wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2024 – 08:27 AM EST

PDB ID	:	4MZU
Title	:	Crystal structure of FdtD, a bifunctional ketoisomerase/N-acetyltransferase from Shewanella denitrificans
Authors	:	Chantigian, D.P.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2013-09-30
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

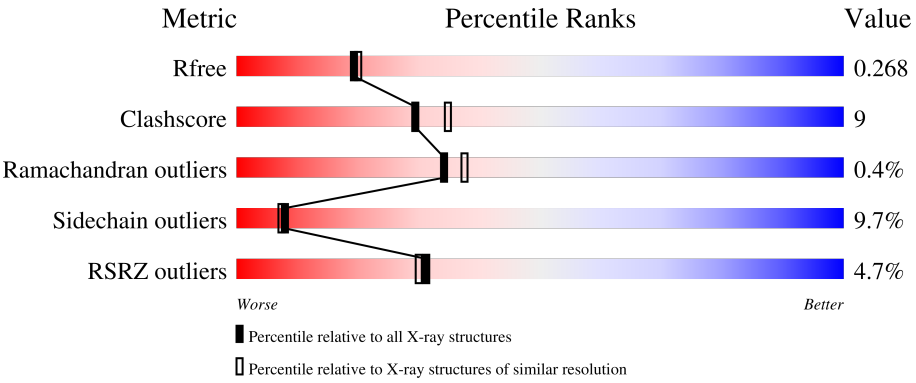
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	2% 69% 17% • • 9%
1	B	312	4% 76% 15% • 7%
1	C	312	2% 73% 14% • • 9%
1	D	312	4% 68% 21% • 9%
1	E	312	3% 66% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	312	5% 73% 17% 6%
1	G	312	2% 70% 19% 9%
1	H	312	9% 58% 28% 11%
1	I	312	4% 66% 22% 9%
1	J	312	7% 65% 18% 12%
1	K	312	5% 71% 17% 9%
1	L	312	3% 66% 22% 8%

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
4	TDR	A	403	-	X	-	-
4	TDR	B	403	-	X	-	-
4	TDR	C	403	-	X	-	-
4	TDR	D	403	-	X	-	-
4	TDR	E	403	-	X	-	-
4	TDR	J	403	-	X	-	-
4	TDR	L	403	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28412 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called WxcM-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2220	1412	379	418	11			
1	B	290	Total	C	N	O	S	0	0	0
			2262	1438	387	426	11			
1	C	285	Total	C	N	O	S	0	1	0
			2222	1416	379	416	11			
1	D	283	Total	C	N	O	S	0	0	0
			2204	1403	375	415	11			
1	E	286	Total	C	N	O	S	0	0	0
			2231	1422	379	419	11			
1	F	294	Total	C	N	O	S	0	0	0
			2288	1455	393	429	11			
1	G	283	Total	C	N	O	S	0	1	0
			2206	1404	376	415	11			
1	H	278	Total	C	N	O	S	0	0	0
			2159	1379	364	405	11			
1	I	285	Total	C	N	O	S	0	0	0
			2217	1412	377	417	11			
1	J	275	Total	C	N	O	S	0	1	0
			2140	1368	361	401	10			
1	K	285	Total	C	N	O	S	0	1	0
			2226	1418	378	419	11			
1	L	286	Total	C	N	O	S	0	1	0
			2228	1418	380	419	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	LEU	-	expression tag	UNP Q12KT8
A	306	GLU	-	expression tag	UNP Q12KT8
A	307	HIS	-	expression tag	UNP Q12KT8
A	308	HIS	-	expression tag	UNP Q12KT8
A	309	HIS	-	expression tag	UNP Q12KT8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	expression tag	UNP Q12KT8
A	311	HIS	-	expression tag	UNP Q12KT8
A	312	HIS	-	expression tag	UNP Q12KT8
B	305	LEU	-	expression tag	UNP Q12KT8
B	306	GLU	-	expression tag	UNP Q12KT8
B	307	HIS	-	expression tag	UNP Q12KT8
B	308	HIS	-	expression tag	UNP Q12KT8
B	309	HIS	-	expression tag	UNP Q12KT8
B	310	HIS	-	expression tag	UNP Q12KT8
B	311	HIS	-	expression tag	UNP Q12KT8
B	312	HIS	-	expression tag	UNP Q12KT8
C	305	LEU	-	expression tag	UNP Q12KT8
C	306	GLU	-	expression tag	UNP Q12KT8
C	307	HIS	-	expression tag	UNP Q12KT8
C	308	HIS	-	expression tag	UNP Q12KT8
C	309	HIS	-	expression tag	UNP Q12KT8
C	310	HIS	-	expression tag	UNP Q12KT8
C	311	HIS	-	expression tag	UNP Q12KT8
C	312	HIS	-	expression tag	UNP Q12KT8
D	305	LEU	-	expression tag	UNP Q12KT8
D	306	GLU	-	expression tag	UNP Q12KT8
D	307	HIS	-	expression tag	UNP Q12KT8
D	308	HIS	-	expression tag	UNP Q12KT8
D	309	HIS	-	expression tag	UNP Q12KT8
D	310	HIS	-	expression tag	UNP Q12KT8
D	311	HIS	-	expression tag	UNP Q12KT8
D	312	HIS	-	expression tag	UNP Q12KT8
E	305	LEU	-	expression tag	UNP Q12KT8
E	306	GLU	-	expression tag	UNP Q12KT8
E	307	HIS	-	expression tag	UNP Q12KT8
E	308	HIS	-	expression tag	UNP Q12KT8
E	309	HIS	-	expression tag	UNP Q12KT8
E	310	HIS	-	expression tag	UNP Q12KT8
E	311	HIS	-	expression tag	UNP Q12KT8
E	312	HIS	-	expression tag	UNP Q12KT8
F	305	LEU	-	expression tag	UNP Q12KT8
F	306	GLU	-	expression tag	UNP Q12KT8
F	307	HIS	-	expression tag	UNP Q12KT8
F	308	HIS	-	expression tag	UNP Q12KT8
F	309	HIS	-	expression tag	UNP Q12KT8
F	310	HIS	-	expression tag	UNP Q12KT8
F	311	HIS	-	expression tag	UNP Q12KT8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	312	HIS	-	expression tag	UNP Q12KT8
G	305	LEU	-	expression tag	UNP Q12KT8
G	306	GLU	-	expression tag	UNP Q12KT8
G	307	HIS	-	expression tag	UNP Q12KT8
G	308	HIS	-	expression tag	UNP Q12KT8
G	309	HIS	-	expression tag	UNP Q12KT8
G	310	HIS	-	expression tag	UNP Q12KT8
G	311	HIS	-	expression tag	UNP Q12KT8
G	312	HIS	-	expression tag	UNP Q12KT8
H	305	LEU	-	expression tag	UNP Q12KT8
H	306	GLU	-	expression tag	UNP Q12KT8
H	307	HIS	-	expression tag	UNP Q12KT8
H	308	HIS	-	expression tag	UNP Q12KT8
H	309	HIS	-	expression tag	UNP Q12KT8
H	310	HIS	-	expression tag	UNP Q12KT8
H	311	HIS	-	expression tag	UNP Q12KT8
H	312	HIS	-	expression tag	UNP Q12KT8
I	305	LEU	-	expression tag	UNP Q12KT8
I	306	GLU	-	expression tag	UNP Q12KT8
I	307	HIS	-	expression tag	UNP Q12KT8
I	308	HIS	-	expression tag	UNP Q12KT8
I	309	HIS	-	expression tag	UNP Q12KT8
I	310	HIS	-	expression tag	UNP Q12KT8
I	311	HIS	-	expression tag	UNP Q12KT8
I	312	HIS	-	expression tag	UNP Q12KT8
J	305	LEU	-	expression tag	UNP Q12KT8
J	306	GLU	-	expression tag	UNP Q12KT8
J	307	HIS	-	expression tag	UNP Q12KT8
J	308	HIS	-	expression tag	UNP Q12KT8
J	309	HIS	-	expression tag	UNP Q12KT8
J	310	HIS	-	expression tag	UNP Q12KT8
J	311	HIS	-	expression tag	UNP Q12KT8
J	312	HIS	-	expression tag	UNP Q12KT8
K	305	LEU	-	expression tag	UNP Q12KT8
K	306	GLU	-	expression tag	UNP Q12KT8
K	307	HIS	-	expression tag	UNP Q12KT8
K	308	HIS	-	expression tag	UNP Q12KT8
K	309	HIS	-	expression tag	UNP Q12KT8
K	310	HIS	-	expression tag	UNP Q12KT8
K	311	HIS	-	expression tag	UNP Q12KT8
K	312	HIS	-	expression tag	UNP Q12KT8
L	305	LEU	-	expression tag	UNP Q12KT8

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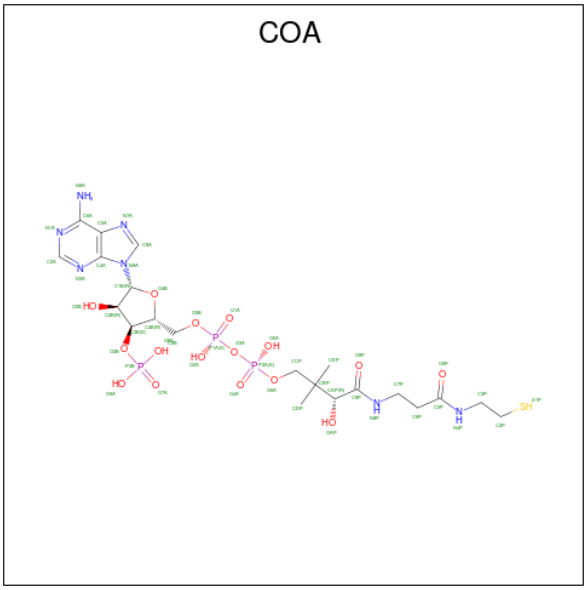
Chain	Residue	Modelled	Actual	Comment	Reference
L	306	GLU	-	expression tag	UNP Q12KT8
L	307	HIS	-	expression tag	UNP Q12KT8
L	308	HIS	-	expression tag	UNP Q12KT8
L	309	HIS	-	expression tag	UNP Q12KT8
L	310	HIS	-	expression tag	UNP Q12KT8
L	311	HIS	-	expression tag	UNP Q12KT8
L	312	HIS	-	expression tag	UNP Q12KT8

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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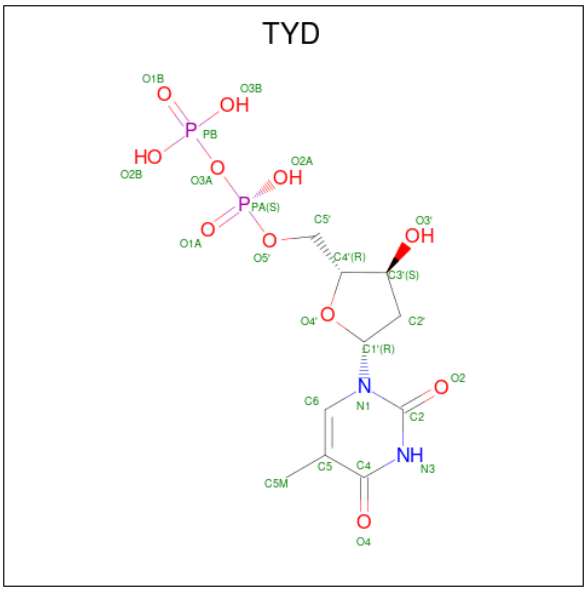
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	E	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	F	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	G	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

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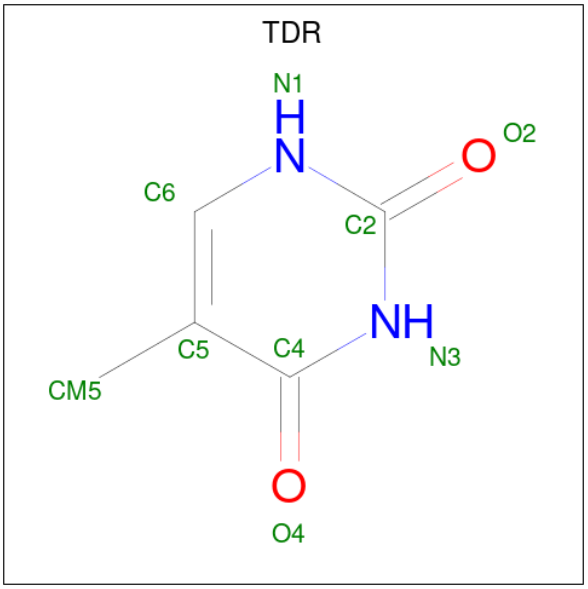
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	I	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	J	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	K	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	L	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 4 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	2	2		
4	B	1	Total	C	N	O	0	0
			9	5	2	2		
4	C	1	Total	C	N	O	0	0
			9	5	2	2		
4	D	1	Total	C	N	O	0	0
			9	5	2	2		
4	E	1	Total	C	N	O	0	0
			9	5	2	2		
4	F	1	Total	C	N	O	0	0
			9	5	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C N O 9 5 2 2	0	0
4	K	1	Total C N O 9 5 2 2	0	0
4	L	1	Total C N O 9 5 2 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	93	Total O 93 93	0	0
6	B	100	Total O 100 100	0	0
6	C	87	Total O 87 87	0	0
6	D	53	Total O 53 53	0	0
6	E	66	Total O 66 66	0	0
6	F	61	Total O 61 61	0	0
6	G	80	Total O 80 80	0	0
6	H	42	Total O 42 42	0	0
6	I	67	Total O 67 67	0	0

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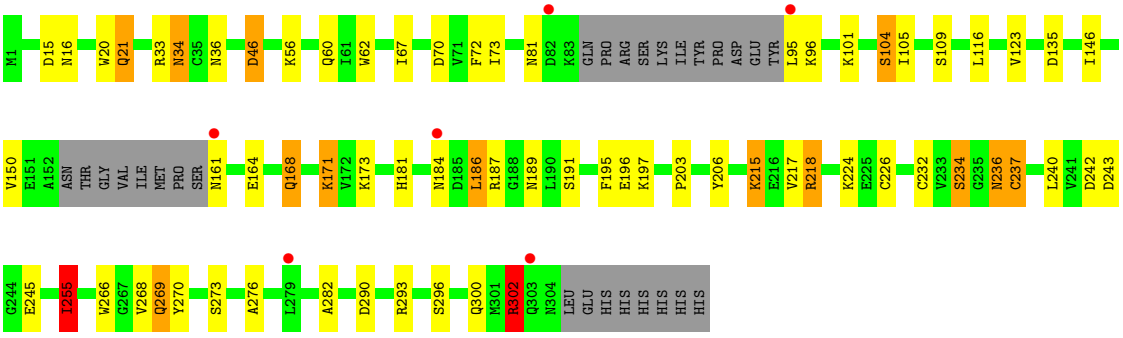
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	54	Total O 54 54	0	0
6	K	82	Total O 82 82	0	0
6	L	62	Total O 62 62	0	0

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.

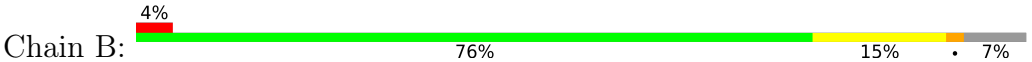
• Molecule 1: WxcM-like protein

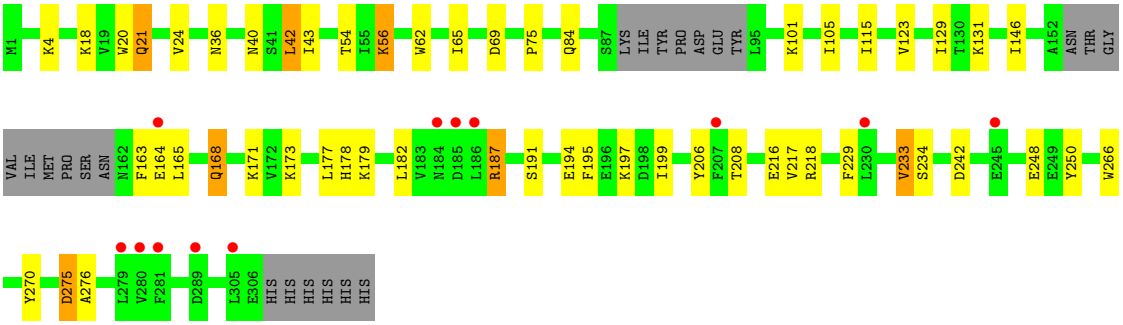
Chain A:



• Molecule 1: WxcM-like protein

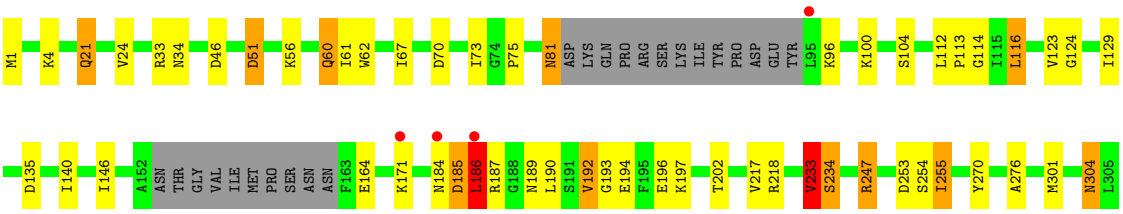
Chain B:

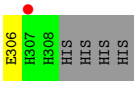




• Molecule 1: WxcM-like protein

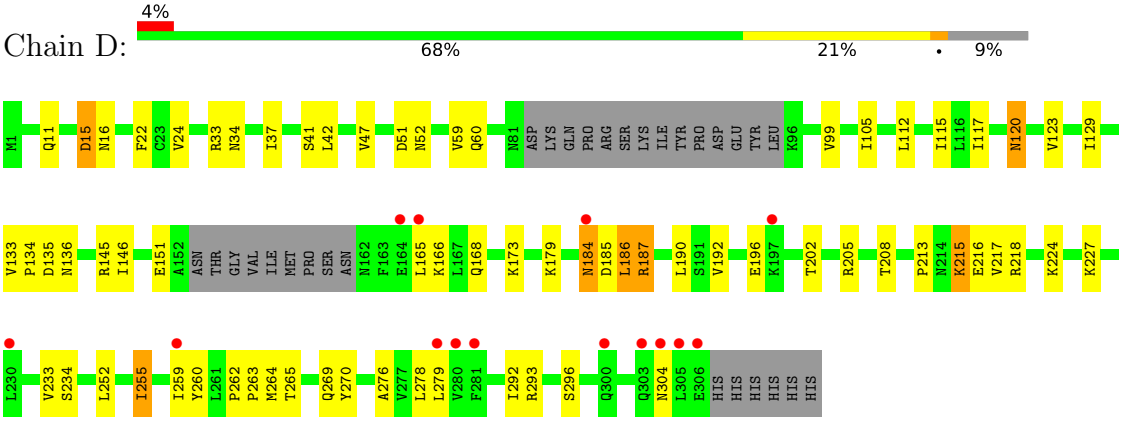
Chain C:





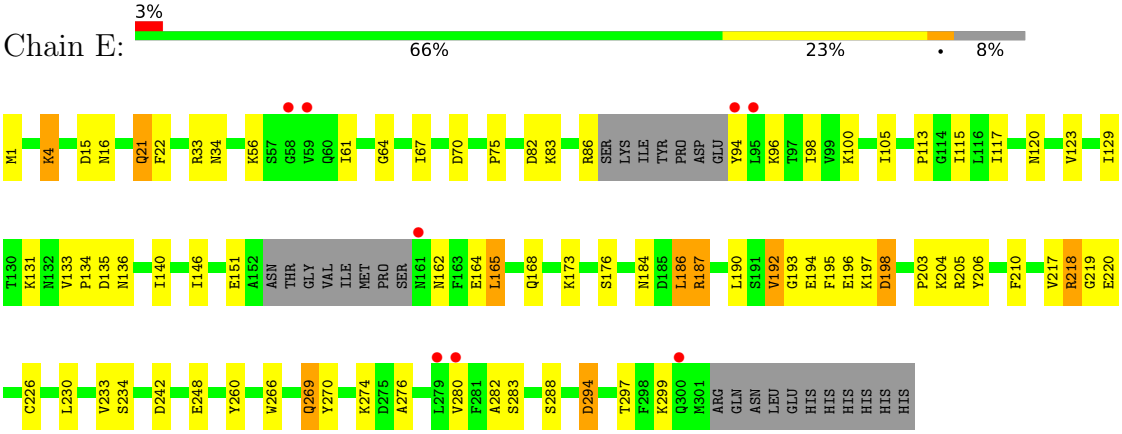
• Molecule 1: WxcM-like protein

Chain D:



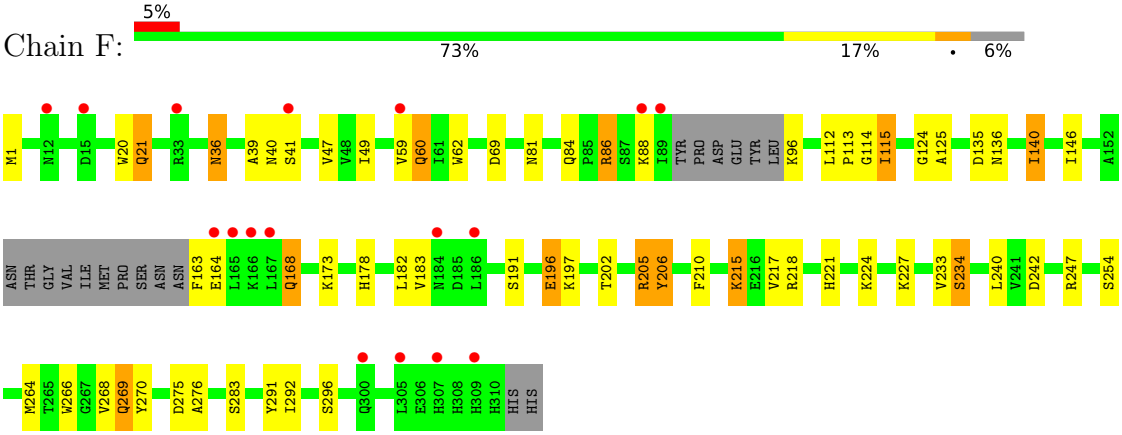
• Molecule 1: WxcM-like protein

Chain E:



