wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 06:42 AM EDT

PDB ID	:	6B5E
Title	:	Mycobacterium tuberculosis RmlA in complex with dTDP-glucose
Authors	:	Brown, H.A.; Holden, H.M.
Deposited on	:	2017-09-29
Resolution	:	1.85 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:

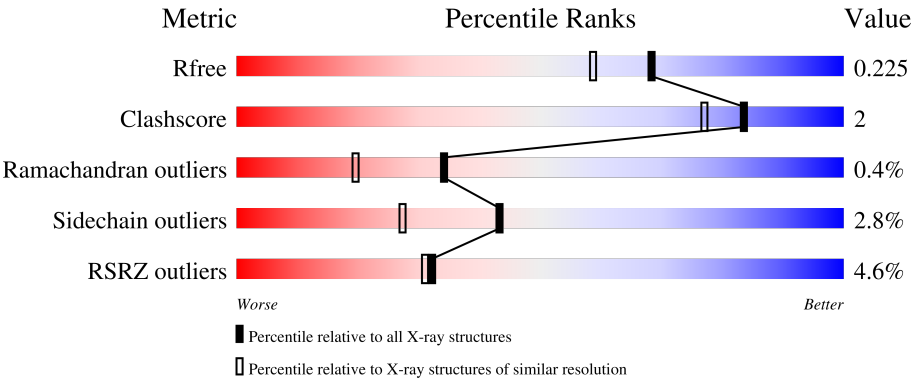
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	296	90% 6%
1	B	296	90% 7%
1	C	296	3% 89% 7%
1	D	296	3% 91% 5%
1	E	296	5% 90% 6%

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Mol	Chain	Length	Quality of chain
1	F	296	6% 89% 6%
1	G	296	4% 89% 6%
1	H	296	11% 85% 8% 6%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19586 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 Glucose-1-phosphate thymidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	3	0
			2191	1407	368	410	6			
1	B	286	Total	C	N	O	S	0	2	0
			2219	1423	378	411	7			
1	C	286	Total	C	N	O	S	0	4	0
			2224	1426	378	412	8			
1	D	286	Total	C	N	O	S	0	1	0
			2187	1403	368	409	7			
1	E	286	Total	C	N	O	S	0	5	0
			2214	1423	373	412	6			
1	F	284	Total	C	N	O	S	0	4	0
			2202	1415	370	409	8			
1	G	284	Total	C	N	O	S	0	3	0
			2204	1415	375	407	7			
1	H	279	Total	C	N	O	S	0	0	0
			2142	1376	361	399	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	LEU	-	expression tag	UNP P9WH13
A	290	GLU	-	expression tag	UNP P9WH13
A	291	HIS	-	expression tag	UNP P9WH13
A	292	HIS	-	expression tag	UNP P9WH13
A	293	HIS	-	expression tag	UNP P9WH13
A	294	HIS	-	expression tag	UNP P9WH13
A	295	HIS	-	expression tag	UNP P9WH13
A	296	HIS	-	expression tag	UNP P9WH13
B	289	LEU	-	expression tag	UNP P9WH13
B	290	GLU	-	expression tag	UNP P9WH13
B	291	HIS	-	expression tag	UNP P9WH13
B	292	HIS	-	expression tag	UNP P9WH13
B	293	HIS	-	expression tag	UNP P9WH13

