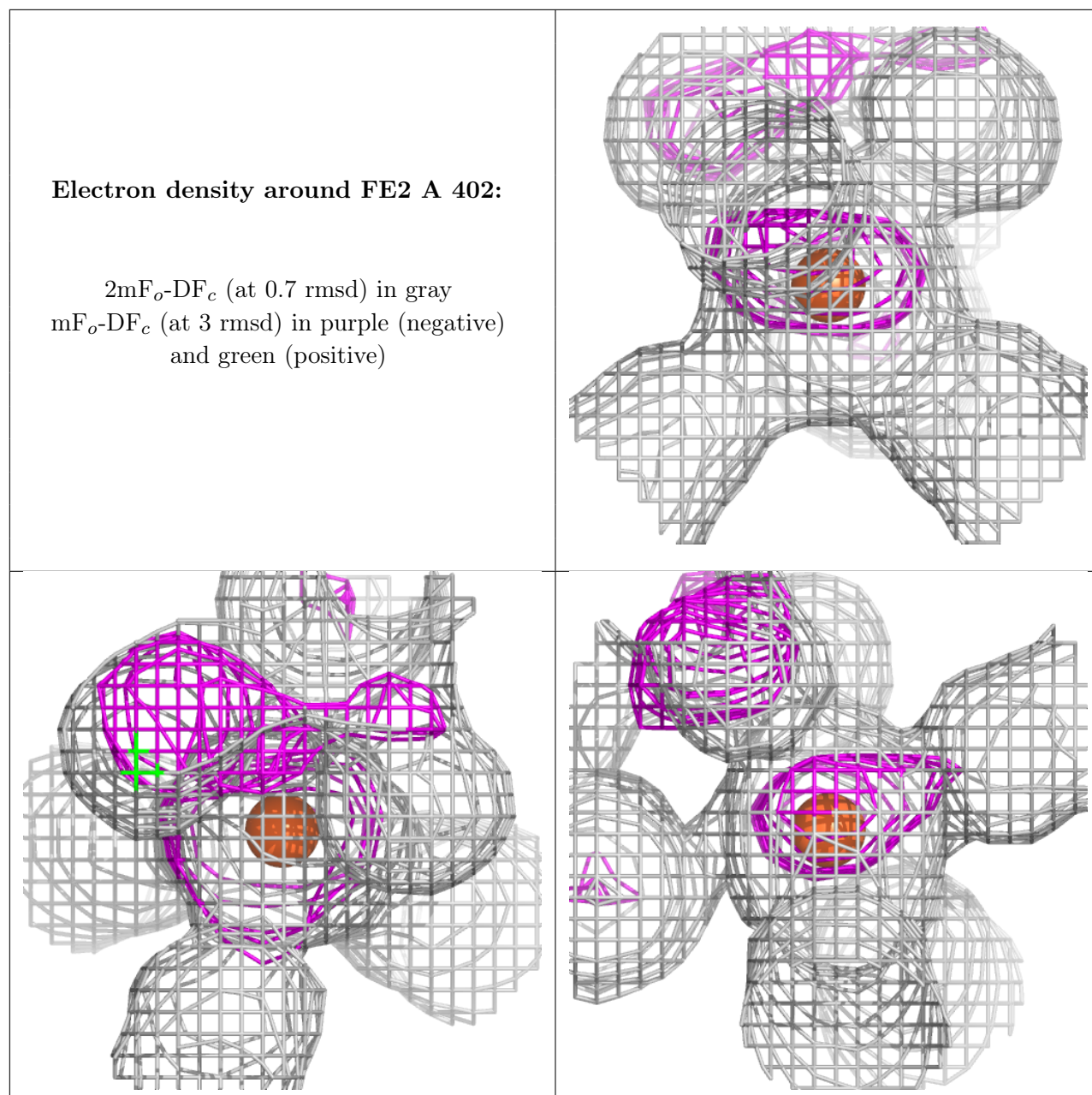
Electron density around CMO A 403 (C):

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

**Electron density around SAH A 408:**

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





4.5 Other polymers [i](#)

There are no such residues in this entry.