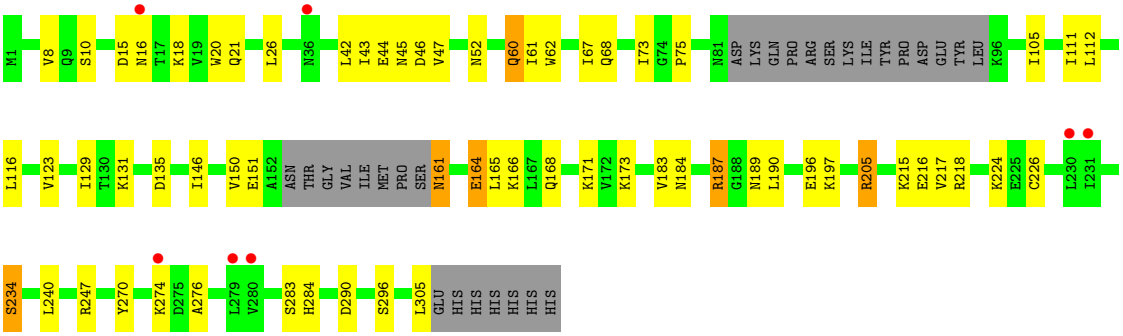
• Molecule 1: WxcM-like protein

Chain F:

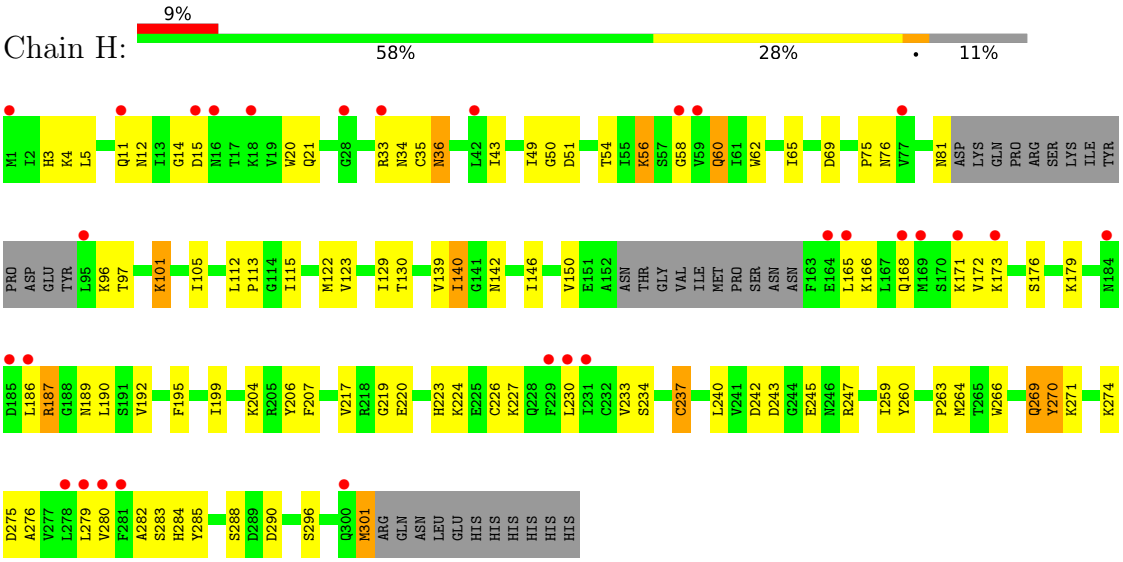


• Molecule 1: WxcM-like protein

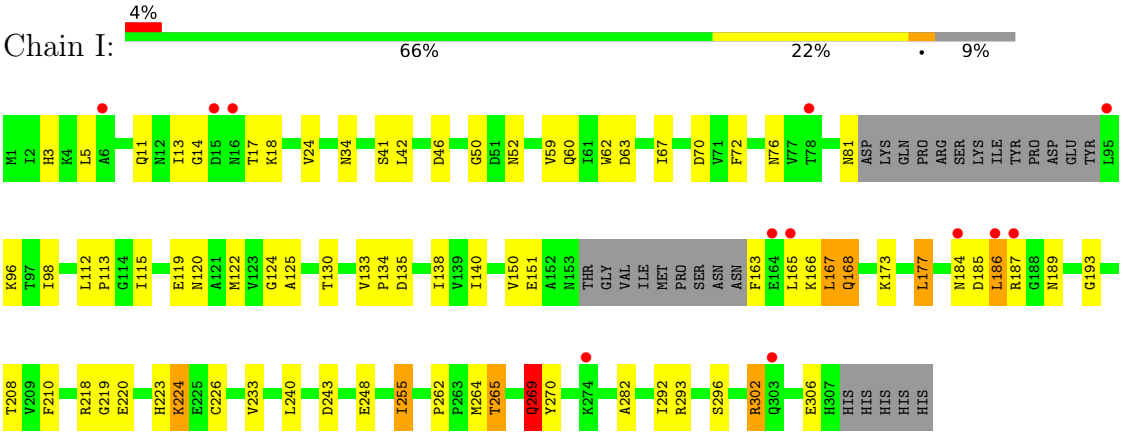
Chain G:



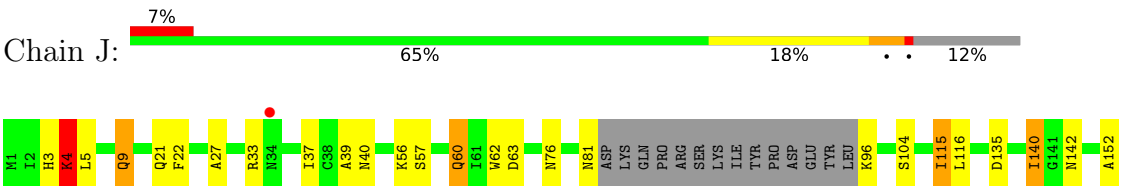
• Molecule 1: WxcM-like protein

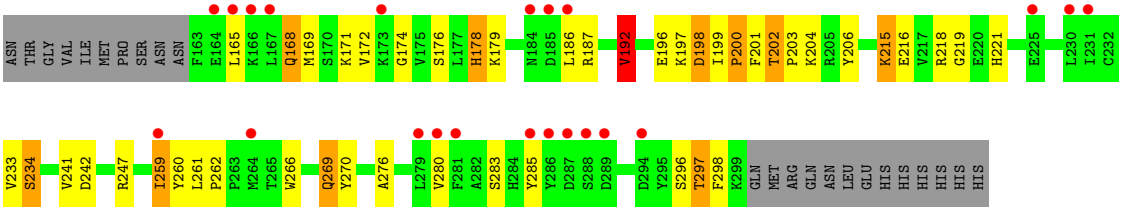


• Molecule 1: WxcM-like protein



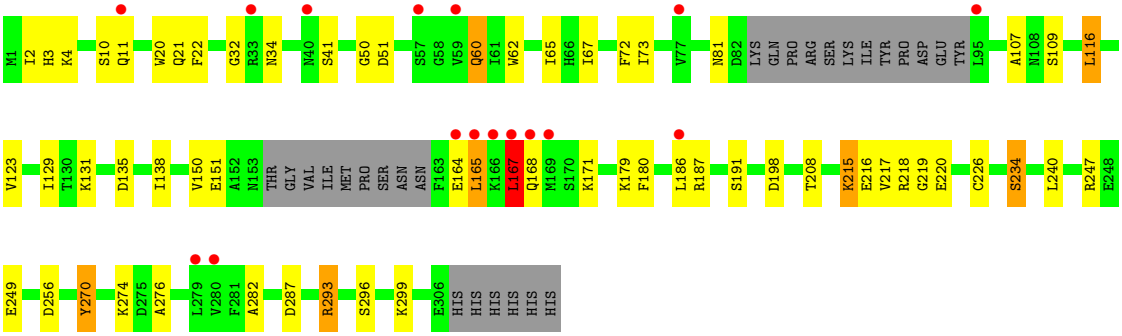
• Molecule 1: WxcM-like protein





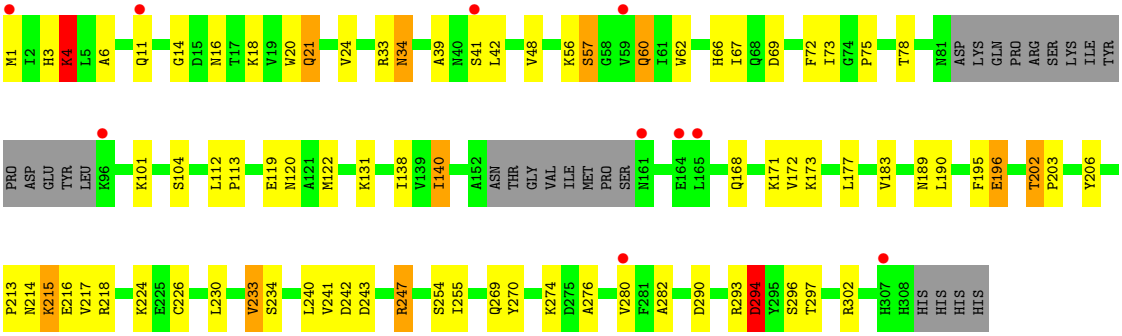
• Molecule 1: WxcM-like protein

Chain K:



• Molecule 1: WxcM-like protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.31Å 109.44Å 127.85Å 79.23° 79.98° 84.89°	Depositor
Resolution (Å)	30.00 – 2.20 28.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.00-2.20) 90.9 (28.75-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.17 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.270 0.204 , 0.268	Depositor DCC
R_{free} test set	10284 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28412	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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: TYD, MG, COA, TDR

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	0.70	1/2261 (0.0%)	1.11	9/3059 (0.3%)
1	B	0.66	0/2304	1.06	4/3117 (0.1%)
1	C	0.68	0/2266	1.13	11/3066 (0.4%)
1	D	0.60	0/2245	1.06	6/3038 (0.2%)
1	E	0.61	0/2274	1.06	7/3078 (0.2%)
1	F	0.64	0/2331	1.09	6/3153 (0.2%)
1	G	0.63	0/2250	1.04	4/3045 (0.1%)
1	H	0.52	1/2200 (0.0%)	0.95	5/2978 (0.2%)
1	I	0.60	0/2258	1.04	4/3056 (0.1%)
1	J	0.56	0/2184	0.98	5/2956 (0.2%)
1	K	0.65	0/2270	1.08	10/3071 (0.3%)
1	L	0.61	0/2272	1.05	3/3074 (0.1%)
All	All	0.62	2/27115 (0.0%)	1.05	74/36691 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	CYS	CB-SG	-6.57	1.71	1.82
1	H	237	CYS	CB-SG	-5.43	1.73	1.81

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	ARG	NE-CZ-NH2	-14.92	112.84	120.30
1	C	247	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	56	LYS	CD-CE-NZ	7.64	129.28	111.70
1	A	237	CYS	N-CA-CB	-7.60	96.93	110.60
1	K	135	ASP	CB-CG-OD1	7.56	125.10	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	233	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2220	0	2214	57	0
1	B	2262	0	2258	38	0
1	C	2222	0	2219	48	0
1	D	2204	0	2197	37	0
1	E	2231	0	2224	45	0
1	F	2288	0	2278	51	0
1	G	2206	0	2202	48	0
1	H	2159	0	2158	61	0
1	I	2217	0	2210	57	0
1	J	2140	0	2143	45	0
1	K	2226	0	2225	37	0
1	L	2228	0	2220	49	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	0	0
2	D	48	0	32	1	0
2	E	48	0	32	0	0
2	F	48	0	32	0	0
2	G	96	0	64	1	0
2	I	48	0	32	2	0
2	J	48	0	32	4	0
2	K	48	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	48	0	32	3	0
3	A	25	0	13	0	0
3	B	25	0	13	0	0
3	C	25	0	13	0	0
3	D	25	0	13	2	0
3	E	25	0	13	4	0
3	F	25	0	13	1	0
3	G	25	0	13	1	0
3	H	25	0	13	1	0
3	I	25	0	13	0	0
3	J	25	0	13	0	0
3	K	25	0	13	0	0
3	L	25	0	13	1	0
4	A	9	0	6	1	0
4	B	9	0	6	0	0
4	C	9	0	6	0	0
4	D	9	0	6	0	0
4	E	9	0	6	0	0
4	F	9	0	6	0	0
4	J	9	0	6	0	0
4	K	9	0	6	0	0
4	L	9	0	6	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	93	0	0	1	0
6	B	100	0	0	2	0
6	C	87	0	0	1	0
6	D	53	0	0	0	0
6	E	66	0	0	1	0
6	F	61	0	0	3	0
6	G	80	0	0	1	1
6	H	42	0	0	1	0
6	I	67	0	0	1	0
6	J	54	0	0	1	1
6	K	82	0	0	2	0
6	L	62	0	0	2	0
All	All	28412	0	27142	517	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 9.

The worst 5 of 517 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:236:ASN:HD21	1:A:273:SER:HB3	1.05	1.12
1:A:236:ASN:ND2	1:A:273:SER:HB3	1.64	1.11
1:A:60:GLN:HG3	1:A:62:TRP:CZ2	1.91	1.05
1:A:184:ASN:HB3	1:A:189:ASN:HD22	1.23	1.04
1:K:215[A]:LYS:HE3	1:K:215[A]:LYS:H	1.22	1.03

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)
6:G:566:HOH:O	6:J:526:HOH:O[1_545]	1.99	0.21

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	279/312 (89%)	269 (96%)	9 (3%)	1 (0%)	34	37
1	B	284/312 (91%)	270 (95%)	14 (5%)	0	100	100
1	C	280/312 (90%)	270 (96%)	10 (4%)	0	100	100
1	D	277/312 (89%)	263 (95%)	13 (5%)	1 (0%)	34	37
1	E	280/312 (90%)	266 (95%)	13 (5%)	1 (0%)	34	37
1	F	288/312 (92%)	268 (93%)	20 (7%)	0	100	100
1	G	278/312 (89%)	267 (96%)	10 (4%)	1 (0%)	34	37
1	H	272/312 (87%)	252 (93%)	19 (7%)	1 (0%)	34	37
1	I	279/312 (89%)	261 (94%)	16 (6%)	2 (1%)	22	22
1	J	270/312 (86%)	258 (96%)	9 (3%)	3 (1%)	14	12
1	K	280/312 (90%)	261 (93%)	16 (6%)	3 (1%)	14	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	281/312 (90%)	260 (92%)	19 (7%)	2 (1%)	22 22
All	All	3348/3744 (89%)	3165 (94%)	168 (5%)	15 (0%)	34 37

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	H	14	GLY
1	K	3	HIS
1	J	297	THR
1	E	197	LYS

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	246/272 (90%)	220 (89%)	26 (11%)	6 6
1	B	251/272 (92%)	230 (92%)	21 (8%)	11 11
1	C	245/272 (90%)	224 (91%)	21 (9%)	10 10
1	D	244/272 (90%)	218 (89%)	26 (11%)	6 6
1	E	247/272 (91%)	220 (89%)	27 (11%)	6 5
1	F	252/272 (93%)	231 (92%)	21 (8%)	11 11
1	G	245/272 (90%)	225 (92%)	20 (8%)	11 11
1	H	239/272 (88%)	211 (88%)	28 (12%)	5 4
1	I	245/272 (90%)	228 (93%)	17 (7%)	15 16
1	J	237/272 (87%)	206 (87%)	31 (13%)	4 3
1	K	247/272 (91%)	225 (91%)	22 (9%)	9 9
1	L	246/272 (90%)	217 (88%)	29 (12%)	5 4
All	All	2944/3264 (90%)	2655 (90%)	289 (10%)	8 7

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	215[A]	LYS
1	L	293	ARG
1	K	4	LYS
1	L	4	LYS
1	E	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	269	GLN
1	K	136	ASN
1	F	40	ASN
1	E	269	GLN
1	K	184	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 5 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	TDR	B	403	-	9,9,9	2.39	2 (22%)	12,12,12	2.73	7 (58%)
2	COA	G	401	-	41,50,50	0.82	1 (2%)	52,75,75	1.76	14 (26%)
2	COA	F	401	-	41,50,50	0.78	2 (4%)	52,75,75	1.76	10 (19%)
2	COA	L	401	-	41,50,50	0.76	1 (2%)	52,75,75	1.66	13 (25%)
3	TYD	H	401	-	21,26,26	0.71	0	27,40,40	1.81	2 (7%)
3	TYD	J	402	-	21,26,26	0.72	0	27,40,40	1.55	1 (3%)
3	TYD	A	402	-	21,26,26	0.73	0	27,40,40	1.69	1 (3%)
4	TDR	L	403	-	9,9,9	2.08	3 (33%)	12,12,12	3.66	8 (66%)
3	TYD	D	402	-	21,26,26	0.69	0	27,40,40	1.45	3 (11%)
4	TDR	A	403	-	9,9,9	2.10	2 (22%)	12,12,12	4.75	8 (66%)
3	TYD	B	402	-	21,26,26	0.60	0	27,40,40	1.62	3 (11%)
2	COA	K	401	-	41,50,50	0.72	1 (2%)	52,75,75	1.62	9 (17%)
2	COA	I	401	-	41,50,50	0.83	2 (4%)	52,75,75	1.58	8 (15%)
4	TDR	K	403	-	9,9,9	2.03	2 (22%)	12,12,12	2.55	5 (41%)
2	COA	J	401	-	41,50,50	0.75	1 (2%)	52,75,75	1.99	11 (21%)
3	TYD	L	402	-	21,26,26	0.69	0	27,40,40	1.57	2 (7%)
2	COA	C	401	-	41,50,50	0.86	2 (4%)	52,75,75	1.98	11 (21%)
4	TDR	F	403	-	9,9,9	2.13	2 (22%)	12,12,12	2.93	6 (50%)
3	TYD	K	402	-	21,26,26	0.63	0	27,40,40	1.83	4 (14%)
2	COA	E	401	-	41,50,50	0.72	1 (2%)	52,75,75	1.67	12 (23%)
4	TDR	J	403	-	9,9,9	2.16	2 (22%)	12,12,12	3.28	7 (58%)
3	TYD	I	402	-	21,26,26	0.65	0	27,40,40	1.41	4 (14%)
4	TDR	C	403	-	9,9,9	2.21	3 (33%)	12,12,12	3.50	7 (58%)
2	COA	D	401	-	41,50,50	0.75	1 (2%)	52,75,75	1.58	12 (23%)
3	TYD	F	402	-	21,26,26	0.59	0	27,40,40	1.46	3 (11%)
4	TDR	E	403	-	9,9,9	2.14	3 (33%)	12,12,12	2.97	7 (58%)
3	TYD	C	402	-	21,26,26	0.67	0	27,40,40	1.59	3 (11%)
3	TYD	G	402	-	21,26,26	0.63	0	27,40,40	1.59	5 (18%)
2	COA	A	401	-	41,50,50	0.91	2 (4%)	52,75,75	1.84	15 (28%)
2	COA	B	401	-	41,50,50	0.83	2 (4%)	52,75,75	1.70	13 (25%)
2	COA	G	403	-	41,50,50	0.73	0	52,75,75	1.54	9 (17%)
3	TYD	E	402	-	21,26,26	0.64	0	27,40,40	1.67	5 (18%)
4	TDR	D	403	-	9,9,9	2.21	3 (33%)	12,12,12	3.56	8 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TDR	B	403	-	-	-	0/1/1/1
2	COA	G	401	-	-	5/44/64/64	0/3/3/3
2	COA	F	401	-	-	6/44/64/64	0/3/3/3
2	COA	L	401	-	-	10/44/64/64	0/3/3/3
3	TYD	H	401	-	-	2/13/28/28	0/2/2/2
3	TYD	J	402	-	-	7/13/28/28	0/2/2/2
3	TYD	A	402	-	-	4/13/28/28	0/2/2/2
4	TDR	L	403	-	-	-	0/1/1/1
3	TYD	D	402	-	-	0/13/28/28	0/2/2/2
4	TDR	A	403	-	-	-	0/1/1/1
3	TYD	B	402	-	-	8/13/28/28	0/2/2/2
2	COA	K	401	-	-	12/44/64/64	0/3/3/3
2	COA	I	401	-	-	4/44/64/64	0/3/3/3
4	TDR	K	403	-	-	-	0/1/1/1
2	COA	J	401	-	-	10/44/64/64	0/3/3/3
3	TYD	L	402	-	-	3/13/28/28	0/2/2/2
2	COA	C	401	-	-	6/44/64/64	0/3/3/3
4	TDR	F	403	-	-	-	0/1/1/1
3	TYD	K	402	-	-	3/13/28/28	0/2/2/2
2	COA	E	401	-	-	9/44/64/64	0/3/3/3
4	TDR	J	403	-	-	-	0/1/1/1
3	TYD	I	402	-	-	7/13/28/28	0/2/2/2
4	TDR	C	403	-	-	-	0/1/1/1
2	COA	D	401	-	-	9/44/64/64	0/3/3/3
3	TYD	F	402	-	-	8/13/28/28	0/2/2/2
4	TDR	E	403	-	-	-	0/1/1/1
3	TYD	C	402	-	-	3/13/28/28	0/2/2/2
3	TYD	G	402	-	-	2/13/28/28	0/2/2/2
2	COA	A	401	-	-	9/44/64/64	0/3/3/3
2	COA	B	401	-	-	5/44/64/64	0/3/3/3
2	COA	G	403	-	-	6/44/64/64	0/3/3/3
3	TYD	E	402	-	-	4/13/28/28	0/2/2/2
4	TDR	D	403	-	-	-	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	TDR	C6-C5	4.75	1.41	1.34
4	A	403	TDR	C6-C5	4.42	1.40	1.34
4	J	403	TDR	C6-C5	4.33	1.40	1.34
4	E	403	TDR	C6-C5	4.24	1.40	1.34
4	F	403	TDR	C6-C5	4.19	1.40	1.34

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	TDR	C5-C4-N3	11.19	124.86	115.31
3	H	401	TYD	C2-N3-C4	7.53	121.50	115.14
3	A	402	TYD	C2-N3-C4	7.49	121.46	115.14
3	K	402	TYD	C2-N3-C4	7.21	121.23	115.14
4	L	403	TDR	CM5-C5-C4	7.17	126.66	118.77

There are no chirality outliers.