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Chain	Residue	Modelled	Actual	Comment	Reference
B	294	HIS	-	expression tag	UNP P9WH13
B	295	HIS	-	expression tag	UNP P9WH13
B	296	HIS	-	expression tag	UNP P9WH13
C	289	LEU	-	expression tag	UNP P9WH13
C	290	GLU	-	expression tag	UNP P9WH13
C	291	HIS	-	expression tag	UNP P9WH13
C	292	HIS	-	expression tag	UNP P9WH13
C	293	HIS	-	expression tag	UNP P9WH13
C	294	HIS	-	expression tag	UNP P9WH13
C	295	HIS	-	expression tag	UNP P9WH13
C	296	HIS	-	expression tag	UNP P9WH13
D	289	LEU	-	expression tag	UNP P9WH13
D	290	GLU	-	expression tag	UNP P9WH13
D	291	HIS	-	expression tag	UNP P9WH13
D	292	HIS	-	expression tag	UNP P9WH13
D	293	HIS	-	expression tag	UNP P9WH13
D	294	HIS	-	expression tag	UNP P9WH13
D	295	HIS	-	expression tag	UNP P9WH13
D	296	HIS	-	expression tag	UNP P9WH13
E	289	LEU	-	expression tag	UNP P9WH13
E	290	GLU	-	expression tag	UNP P9WH13
E	291	HIS	-	expression tag	UNP P9WH13
E	292	HIS	-	expression tag	UNP P9WH13
E	293	HIS	-	expression tag	UNP P9WH13
E	294	HIS	-	expression tag	UNP P9WH13
E	295	HIS	-	expression tag	UNP P9WH13
E	296	HIS	-	expression tag	UNP P9WH13
F	289	LEU	-	expression tag	UNP P9WH13
F	290	GLU	-	expression tag	UNP P9WH13
F	291	HIS	-	expression tag	UNP P9WH13
F	292	HIS	-	expression tag	UNP P9WH13
F	293	HIS	-	expression tag	UNP P9WH13
F	294	HIS	-	expression tag	UNP P9WH13
F	295	HIS	-	expression tag	UNP P9WH13
F	296	HIS	-	expression tag	UNP P9WH13
G	289	LEU	-	expression tag	UNP P9WH13
G	290	GLU	-	expression tag	UNP P9WH13
G	291	HIS	-	expression tag	UNP P9WH13
G	292	HIS	-	expression tag	UNP P9WH13
G	293	HIS	-	expression tag	UNP P9WH13
G	294	HIS	-	expression tag	UNP P9WH13
G	295	HIS	-	expression tag	UNP P9WH13

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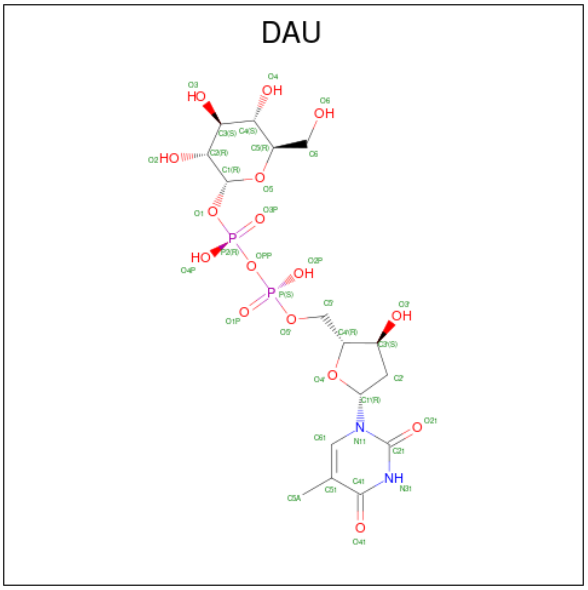
Chain	Residue	Modelled	Actual	Comment	Reference
G	296	HIS	-	expression tag	UNP P9WH13
H	289	LEU	-	expression tag	UNP P9WH13
H	290	GLU	-	expression tag	UNP P9WH13
H	291	HIS	-	expression tag	UNP P9WH13
H	292	HIS	-	expression tag	UNP P9WH13
H	293	HIS	-	expression tag	UNP P9WH13
H	294	HIS	-	expression tag	UNP P9WH13
H	295	HIS	-	expression tag	UNP P9WH13
H	296	HIS	-	expression tag	UNP P9WH13

- Molecule 2 is 2'DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: $C_{16}H_{26}N_2O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

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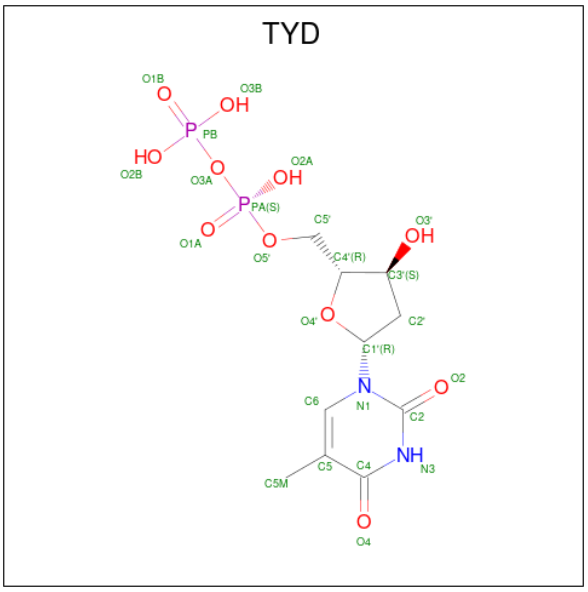
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
2	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).

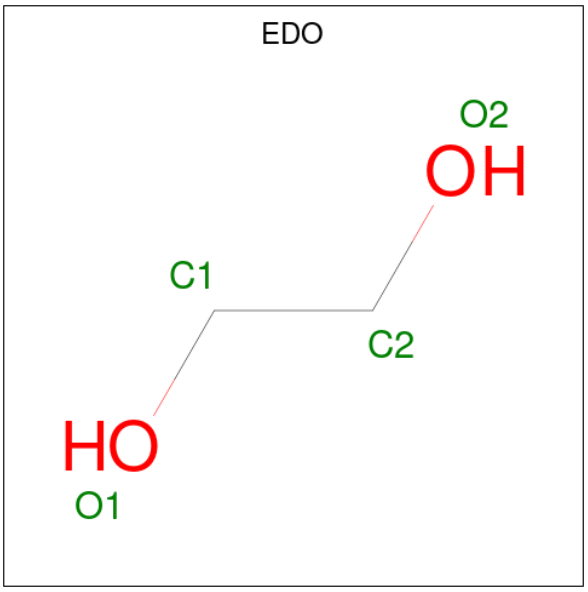


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	G	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	H	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	249	Total O 249 249	0	0
8	B	254	Total O 254 254	0	0
8	C	188	Total O 188 188	0	0
8	D	148	Total O 148 148	0	0
8	E	191	Total O 191 191	0	0
8	F	167	Total O 167 167	0	0

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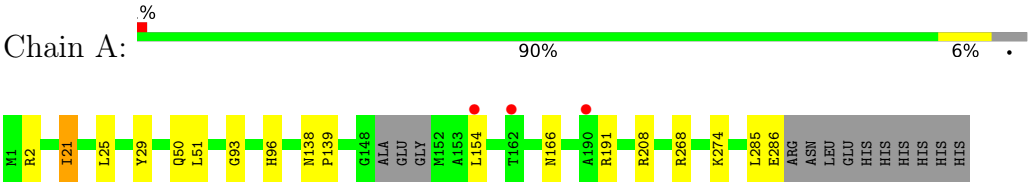
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	181	Total O 181 181	0	0
8	H	99	Total O 99 99	0	0

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.

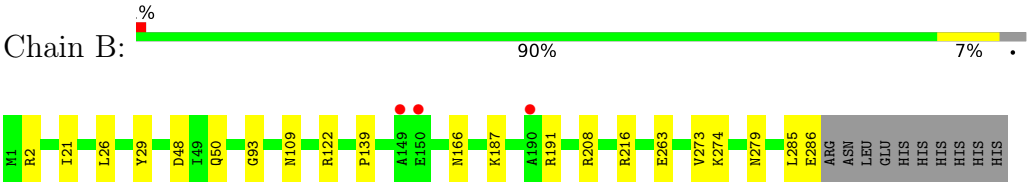
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain A:



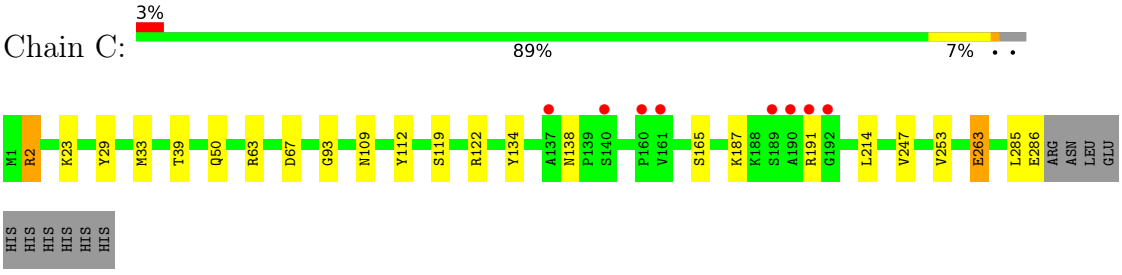
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain B:



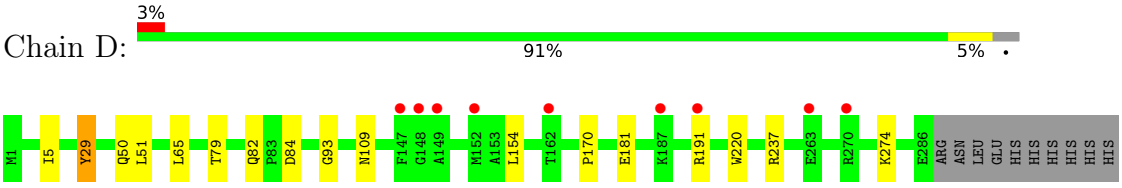
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain C:



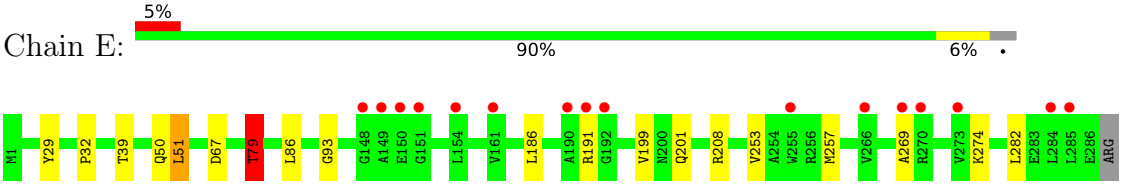
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain D:



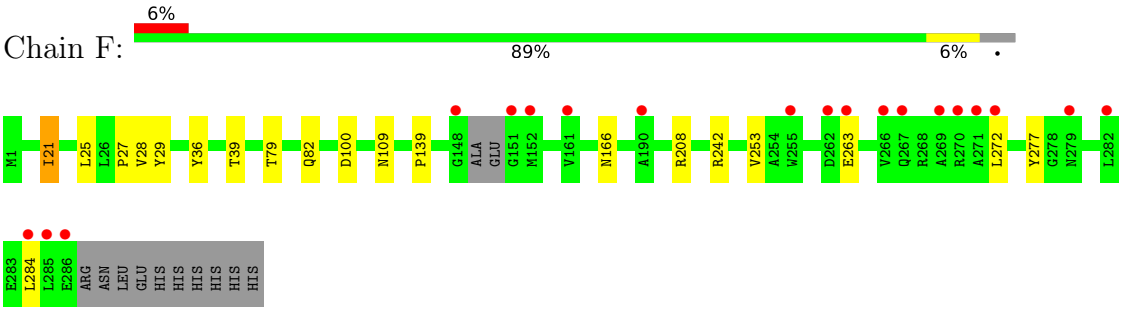
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain E:



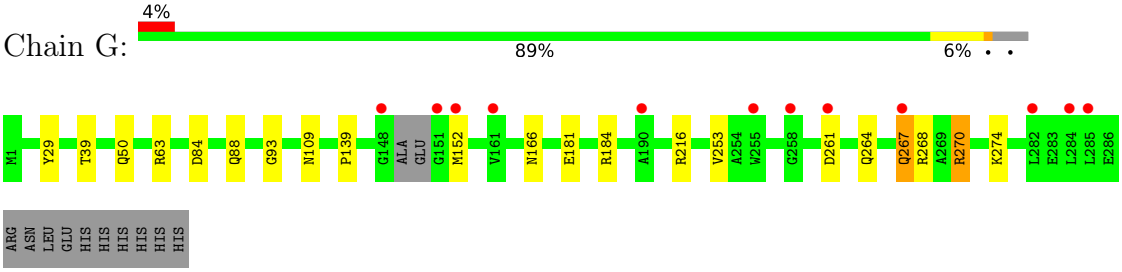
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain F:



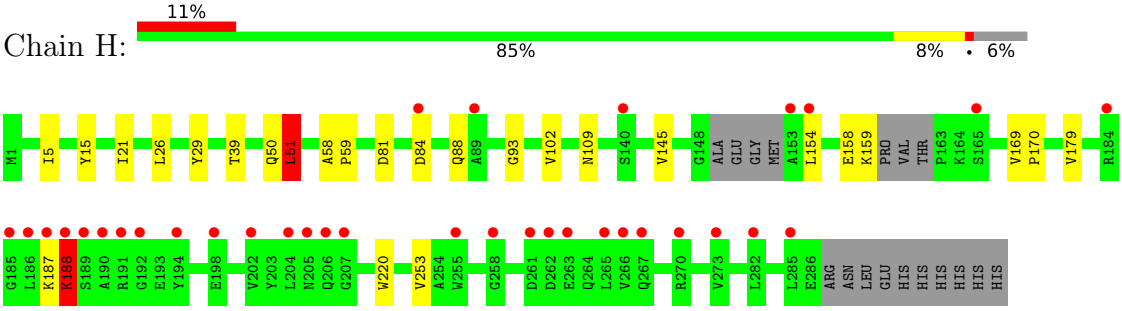
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain G:



• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.32Å 111.26Å 290.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 37.82 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-1.85) 97.8 (37.82-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	15.80 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.171 , 0.218 0.182 , 0.225	Depositor DCC
R_{free} test set	9779 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19586	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: DAU, CL, TYD, MG, EDO, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.73	0/2247	0.82	0/3054
1	B	0.72	0/2273	0.84	1/3086 (0.0%)
1	C	0.63	0/2284	0.76	2/3099 (0.1%)
1	D	0.56	0/2238	0.74	1/3043 (0.0%)
1	E	0.66	1/2277 (0.0%)	0.79	4/3096 (0.1%)
1	F	0.61	0/2261	0.75	2/3070 (0.1%)
1	G	0.58	0/2260	0.77	2/3069 (0.1%)
1	H	0.59	0/2187	0.74	3/2969 (0.1%)
All	All	0.64	1/18027 (0.0%)	0.78	15/24486 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	THR	CB-CG2	-5.35	1.34	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	270	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	G	270	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	F	100	ASP	CB-CG-OD1	7.62	125.15	118.30
1	H	188	LYS	N-CA-C	6.79	129.32	111.00
1	E	208	ARG	NE-CZ-NH2	6.09	123.35	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2191	0	2178	10	0
1	B	2219	0	2225	9	0
1	C	2224	0	2225	12	0
1	D	2187	0	2162	6	0
1	E	2214	0	2217	8	0
1	F	2202	0	2208	11	0
1	G	2204	0	2210	15	0
1	H	2142	0	2126	19	0
2	A	36	0	24	1	0
2	B	36	0	24	0	0
2	C	36	0	24	1	0
2	D	36	0	24	0	0
2	E	72	0	48	0	0
2	F	72	0	48	0	0
2	G	36	0	24	0	0
2	H	36	0	24	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	25	0	13	0	0
4	B	25	0	13	0	0
4	C	25	0	13	0	0
4	D	25	0	13	0	0
4	G	25	0	13	0	0
4	H	25	0	13	0	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	249	0	0	3	0
8	B	254	0	0	1	0
8	C	188	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	148	0	0	0	0
8	E	191	0	0	2	0
8	F	167	0	0	1	0
8	G	181	0	0	2	0
8	H	99	0	0	0	0
All	All	19586	0	17875	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 87 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:G:268[B]:ARG:HH21	1:G:268[B]:ARG:HG3	1.01	1.13
1:A:21:ILE:HD12	1:B:21:ILE:HD12	1.36	1.08
1:A:268[B]:ARG:NH1	8:A:401:HOH:O	1.91	0.95
1:F:21:ILE:HD12	1:H:21:ILE:HD12	1.50	0.92
1:G:268[B]:ARG:HG3	1:G:268[B]:ARG:NH2	1.81	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/296 (95%)	279 (99%)	2 (1%)	1 (0%)	34	19
1	B	286/296 (97%)	282 (99%)	3 (1%)	1 (0%)	41	26
1	C	288/296 (97%)	282 (98%)	5 (2%)	1 (0%)	41	26
1	D	285/296 (96%)	279 (98%)	5 (2%)	1 (0%)	34	19
1	E	289/296 (98%)	285 (99%)	3 (1%)	1 (0%)	41	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	284/296 (96%)	279 (98%)	4 (1%)	1 (0%)	34 19
1	G	283/296 (96%)	280 (99%)	2 (1%)	1 (0%)	34 19
1	H	273/296 (92%)	264 (97%)	7 (3%)	2 (1%)	22 9
All	All	2270/2368 (96%)	2230 (98%)	31 (1%)	9 (0%)	34 19