5 of 142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	COA	OAP-CAP-CBP-CCP
2	A	401	COA	C9P-CAP-CBP-CCP
2	A	401	COA	OAP-CAP-CBP-CDP
2	A	401	COA	C9P-CAP-CBP-CDP
2	A	401	COA	OAP-CAP-CBP-CEP

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	COA	3	0
3	H	401	TYD	1	0
4	L	403	TDR	1	0
3	D	402	TYD	2	0
4	A	403	TDR	1	0
2	K	401	COA	3	0
2	I	401	COA	2	0
2	J	401	COA	4	0
3	L	402	TYD	1	0
2	D	401	COA	1	0
3	F	402	TYD	1	0
3	G	402	TYD	1	0
2	B	401	COA	1	0

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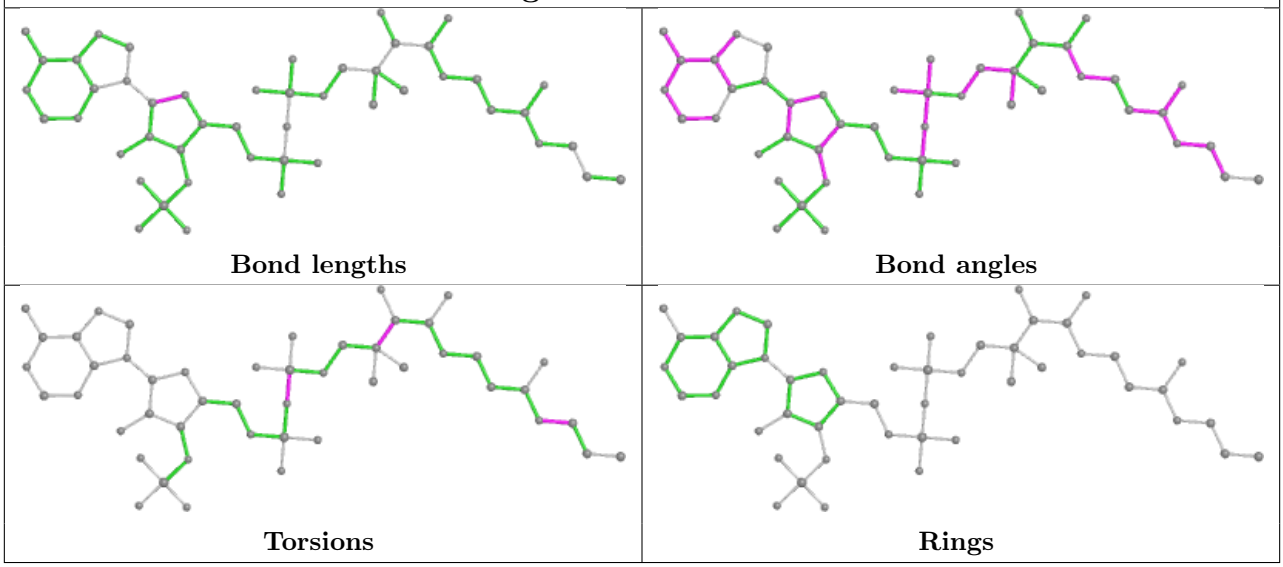
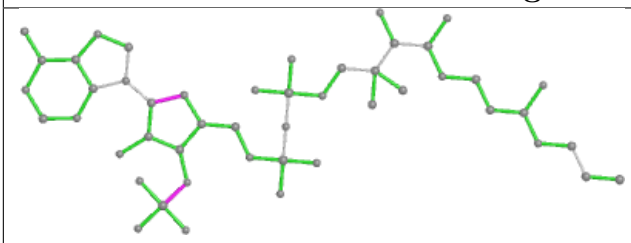
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	403	COA	1	0
3	E	402	TYD	4	0

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.

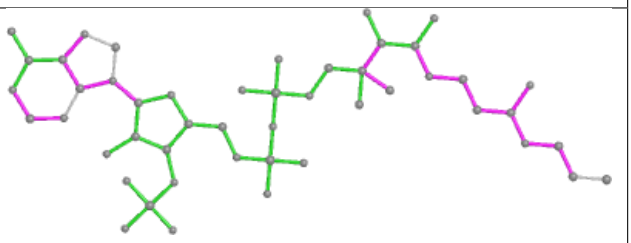
Ligand COA G 401



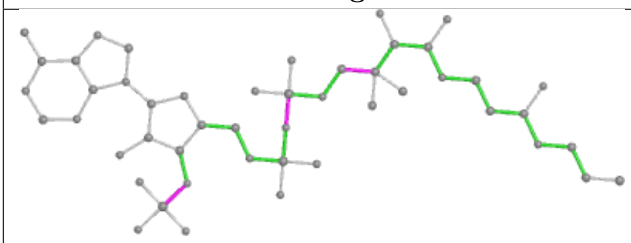
Ligand COA F 401



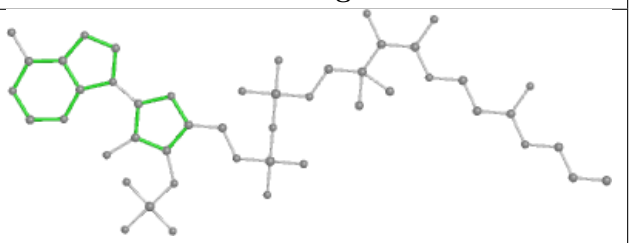
Bond lengths



Bond angles

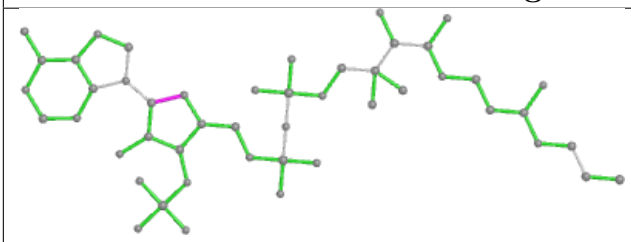


Torsions



Rings

Ligand COA L 401



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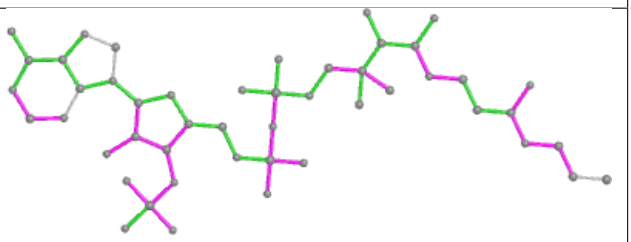
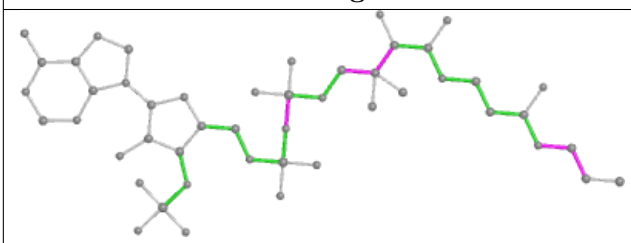


Bond angles



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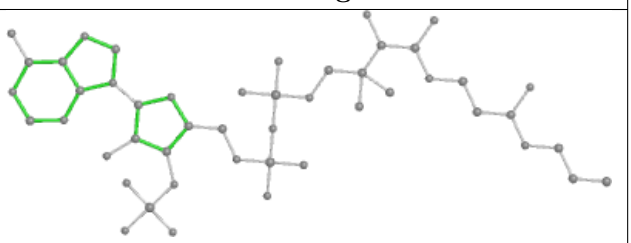
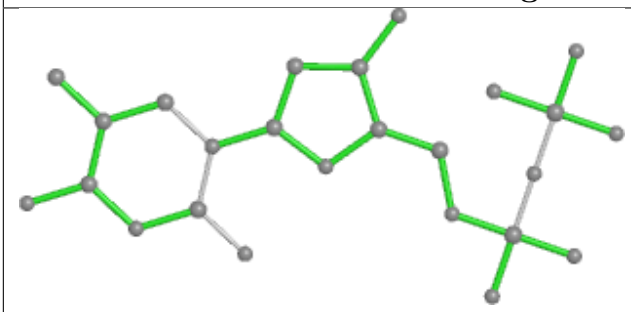


Rings

Ligand TYD H 401



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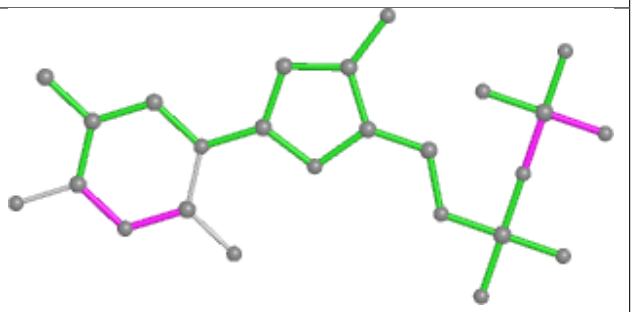
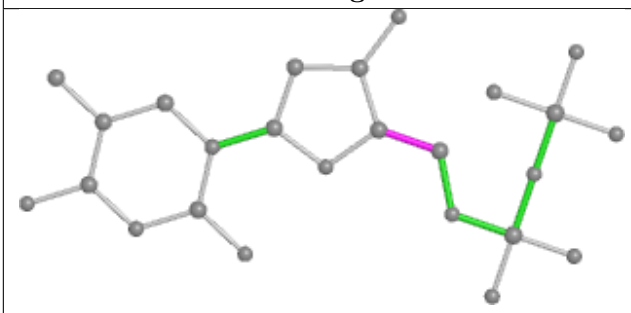


Bond angles



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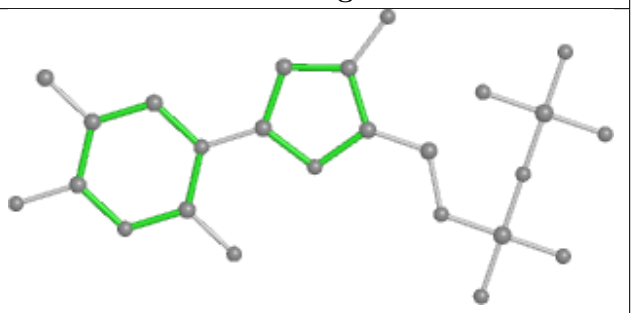
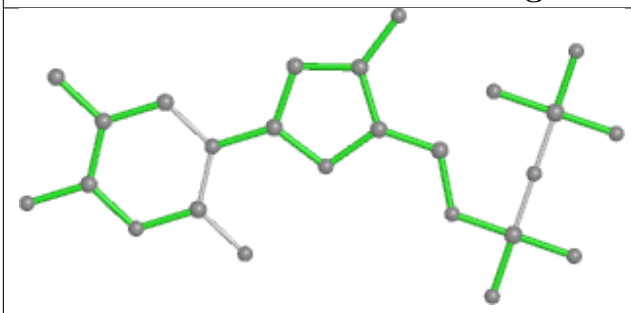


Rings

Ligand TYD J 402



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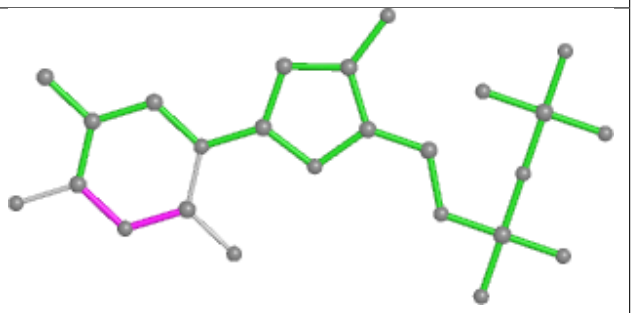
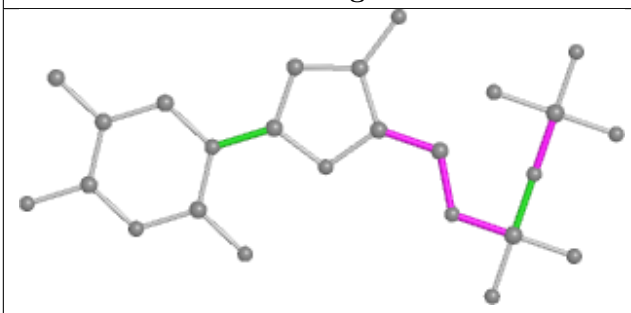


Bond angles



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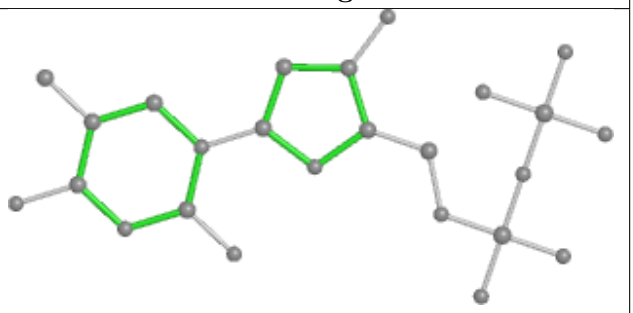
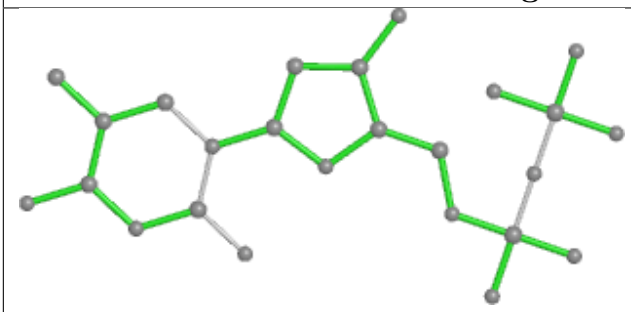
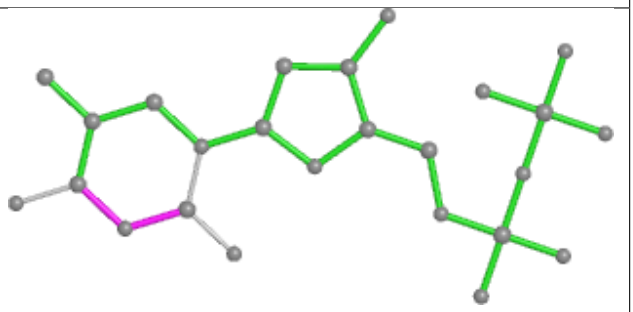
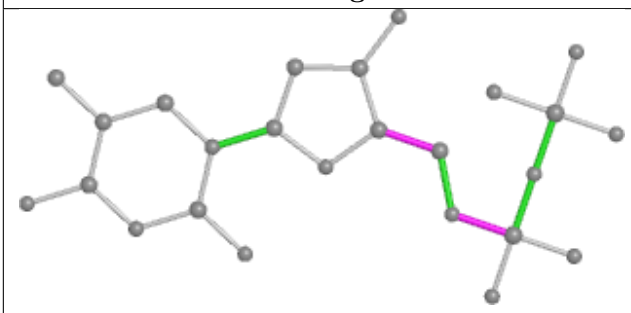
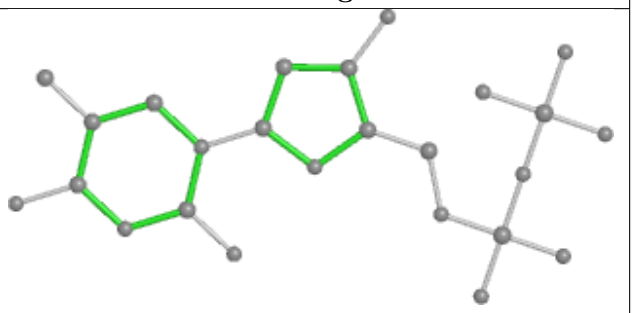


Rings

Ligand TYD A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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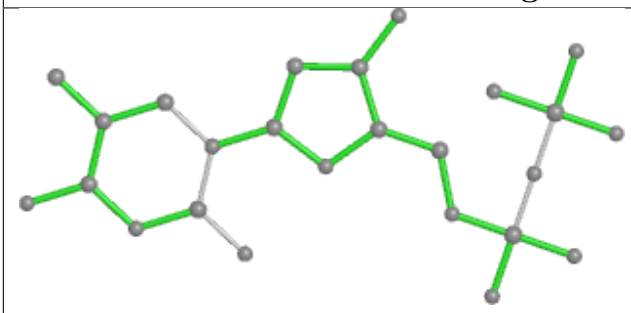
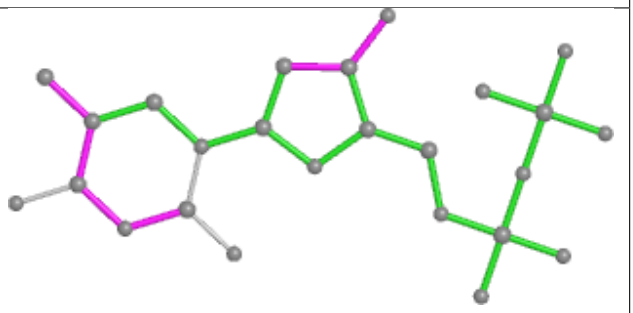
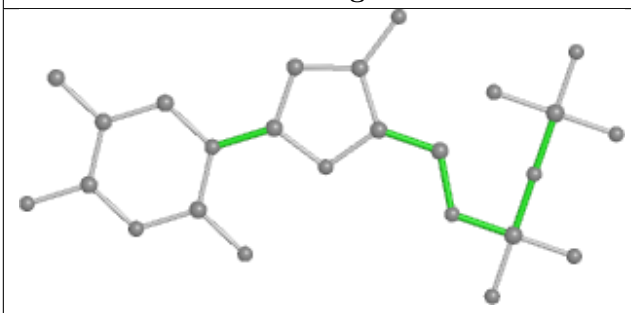
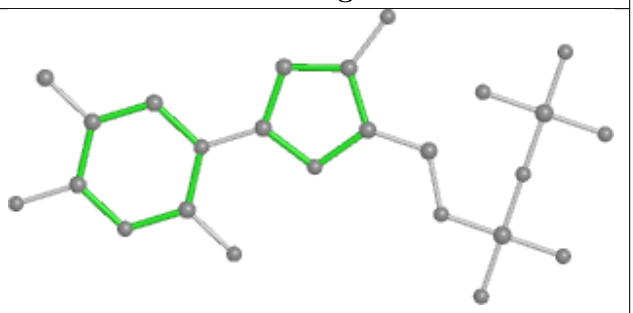
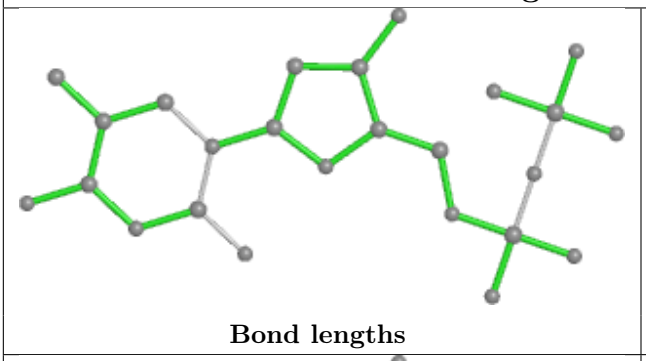
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TYD B 402



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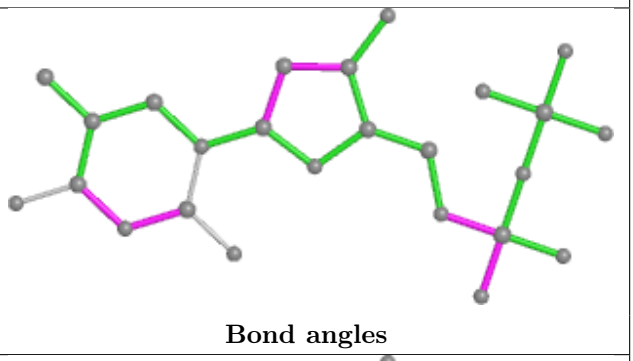
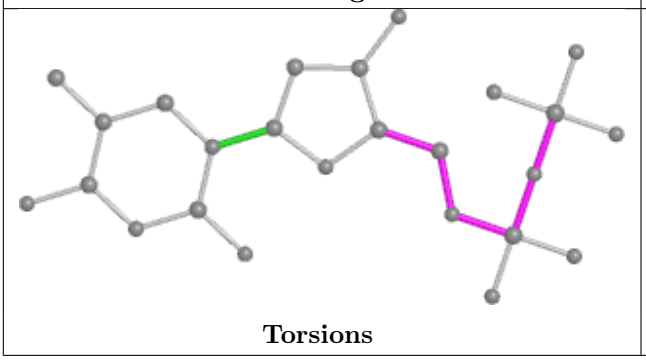


Bond angles



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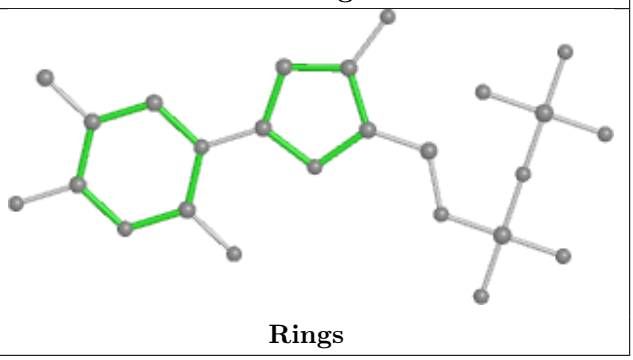
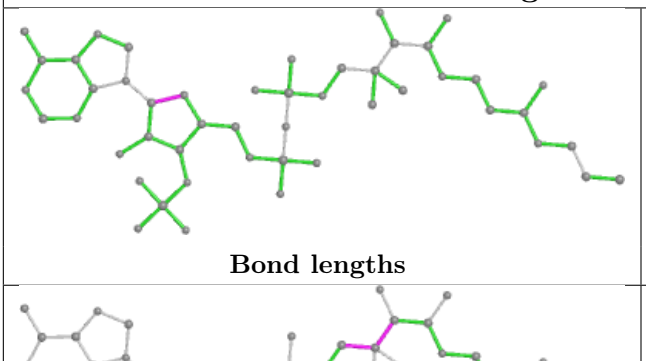


Rings

Ligand COA K 401



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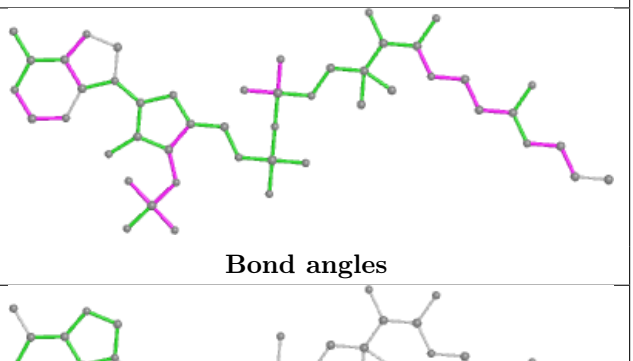
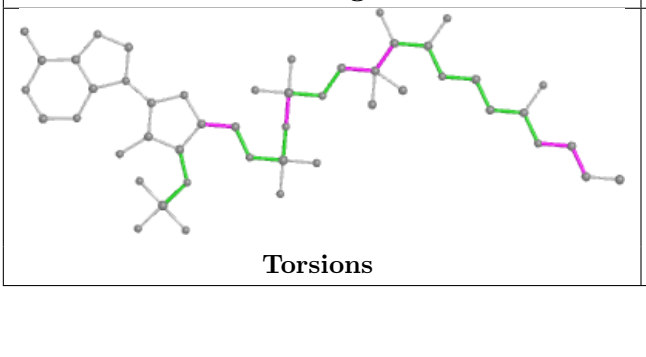


Bond angles



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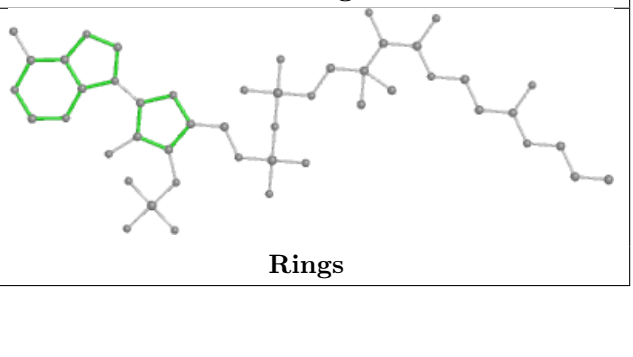
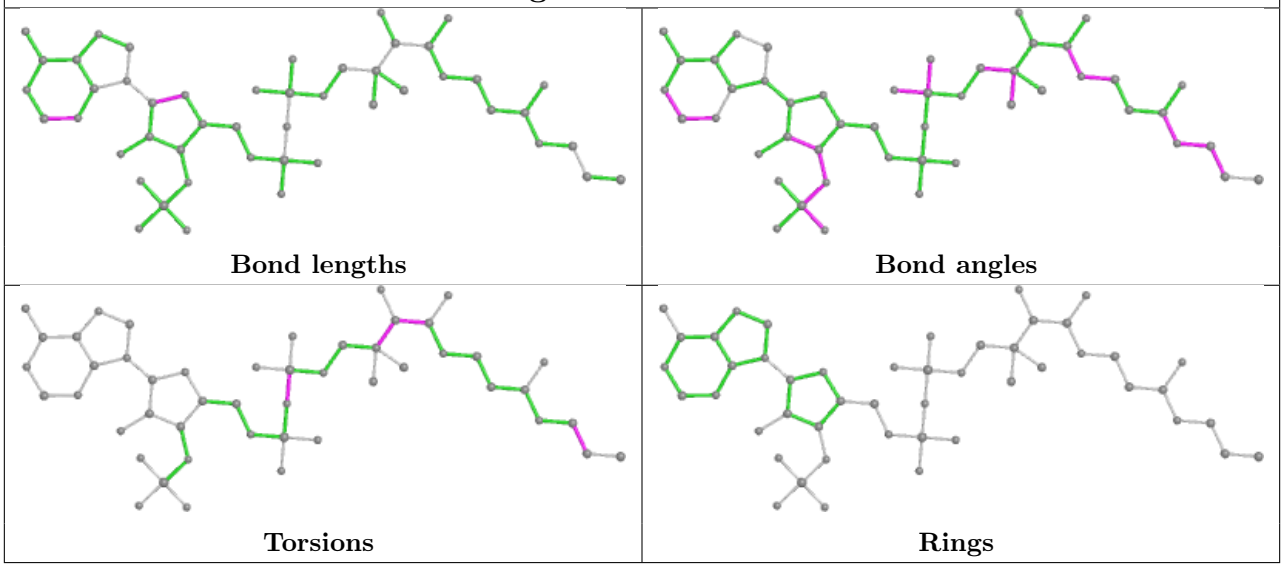


Rings

Ligand COA I 401



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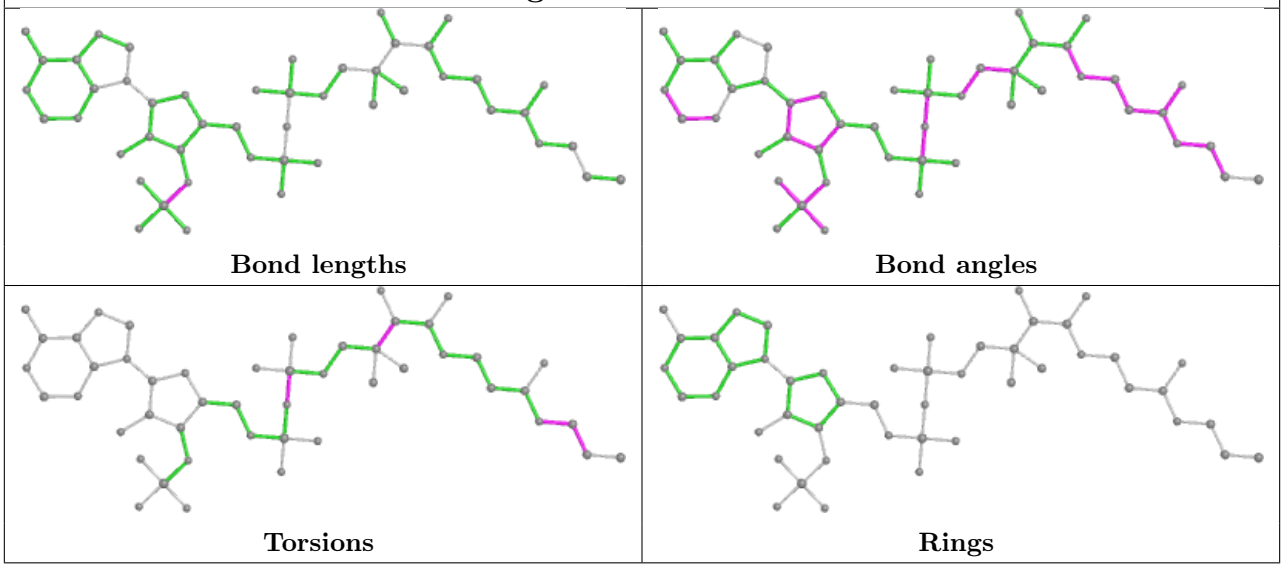
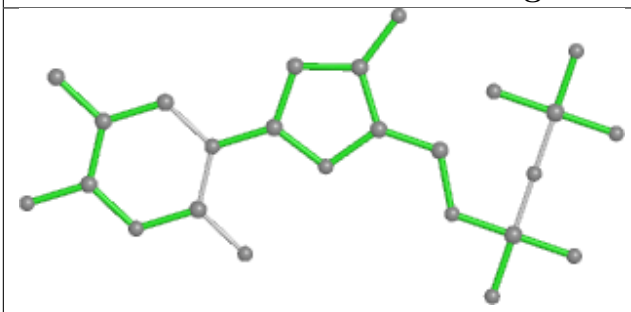
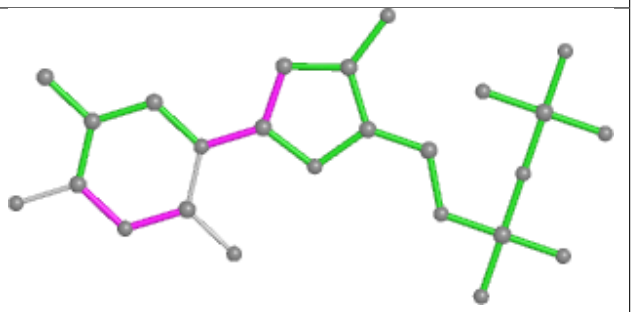


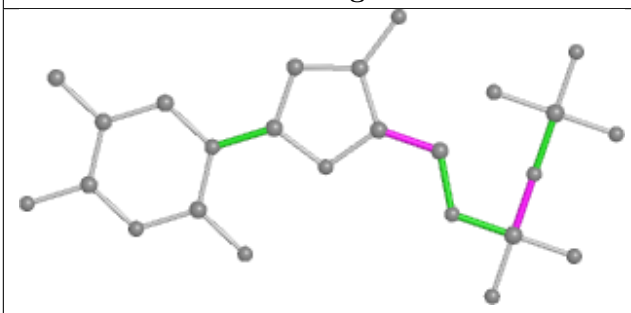
Ligand TYD L 402



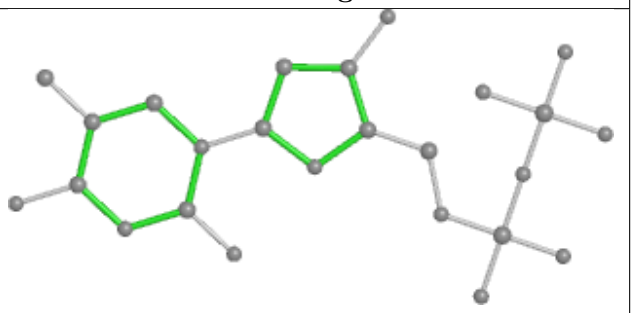
Bond lengths



Bond angles

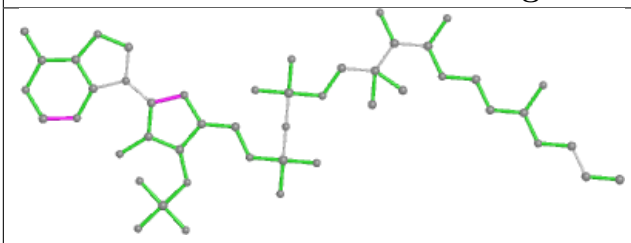


Torsions



Rings

Ligand COA C 401



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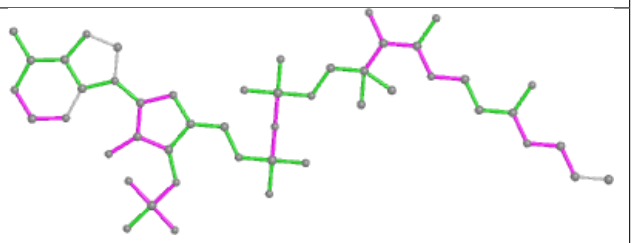
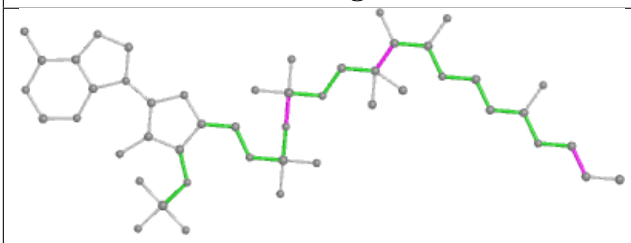


Bond angles



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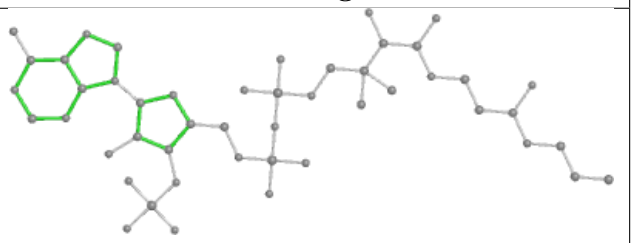
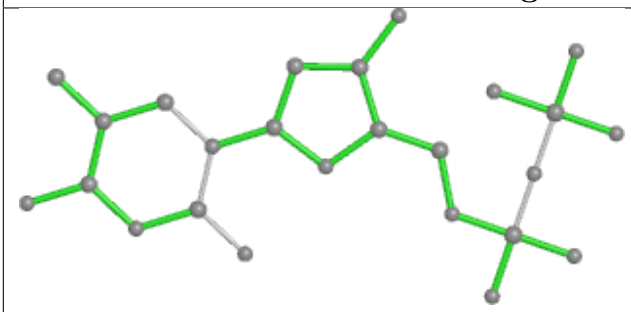


Rings

Ligand TYD K 402



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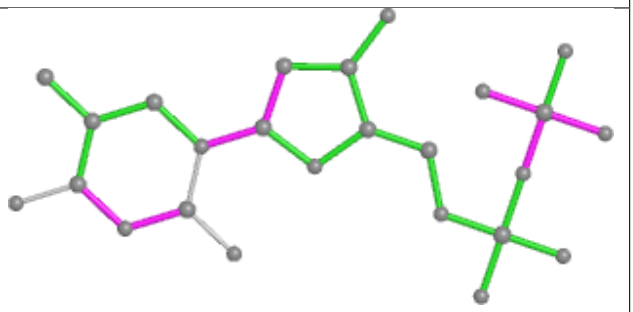
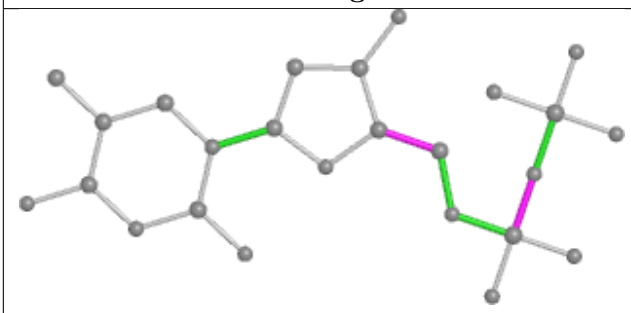
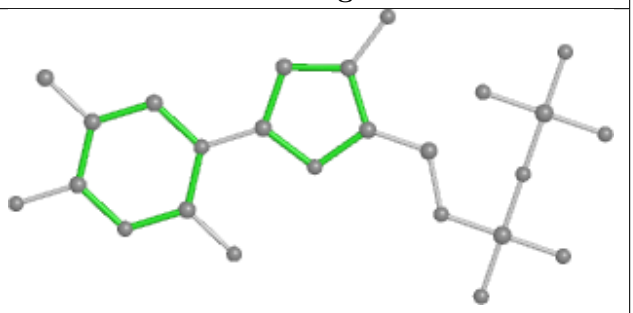


Bond angles

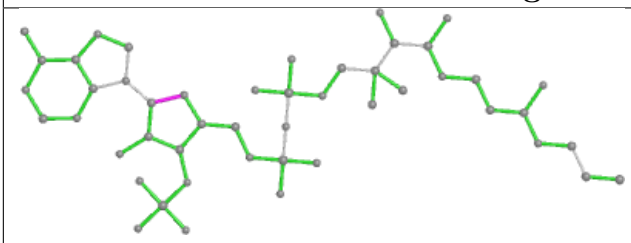


Torsions

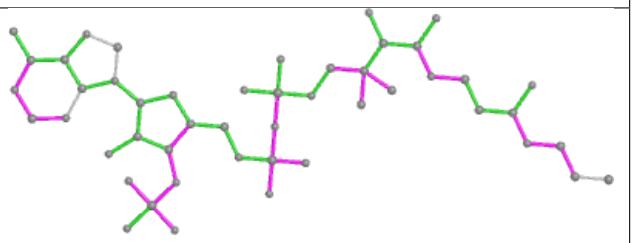


Rings

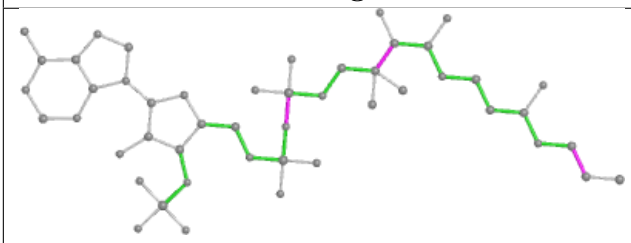
Ligand COA E 401



Bond lengths



Bond angles



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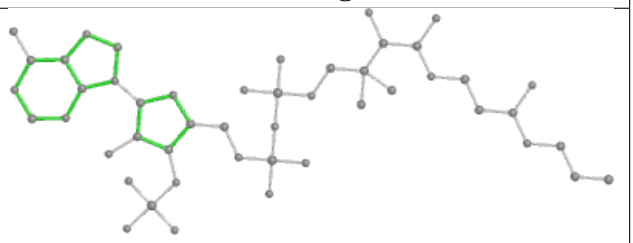
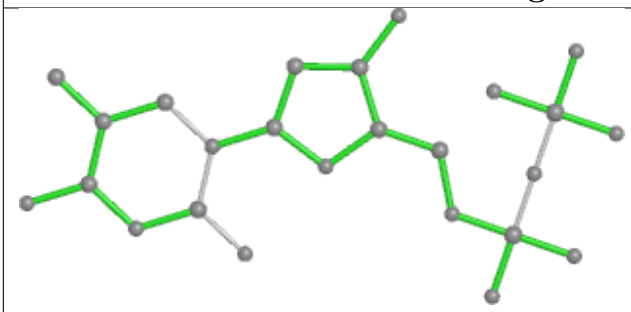
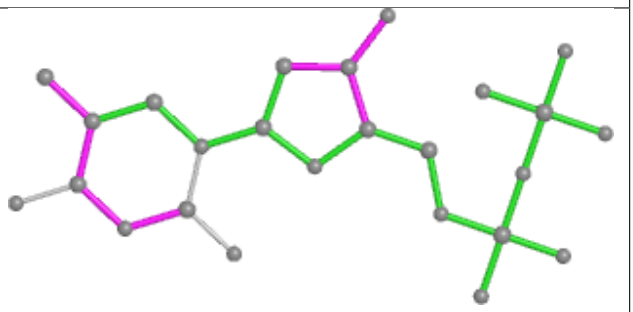


Rings

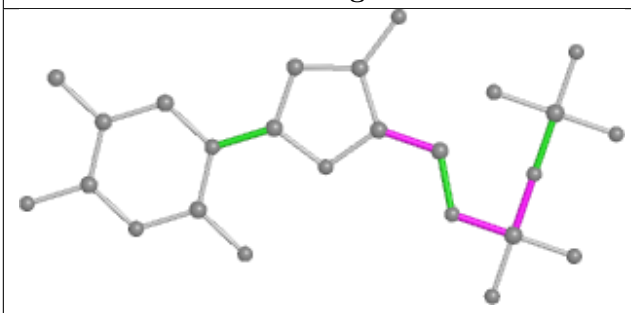
Ligand TYD I 402



Bond lengths



Bond angles



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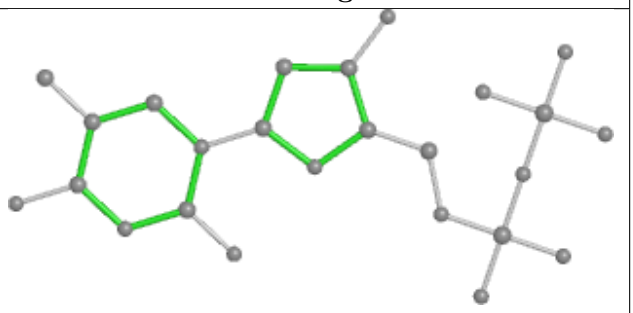
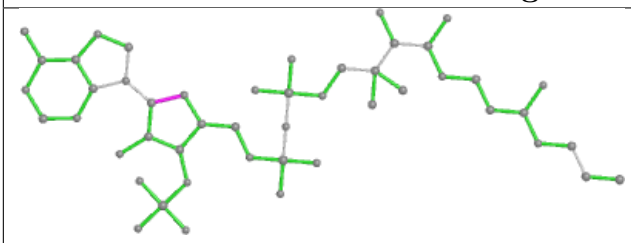
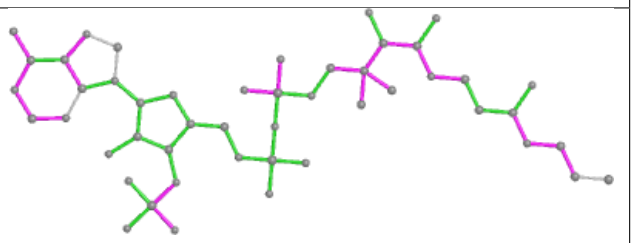