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	188	LYS
1	G	29	TYR
1	A	29	TYR
1	B	29	TYR
1	C	29	TYR

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	226/237 (95%)	220 (97%)	6 (3%)	44 29
1	B	229/237 (97%)	222 (97%)	7 (3%)	40 23
1	C	229/237 (97%)	223 (97%)	6 (3%)	46 30
1	D	223/237 (94%)	216 (97%)	7 (3%)	40 23
1	E	229/237 (97%)	221 (96%)	8 (4%)	36 18
1	F	229/237 (97%)	222 (97%)	7 (3%)	40 23
1	G	228/237 (96%)	222 (97%)	6 (3%)	46 30
1	H	219/237 (92%)	214 (98%)	5 (2%)	50 34
All	All	1812/1896 (96%)	1760 (97%)	52 (3%)	43 26

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51[B]	LEU

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Mol	Chain	Res	Type
1	F	79	THR
1	H	109	ASN
1	E	67	ASP
1	E	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	264	GLN
1	H	95	ASN
1	H	205	ASN
1	H	201	GLN
1	D	82	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	TYD	D	303	-	21,26,26	1.00	1 (4%)	27,40,40	1.94	4 (14%)
6	EDO	A	305	-	3,3,3	0.58	0	2,2,2	0.36	0
4	TYD	H	303	-	21,26,26	1.08	1 (4%)	27,40,40	1.87	4 (14%)
2	DAU	H	301	3	35,38,38	1.14	5 (14%)	53,58,58	1.76	8 (15%)
4	TYD	C	303	-	21,26,26	1.11	1 (4%)	27,40,40	1.92	2 (7%)
2	DAU	B	301	3	35,38,38	1.05	2 (5%)	53,58,58	2.03	9 (16%)
2	DAU	C	301	3	35,38,38	1.19	5 (14%)	53,58,58	2.02	14 (26%)
2	DAU	E	302	-	35,38,38	1.18	5 (14%)	53,58,58	1.50	8 (15%)
2	DAU	F	302	-	35,38,38	1.21	6 (17%)	53,58,58	1.49	9 (16%)
4	TYD	A	303	-	21,26,26	1.20	1 (4%)	27,40,40	1.84	3 (11%)
4	TYD	G	303	-	21,26,26	1.15	2 (9%)	27,40,40	1.91	2 (7%)
2	DAU	E	301	3	35,38,38	1.40	8 (22%)	53,58,58	1.87	15 (28%)
2	DAU	D	301	3	35,38,38	1.11	3 (8%)	53,58,58	1.66	10 (18%)
2	DAU	F	301	3	35,38,38	1.14	4 (11%)	53,58,58	1.98	11 (20%)
2	DAU	G	301	3	35,38,38	1.12	4 (11%)	53,58,58	1.73	10 (18%)
4	TYD	B	304	-	21,26,26	1.17	2 (9%)	27,40,40	1.98	4 (14%)
2	DAU	A	301	3	35,38,38	1.33	4 (11%)	53,58,58	1.97	10 (18%)