Rings

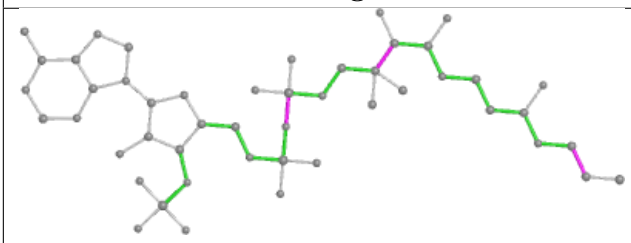
Ligand COA D 401



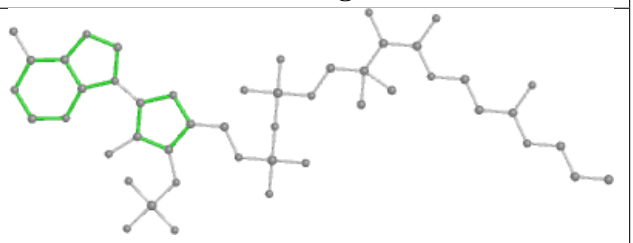
Bond lengths



Bond angles

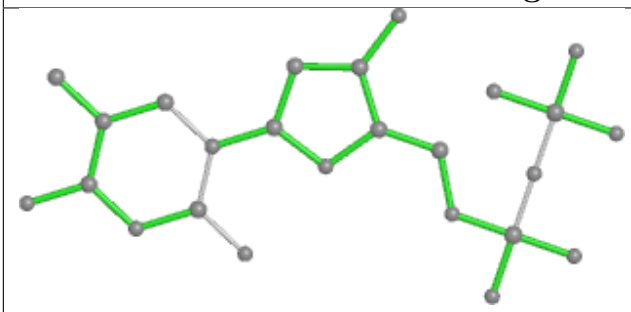


Torsions

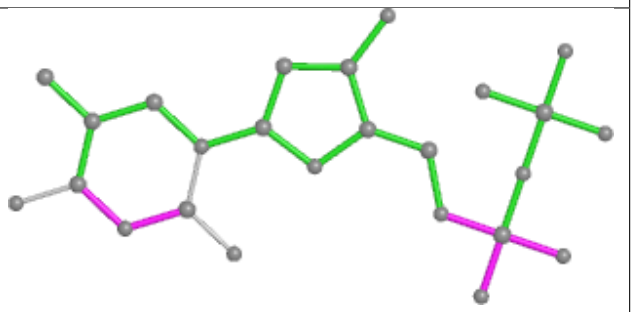


Rings

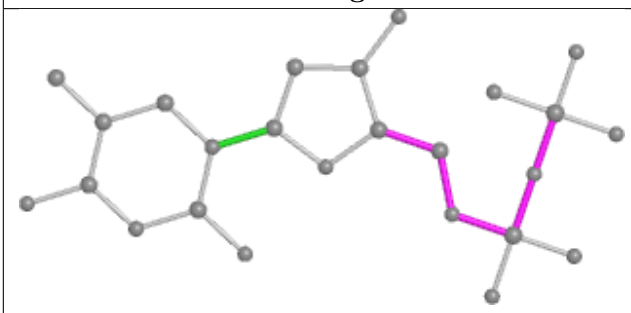
Ligand TYD F 402



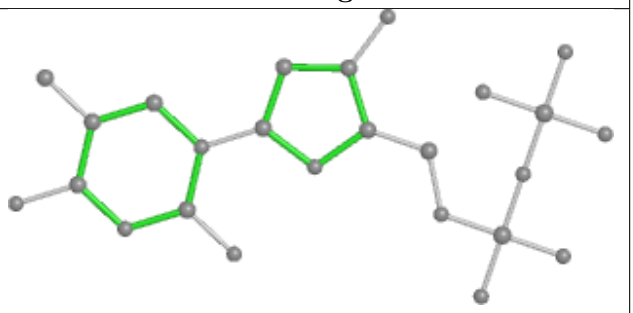
Bond lengths



Bond angles

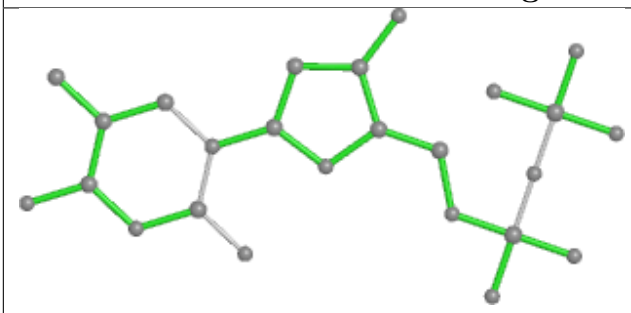


Torsions

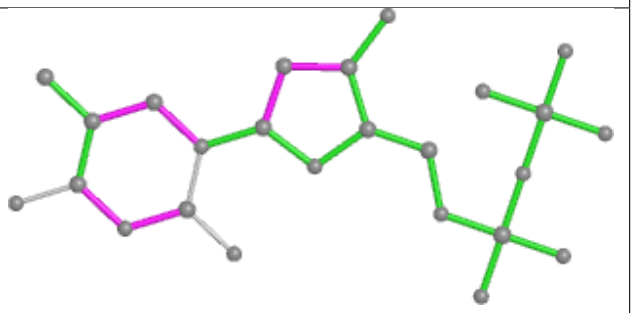


Rings

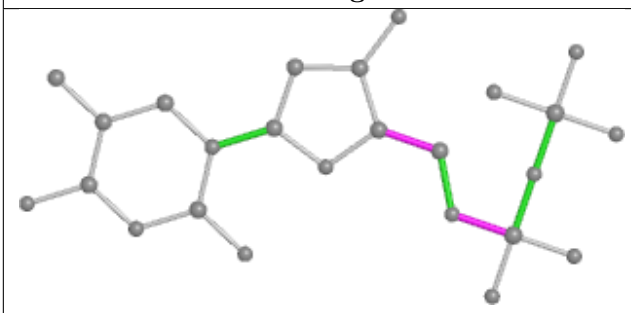
Ligand TYD C 402



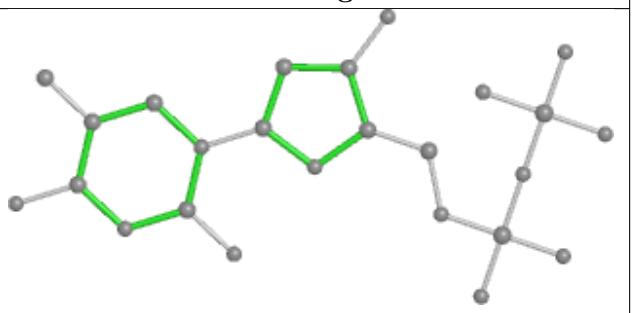
Bond lengths



Bond angles

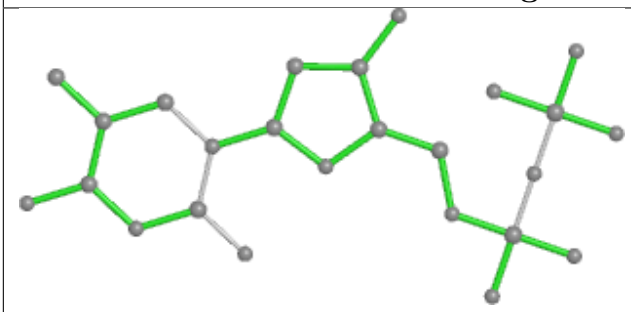


Torsions

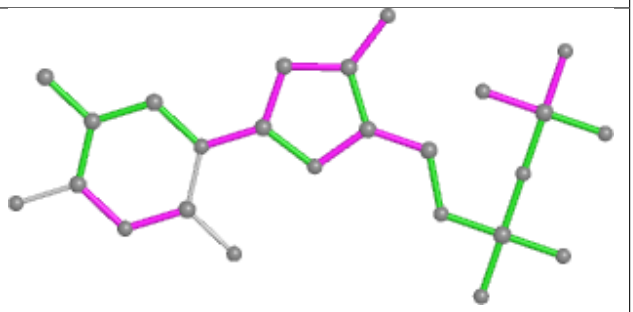


Rings

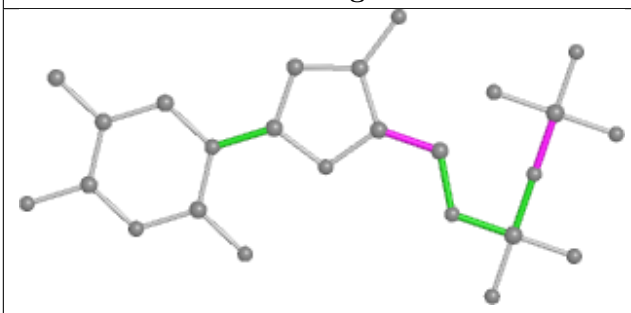
Ligand TYD G 402



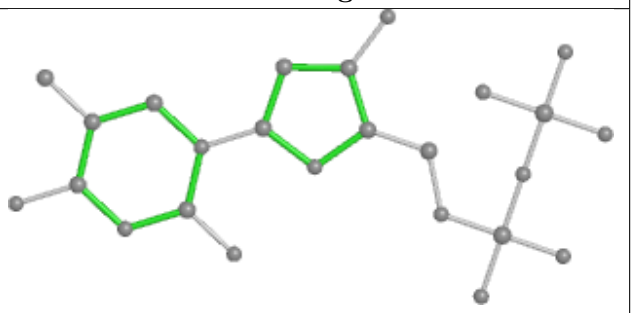
Bond lengths



Bond angles

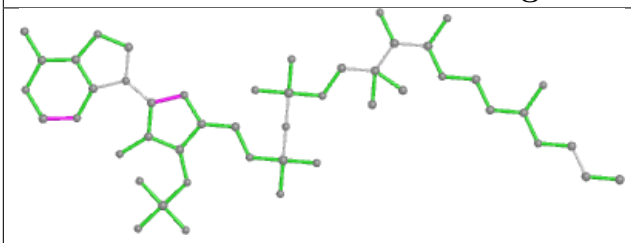


Torsions

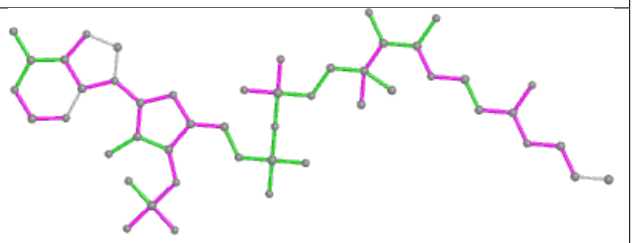


Rings

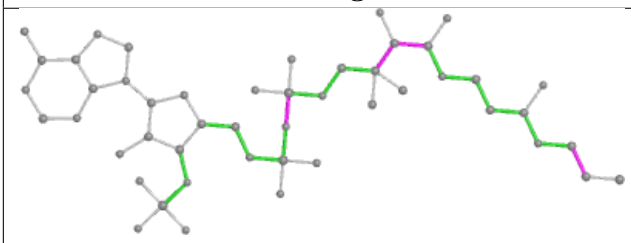
Ligand COA A 401



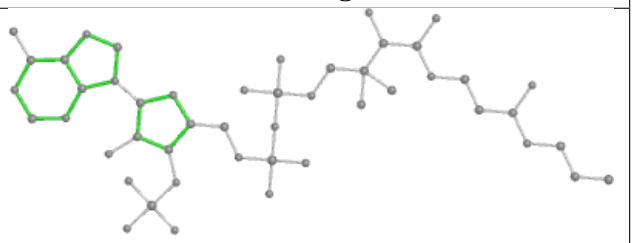
Bond lengths



Bond angles

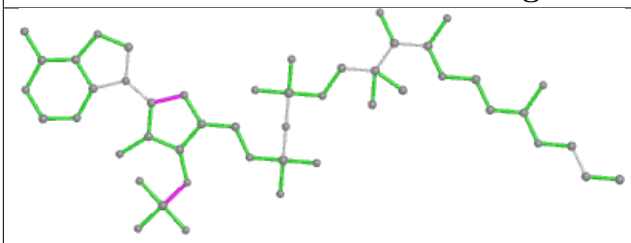


Torsions

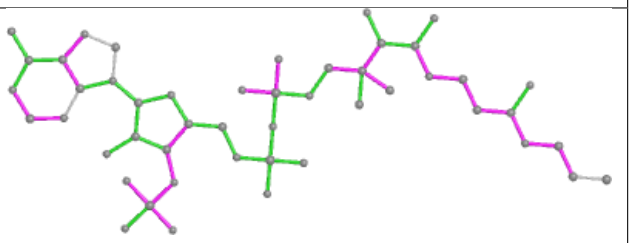


Rings

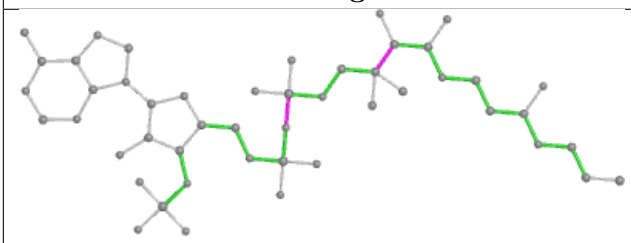
Ligand COA B 401



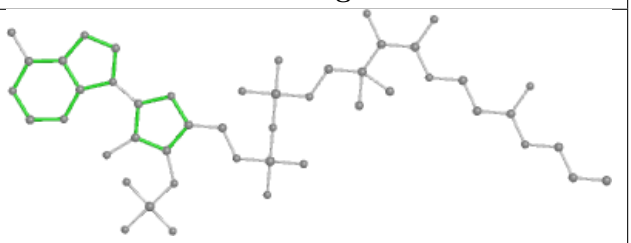
Bond lengths



Bond angles

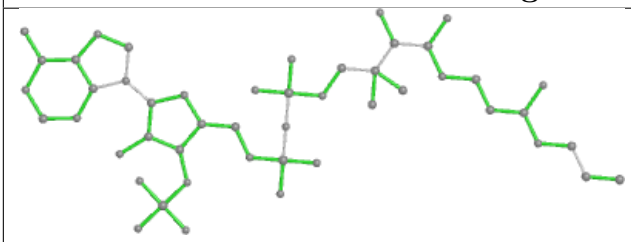


Torsions

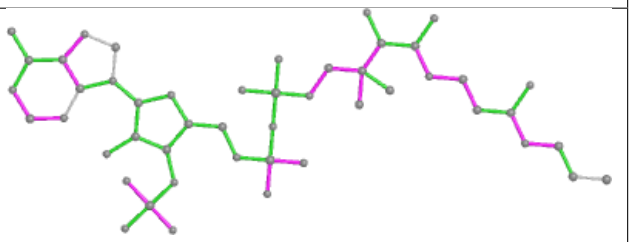


Rings

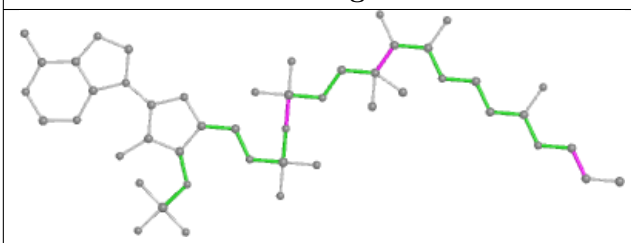
Ligand COA G 403



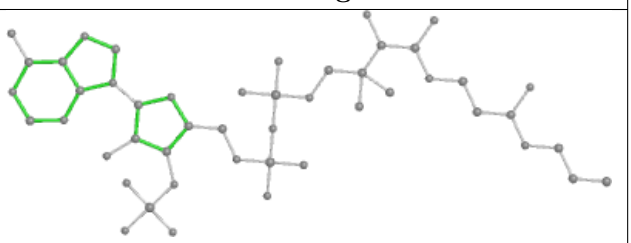
Bond lengths



Bond angles

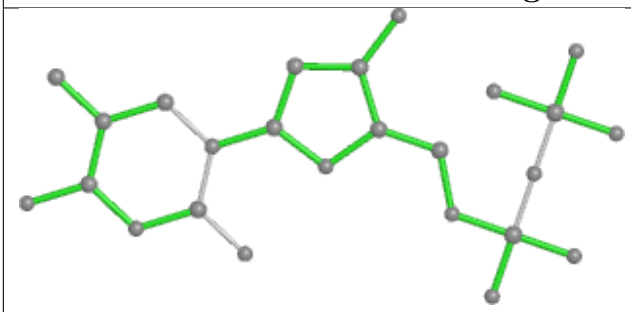


Torsions

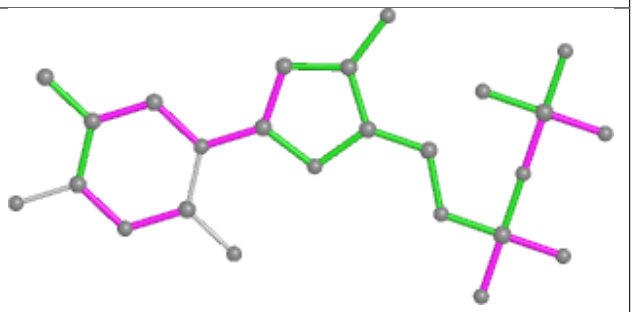


Rings

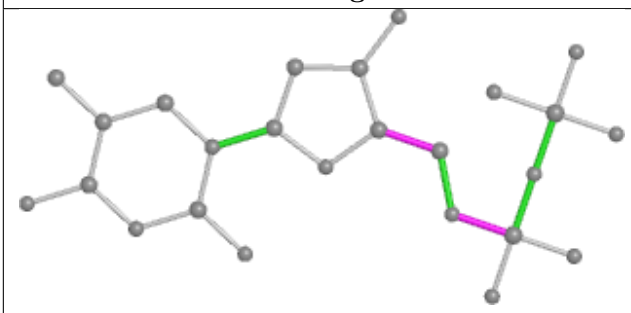
Ligand TYD E 402



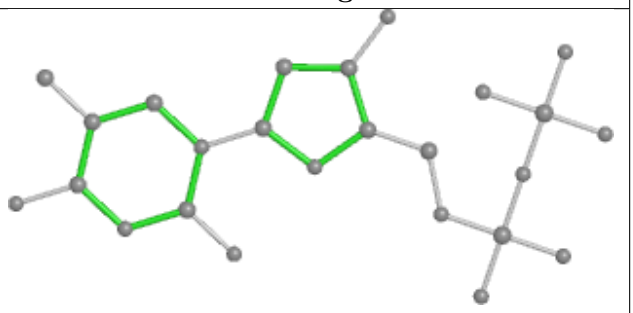
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	285/312 (91%)	-0.03	6 (2%) 63 61	12, 27, 46, 67	0
1	B	290/312 (92%)	0.09	12 (4%) 37 35	12, 28, 51, 65	0
1	C	285/312 (91%)	-0.01	5 (1%) 68 66	14, 28, 47, 66	0
1	D	283/312 (90%)	0.16	14 (4%) 29 28	18, 33, 53, 75	0
1	E	286/312 (91%)	0.12	8 (2%) 53 51	17, 32, 53, 67	0
1	F	294/312 (94%)	0.26	17 (5%) 23 22	20, 33, 54, 67	0
1	G	283/312 (90%)	0.01	7 (2%) 57 55	17, 31, 56, 63	0
1	H	278/312 (89%)	0.53	29 (10%) 6 5	27, 47, 65, 74	0
1	I	285/312 (91%)	0.20	12 (4%) 36 34	18, 34, 58, 65	0
1	J	275/312 (88%)	0.41	23 (8%) 11 9	18, 40, 63, 70	0
1	K	285/312 (91%)	0.16	16 (5%) 24 23	16, 29, 55, 81	0
1	L	286/312 (91%)	0.15	10 (3%) 44 42	20, 32, 58, 65	0
All	All	3415/3744 (91%)	0.17	159 (4%) 31 30	12, 33, 58, 81	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	165	LEU	8.7
1	E	94	TYR	6.6
1	F	165	LEU	6.0
1	K	167	LEU	5.5
1	E	161	ASN	5.2

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 (i)

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
4	TDR	L	403	9/9	0.71	0.20	71,72,73,74	0
4	TDR	D	403	9/9	0.74	0.20	43,47,49,50	0
4	TDR	C	403	9/9	0.75	0.18	51,55,57,59	0
4	TDR	K	403	9/9	0.76	0.20	69,72,74,74	0
4	TDR	J	403	9/9	0.77	0.25	58,62,64,65	0
3	TYD	J	402	25/25	0.82	0.19	69,81,92,93	0
4	TDR	A	403	9/9	0.83	0.17	31,41,43,44	0
4	TDR	B	403	9/9	0.84	0.17	41,43,47,47	0
4	TDR	F	403	9/9	0.85	0.14	52,54,56,56	0
4	TDR	E	403	9/9	0.85	0.13	41,46,48,49	0
3	TYD	G	402	25/25	0.86	0.17	40,58,72,72	0
3	TYD	A	402	25/25	0.88	0.16	39,63,74,75	0
3	TYD	H	401	25/25	0.88	0.14	44,61,73,74	0
3	TYD	D	402	25/25	0.88	0.17	47,71,75,77	0
3	TYD	F	402	25/25	0.88	0.13	35,56,79,79	0
3	TYD	L	402	25/25	0.90	0.14	46,63,71,72	0
3	TYD	C	402	25/25	0.90	0.14	31,56,66,68	0
3	TYD	B	402	25/25	0.91	0.12	34,57,71,73	0
3	TYD	E	402	25/25	0.92	0.13	31,49,61,63	0
3	TYD	K	402	25/25	0.92	0.12	22,39,55,57	0
3	TYD	I	402	25/25	0.92	0.11	22,40,66,68	0
2	COA	I	401	48/48	0.94	0.14	27,43,62,71	0
2	COA	G	401	48/48	0.95	0.11	26,36,41,53	0
2	COA	G	403	48/48	0.95	0.12	35,42,57,70	0
2	COA	D	401	48/48	0.95	0.13	20,41,56,64	0
2	COA	J	401	48/48	0.95	0.12	21,36,48,60	0
2	COA	E	401	48/48	0.95	0.12	20,37,49,59	0
2	COA	F	401	48/48	0.96	0.10	21,35,43,49	0
2	COA	A	401	48/48	0.96	0.12	17,29,42,55	0
2	COA	L	401	48/48	0.96	0.11	15,33,45,53	0
2	COA	C	401	48/48	0.96	0.10	14,32,42,45	0
2	COA	K	401	48/48	0.97	0.12	21,37,64,70	0

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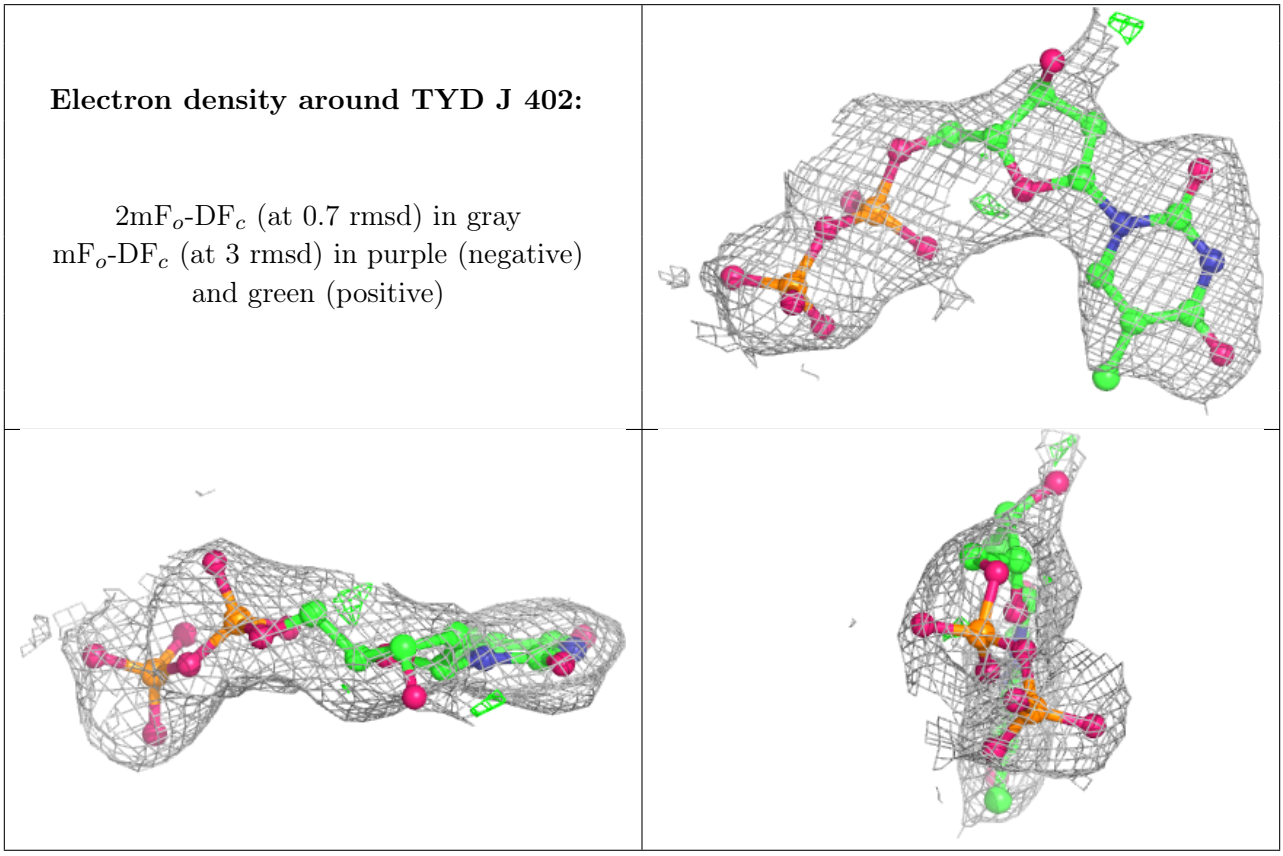
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	C	404	1/1	0.97	0.19	20,20,20,20	0
2	COA	B	401	48/48	0.98	0.09	9,24,33,42	0
5	MG	G	404	1/1	0.98	0.14	27,27,27,27	0
5	MG	J	404	1/1	0.98	0.19	26,26,26,26	0
5	MG	B	404	1/1	0.99	0.20	26,26,26,26	0
5	MG	D	404	1/1	0.99	0.20	21,21,21,21	0

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.

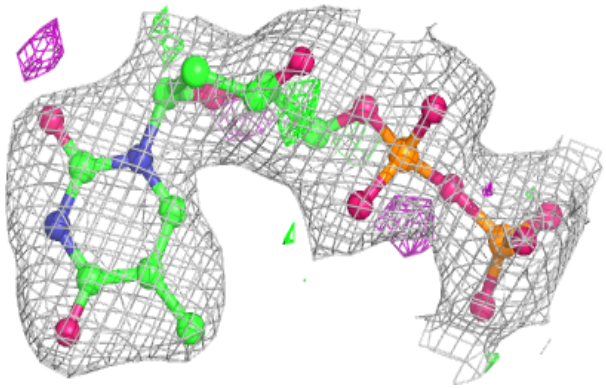
Electron density around TYD J 402:

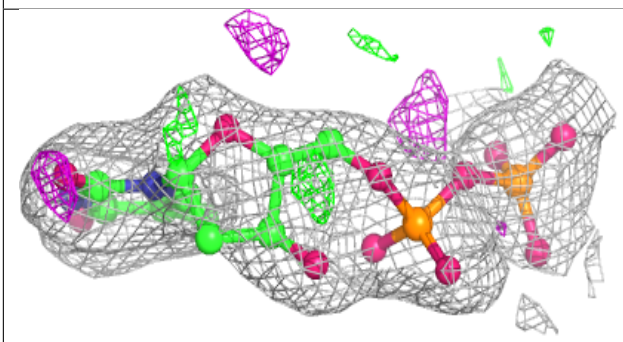
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

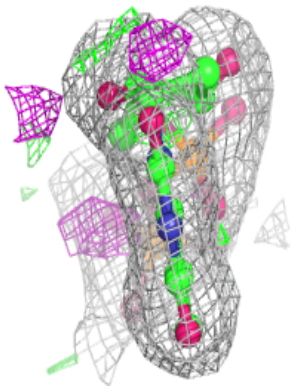


Electron density around TYD G 402:

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

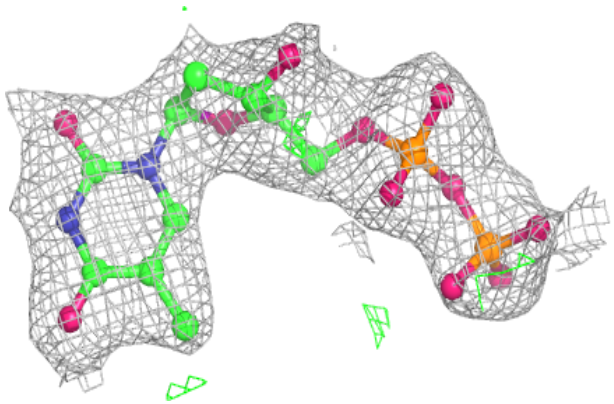


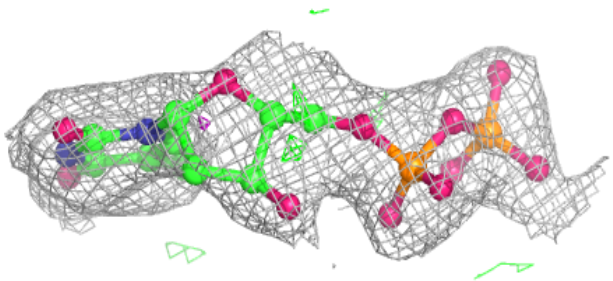


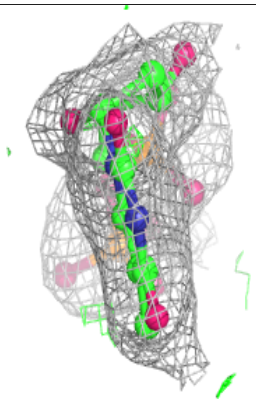


Electron density around TYD A 402:

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

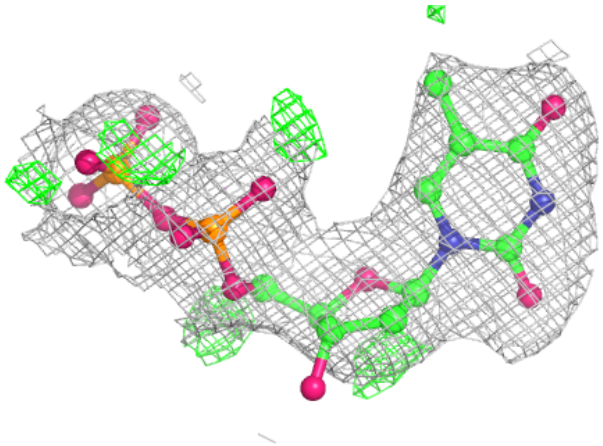


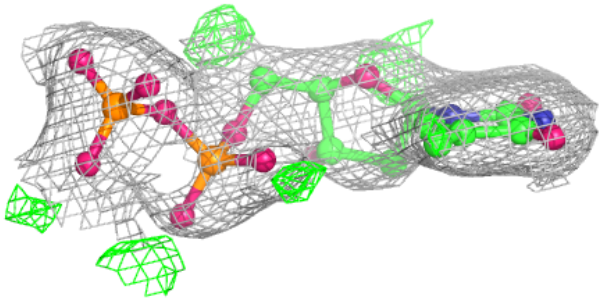


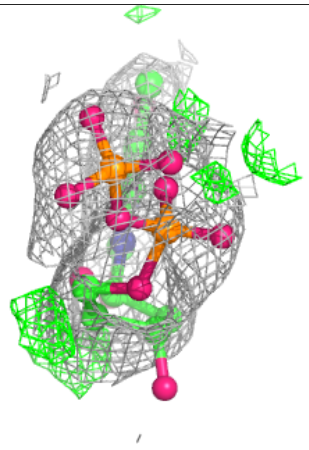


Electron density around TYD H 401:

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

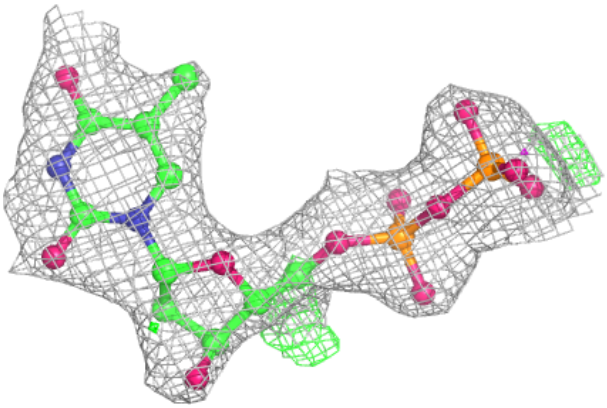


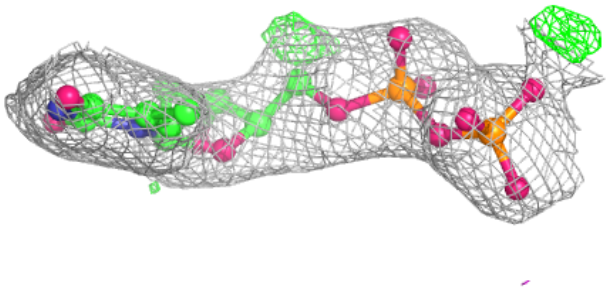


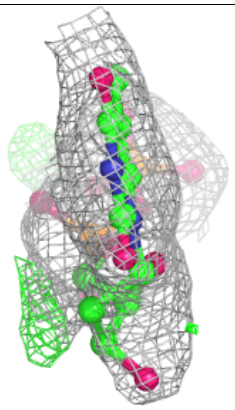


Electron density around TYD D 402:

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

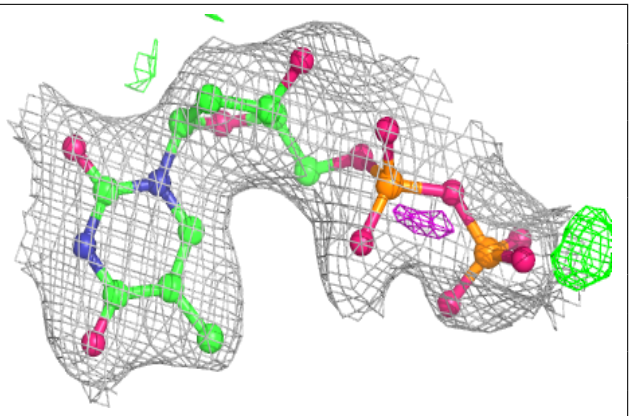


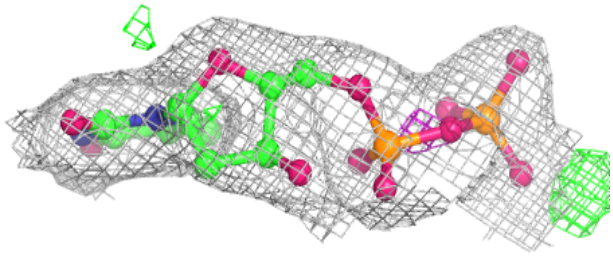


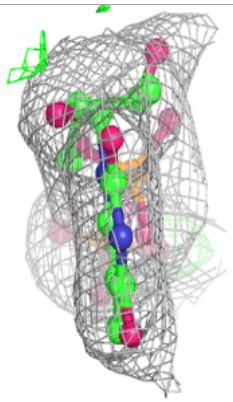


Electron density around TYD F 402:

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

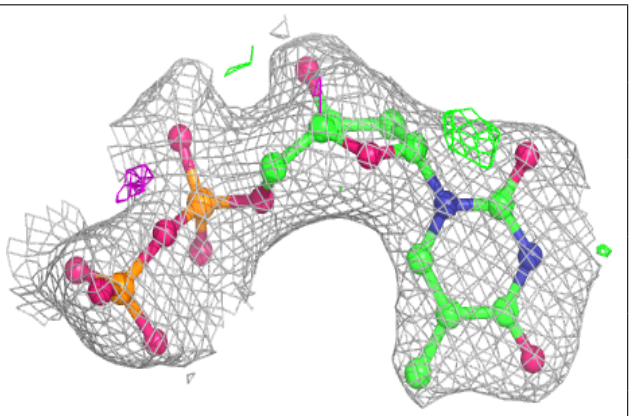


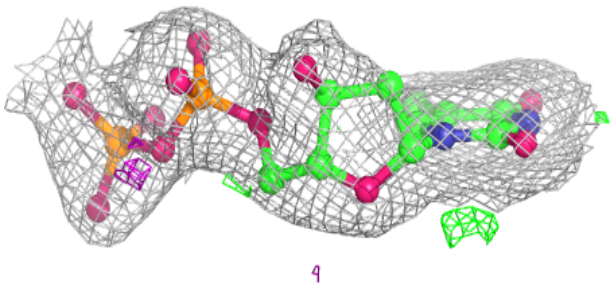


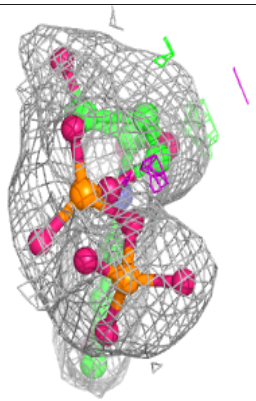


Electron density around TYD L 402:

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

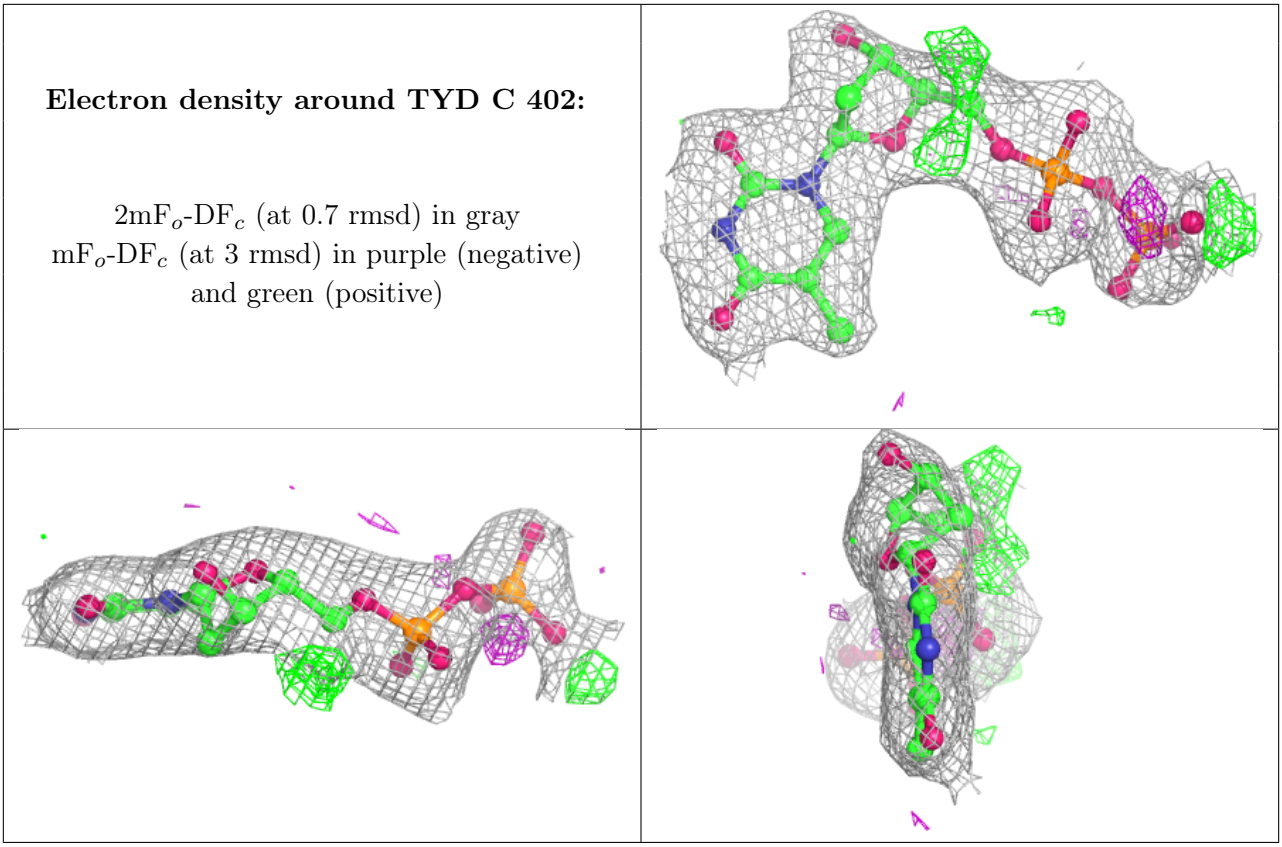






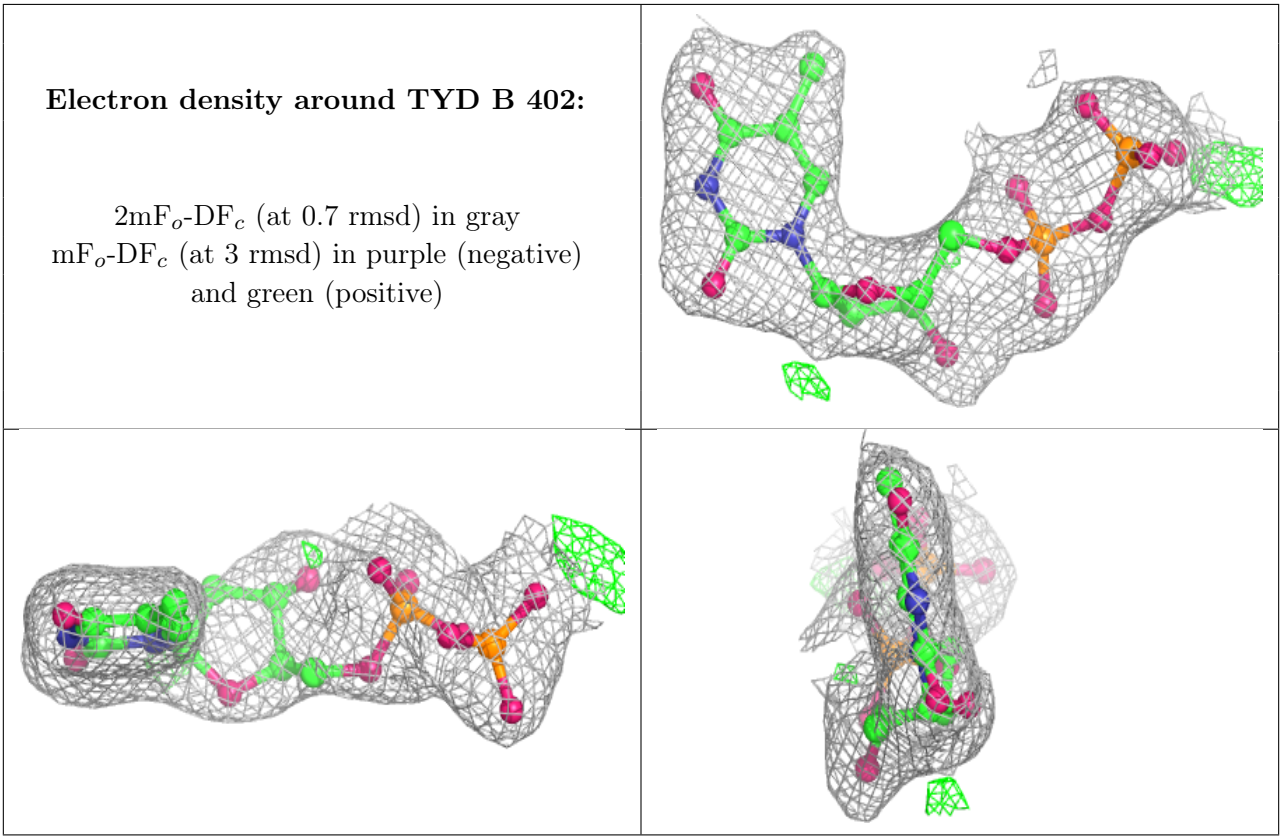
Electron density around TYD C 402:

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



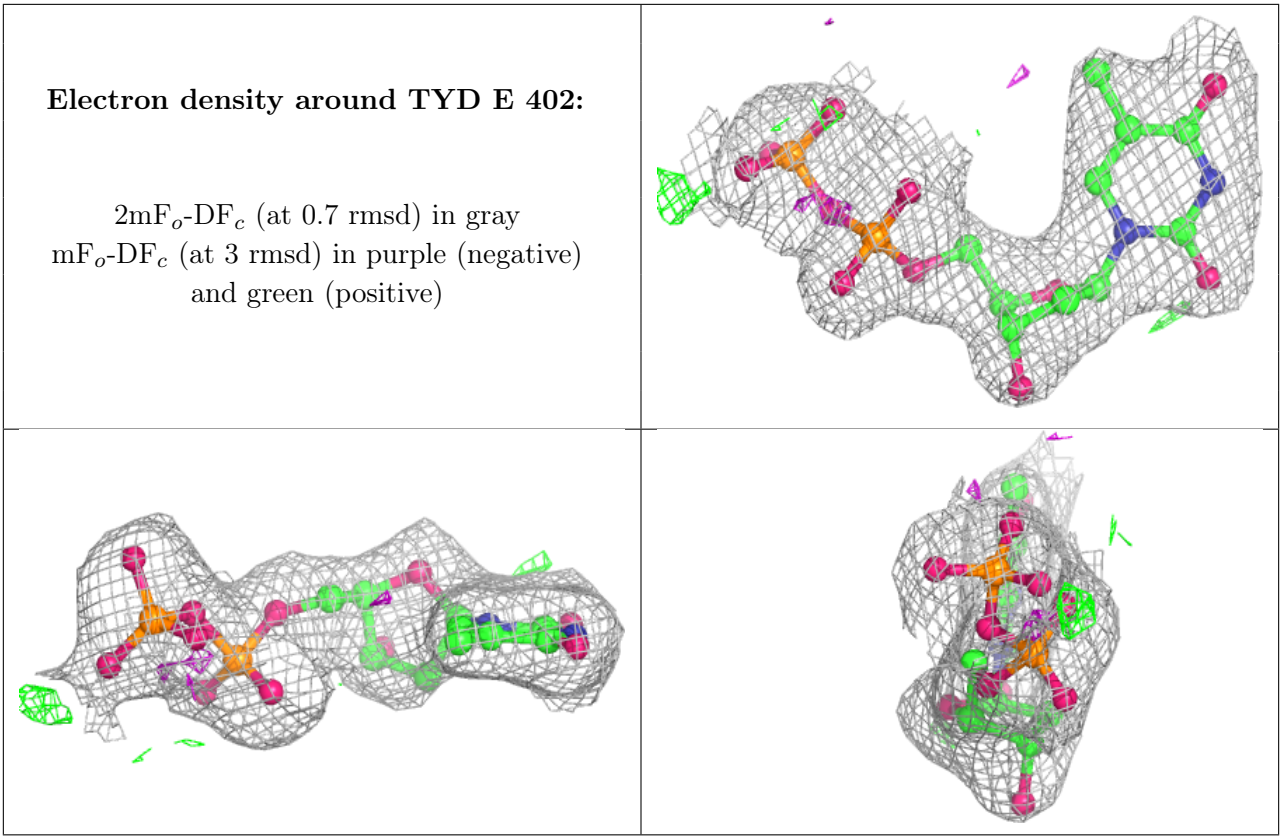
Electron density around TYD B 402:

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



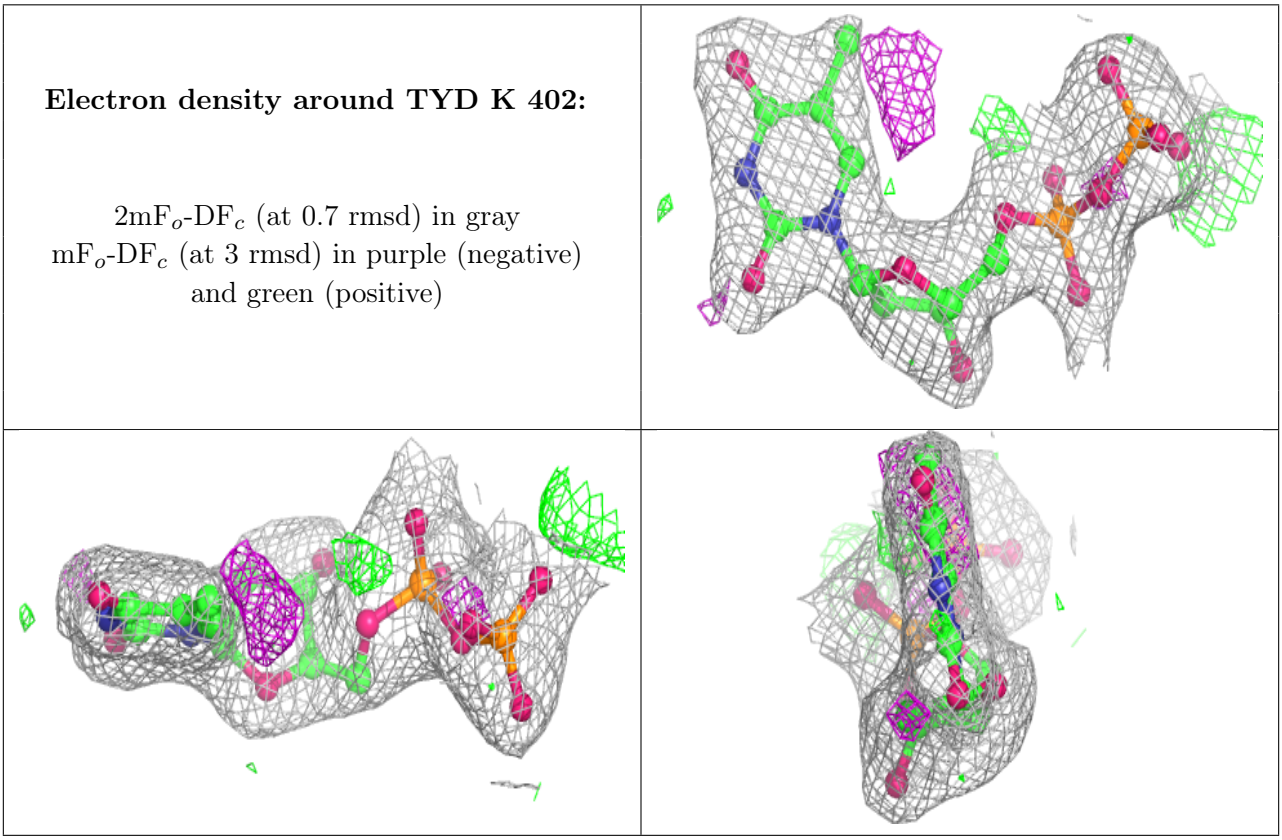
Electron density around TYD E 402:

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



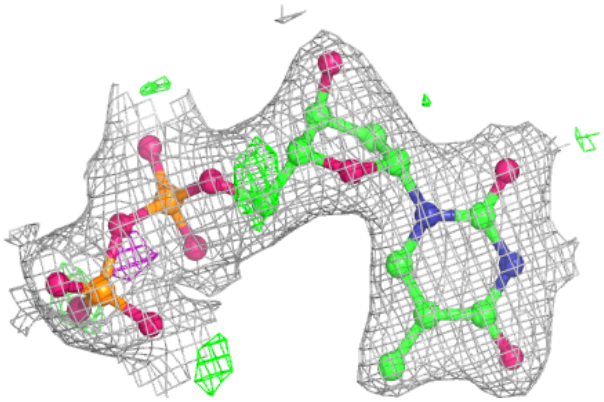
Electron density around TYD K 402:

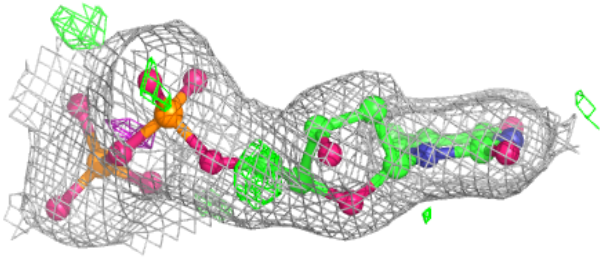
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

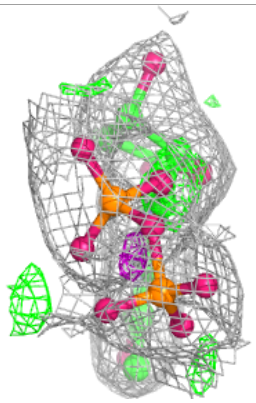


Electron density around TYD I 402:

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

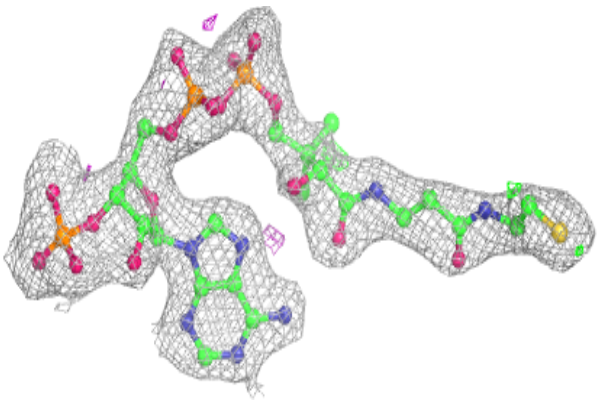


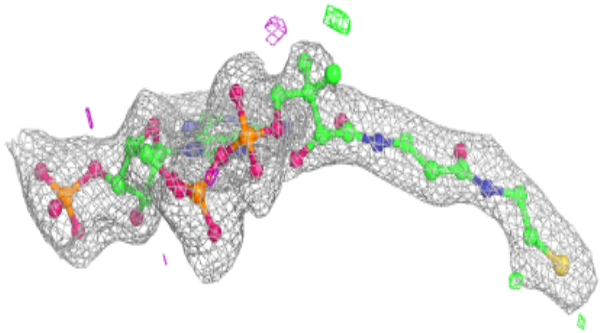


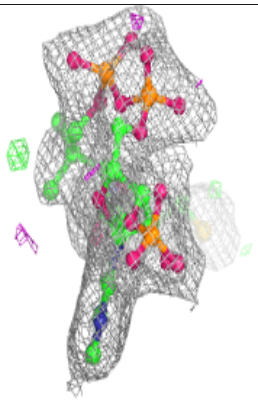


Electron density around COA I 401:

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

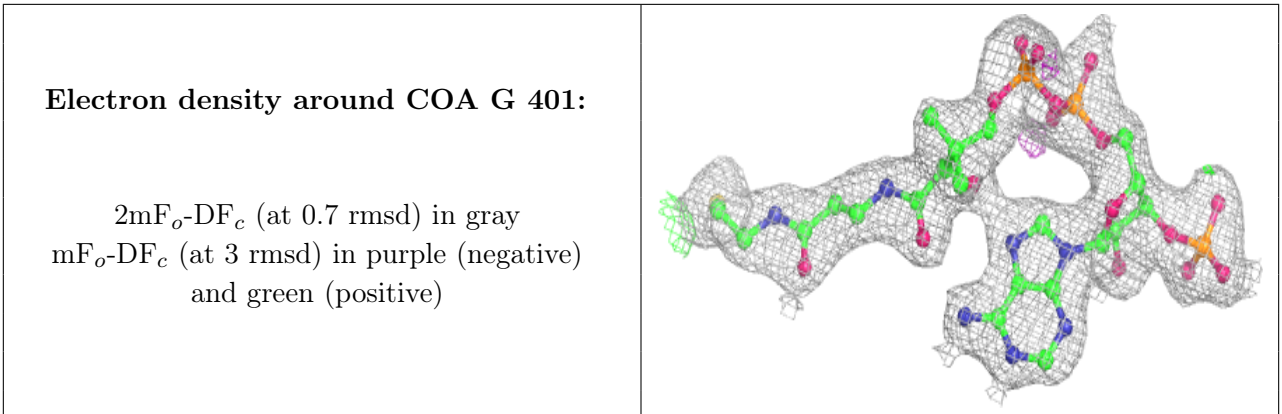


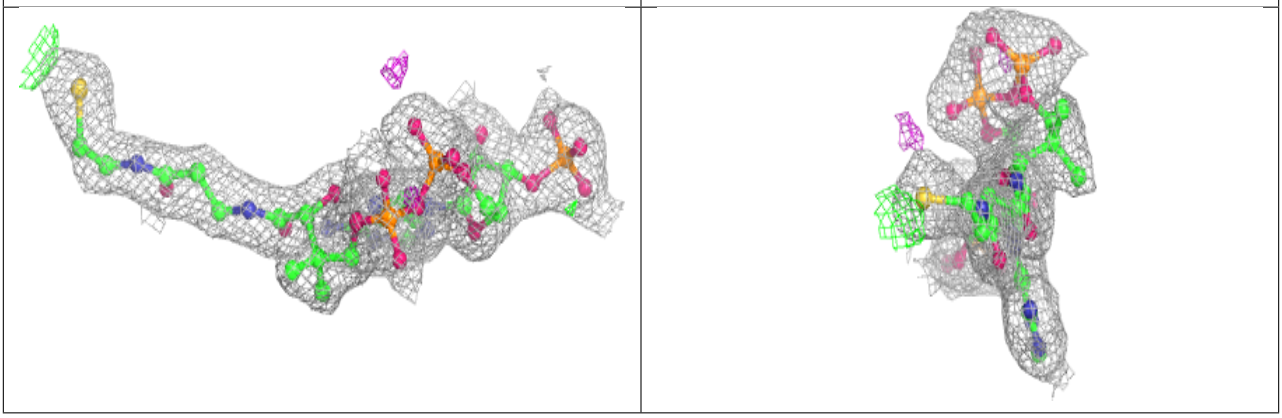




Electron density around COA G 401:

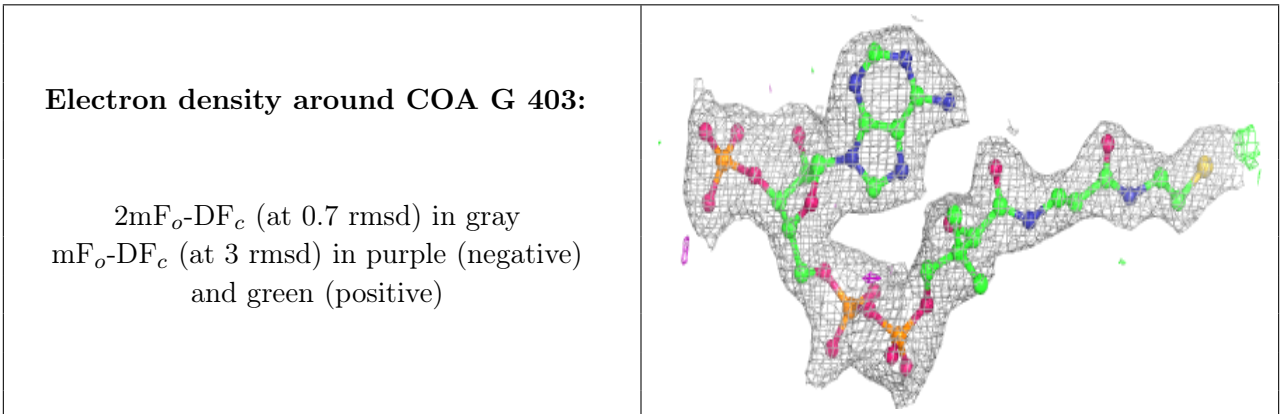
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

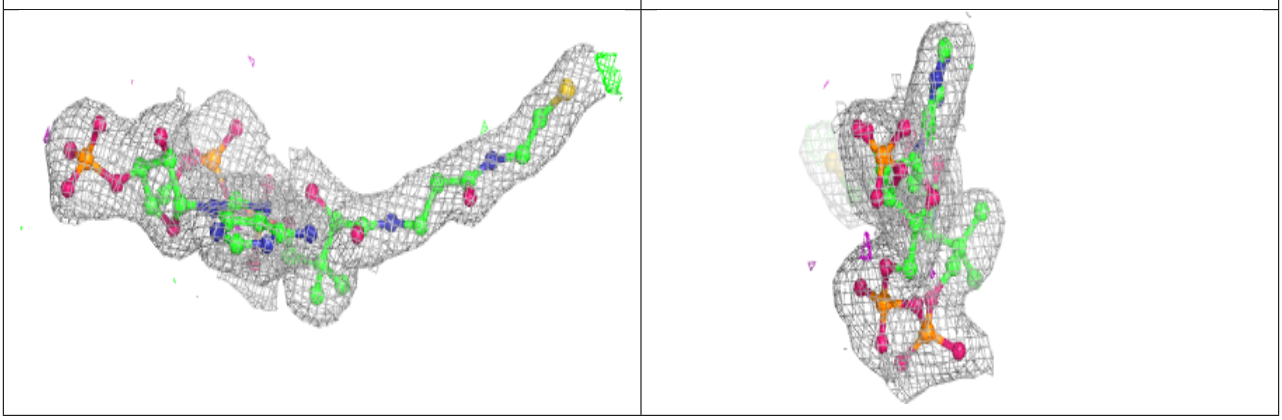




Electron density around COA G 403:

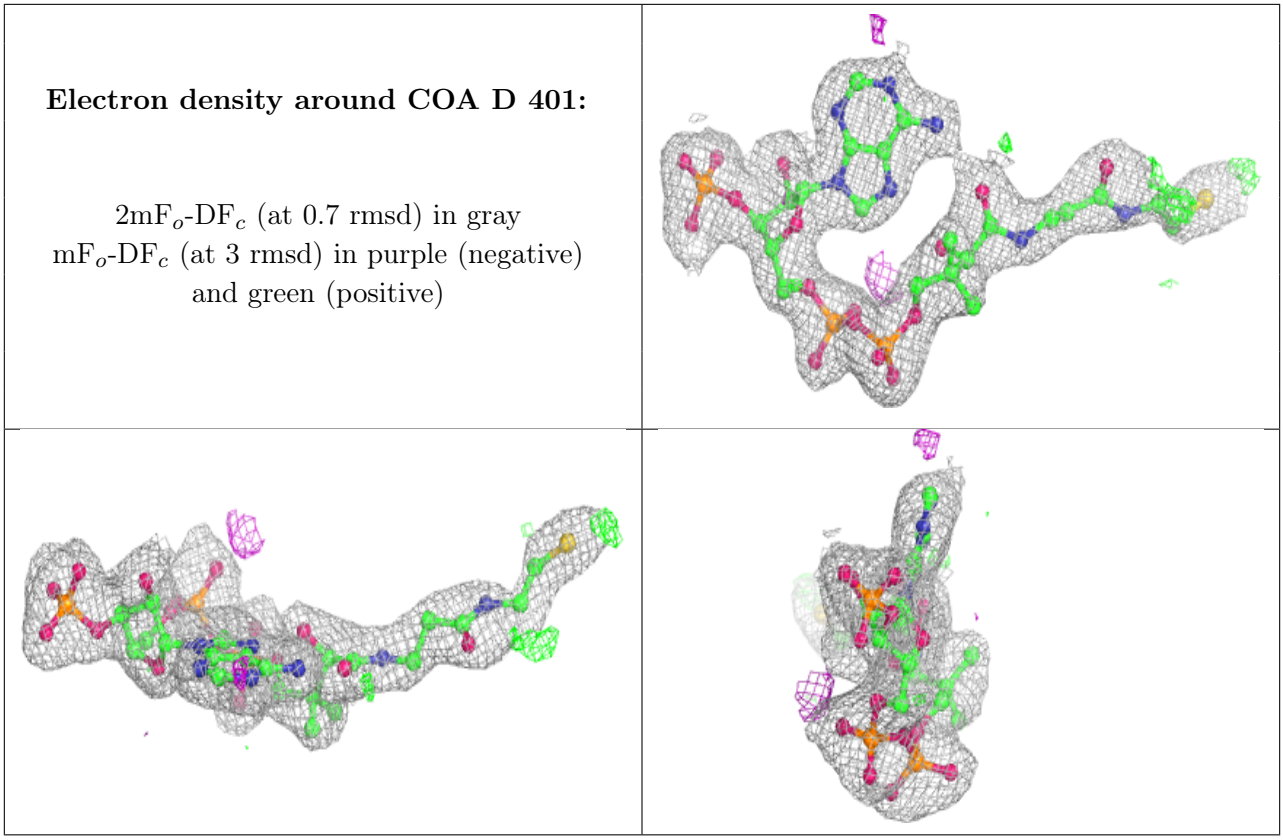
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





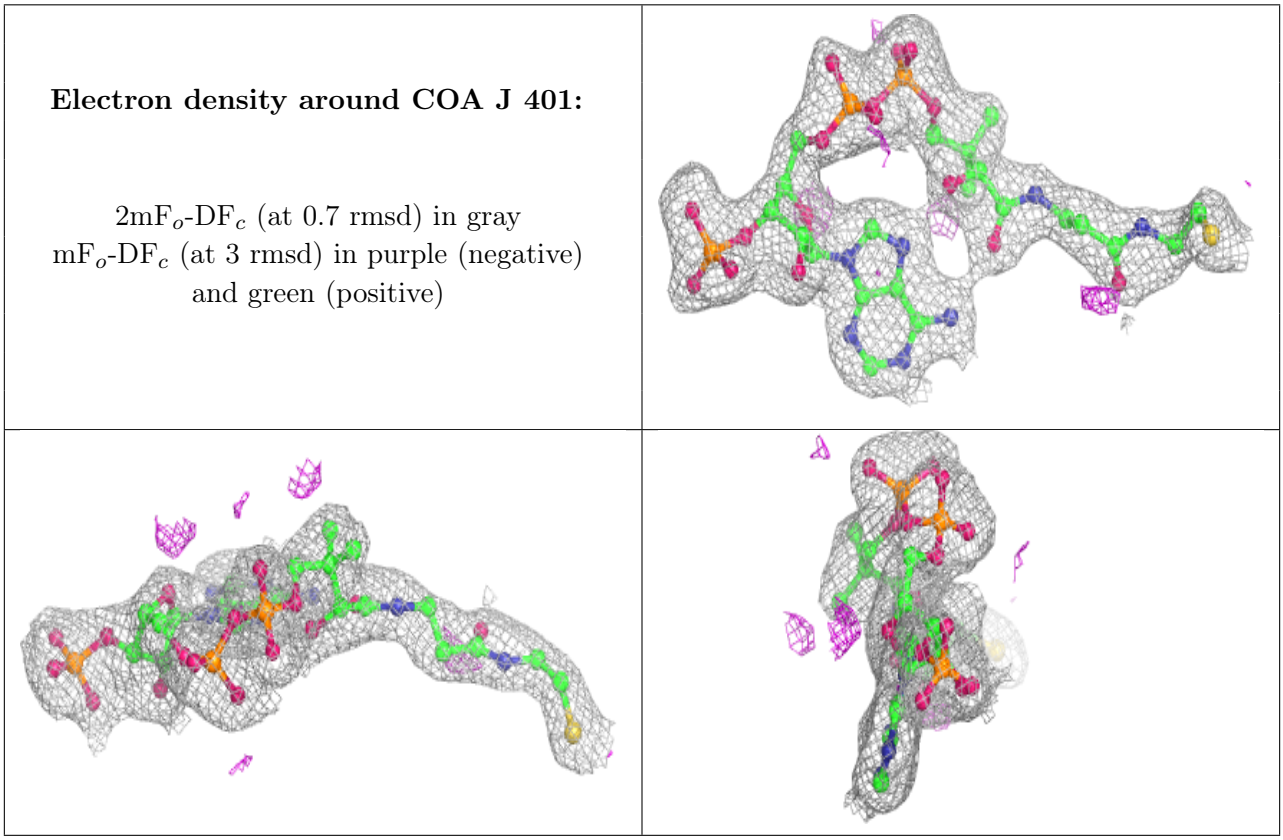
Electron density around COA D 401:

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



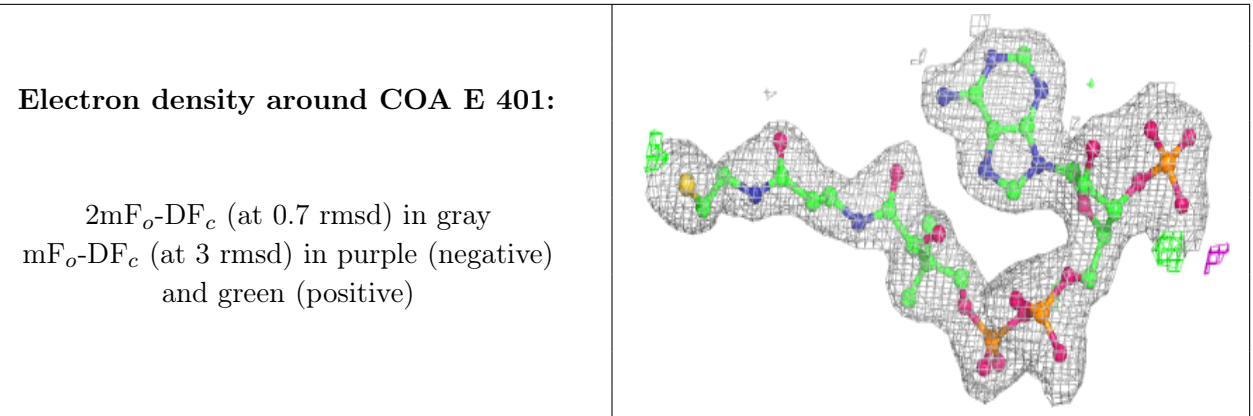
Electron density around COA J 401:

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



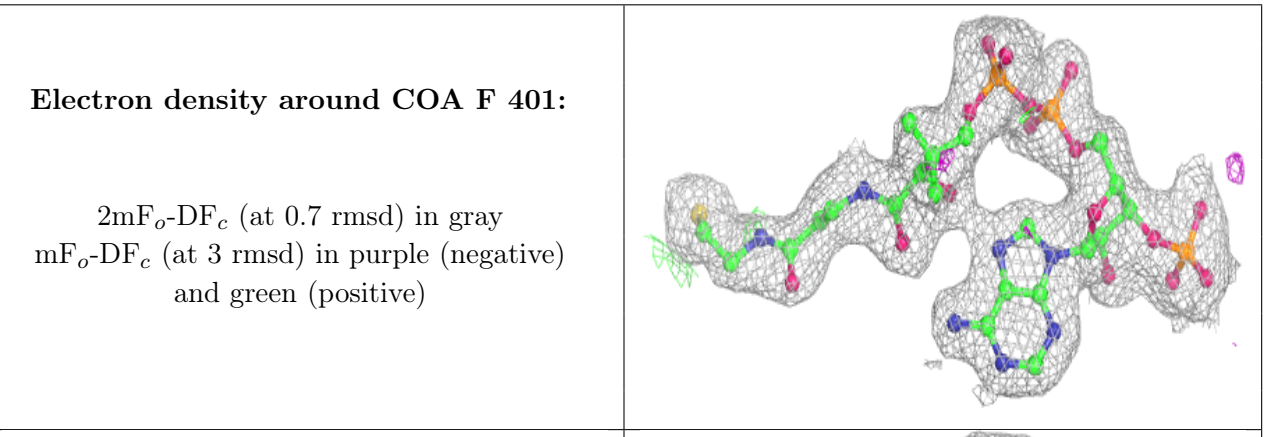
Electron density around COA E 401:

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



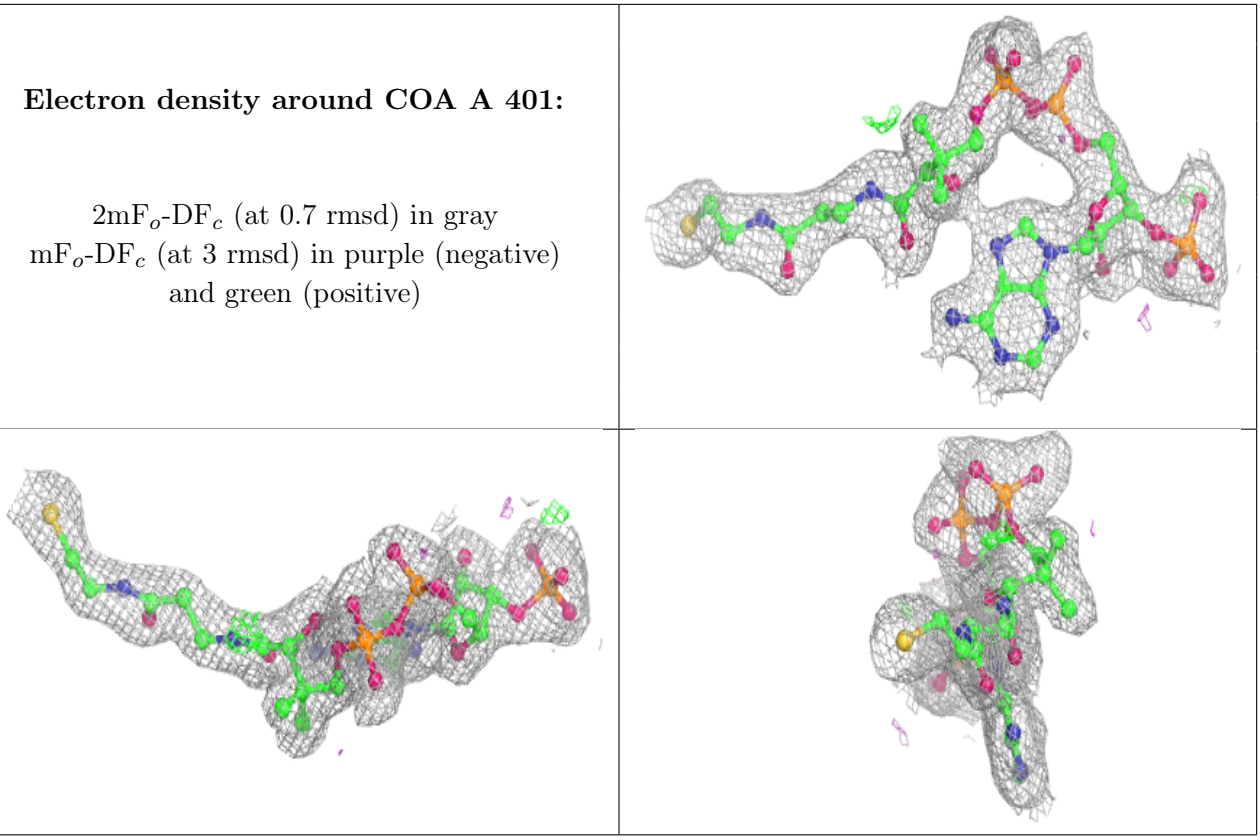
Electron density around COA F 401:

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



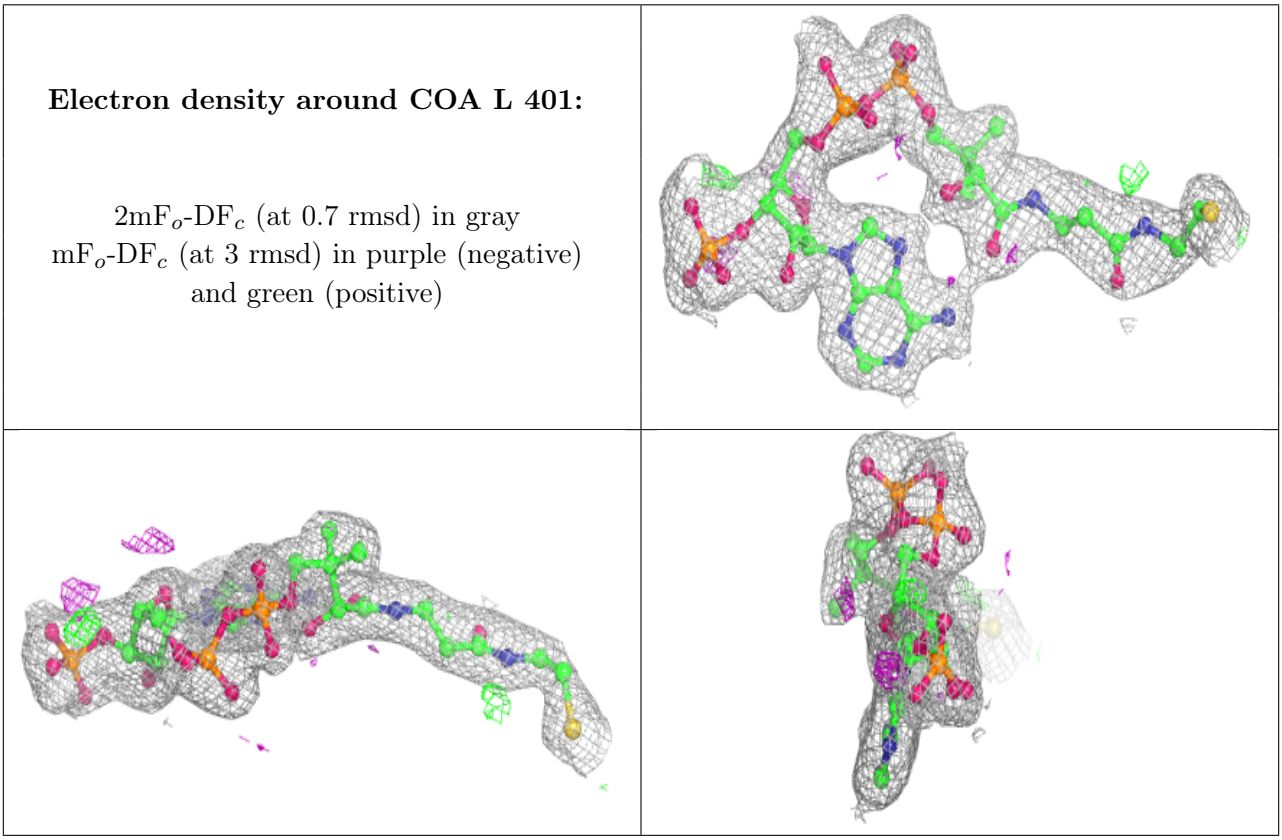
Electron density around COA A 401:

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



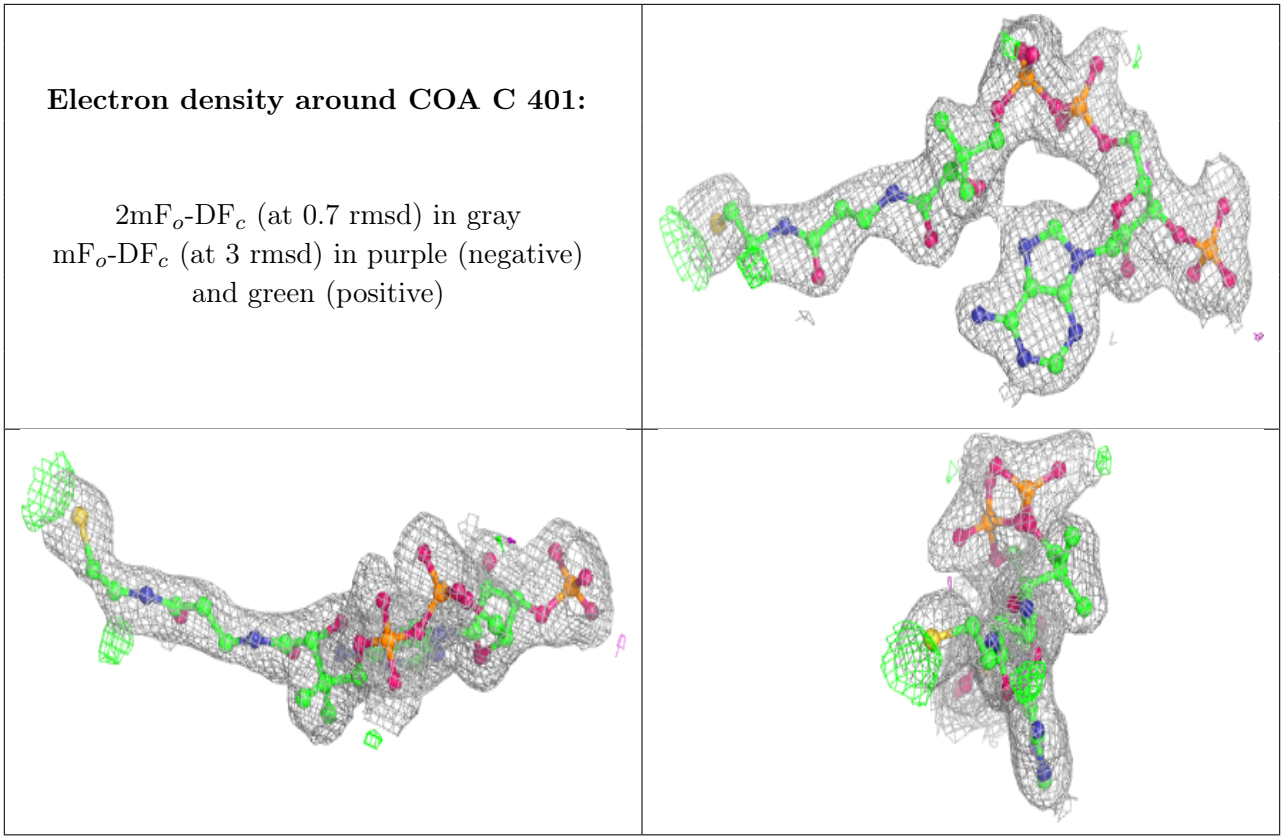
Electron density around COA L 401:

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



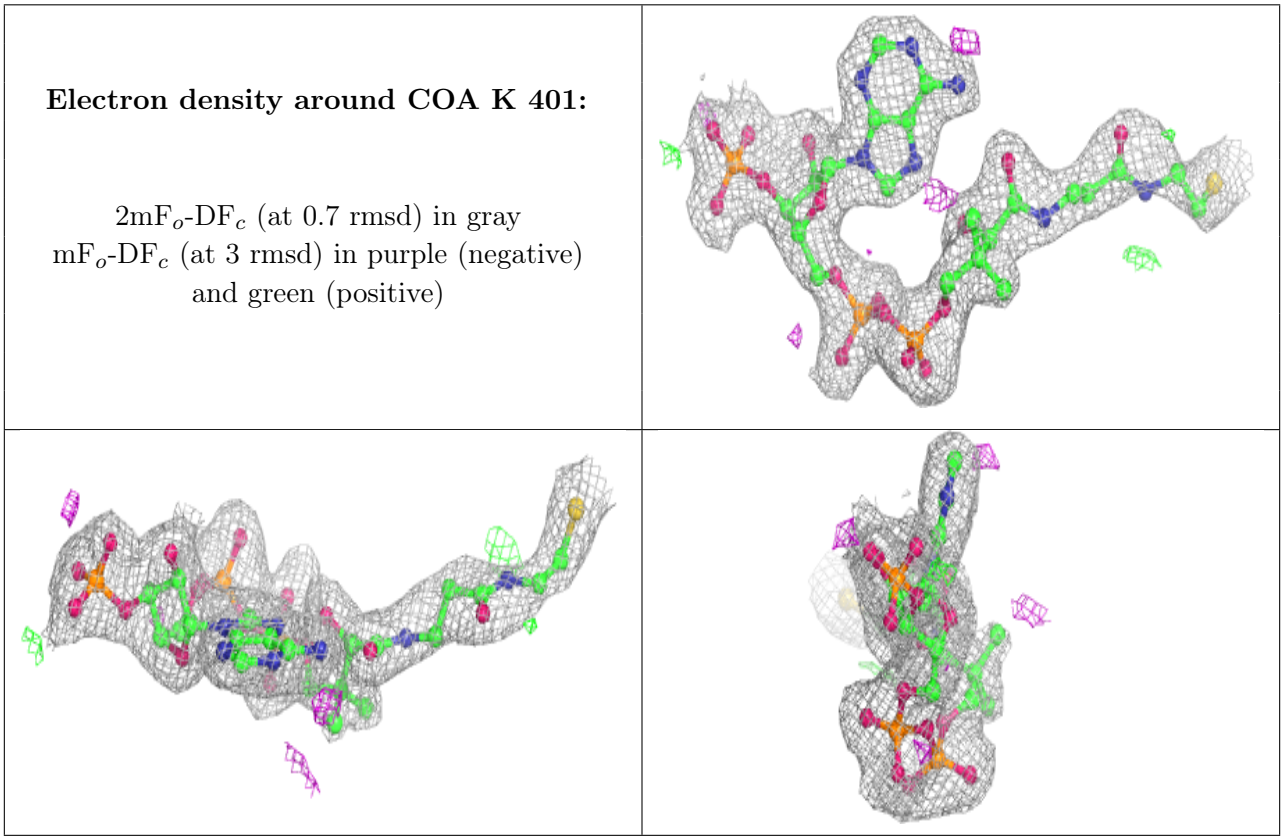
Electron density around COA C 401:

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



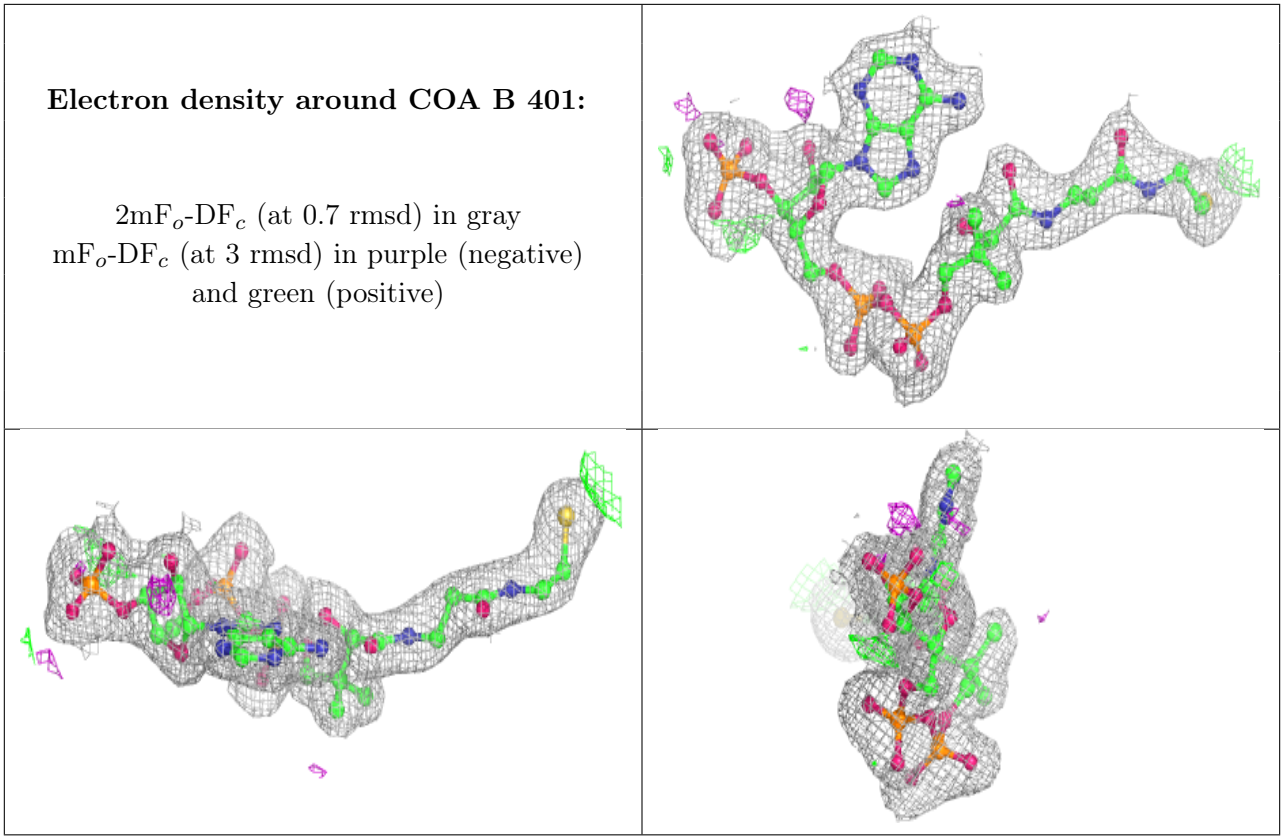
Electron density around COA K 401:

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



Electron density around COA B 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.