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	TYD	D	303	-	-	1/13/28/28	0/2/2/2
6	EDO	A	305	-	-	0/1/1/1	-
4	TYD	H	303	-	-	3/13/28/28	0/2/2/2
2	DAU	H	301	3	-	1/23/55/55	0/3/3/3
4	TYD	C	303	-	-	1/13/28/28	0/2/2/2
2	DAU	B	301	3	-	1/23/55/55	0/3/3/3
2	DAU	C	301	3	-	1/23/55/55	0/3/3/3
2	DAU	E	302	-	-	4/23/55/55	0/3/3/3
2	DAU	F	302	-	-	1/23/55/55	0/3/3/3
4	TYD	A	303	-	-	1/13/28/28	0/2/2/2
4	TYD	G	303	-	-	2/13/28/28	0/2/2/2
2	DAU	E	301	3	-	1/23/55/55	0/3/3/3
2	DAU	D	301	3	-	1/23/55/55	0/3/3/3
2	DAU	F	301	3	-	1/23/55/55	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAU	G	301	3	-	2/23/55/55	0/3/3/3
4	TYD	B	304	-	-	3/13/28/28	0/2/2/2
2	DAU	A	301	3	-	2/23/55/55	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	TYD	C5-C4	3.61	1.49	1.41
4	C	303	TYD	C5-C4	3.58	1.49	1.41
4	H	303	TYD	C5-C4	3.57	1.49	1.41
4	G	303	TYD	C5-C4	3.35	1.48	1.41
4	D	303	TYD	C5-C4	3.31	1.48	1.41

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	303	TYD	C2-N3-C4	8.69	122.48	115.14
4	B	304	TYD	C2-N3-C4	8.52	122.34	115.14
4	G	303	TYD	C2-N3-C4	8.49	122.31	115.14
4	D	303	TYD	C2-N3-C4	8.07	121.95	115.14
4	A	303	TYD	C2-N3-C4	7.71	121.65	115.14

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DAU	C1-O1-P2-OPP
2	F	302	DAU	P2-OPP-P-O5'
4	A	303	TYD	O4'-C1'-N1-C6
4	B	304	TYD	PA-O3A-PB-O3B
4	B	304	TYD	O4'-C1'-N1-C6

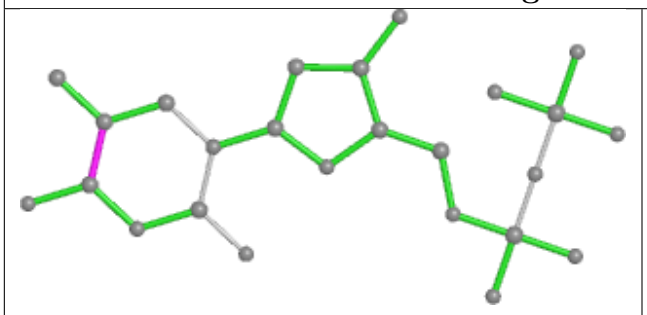
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	DAU	1	0
2	C	301	DAU	1	0
2	A	301	DAU	1	0

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

Ligand TYD D 303



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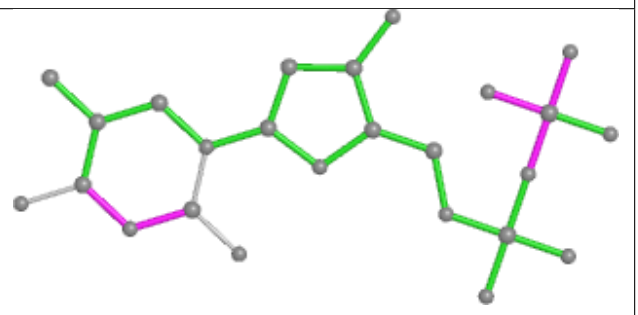

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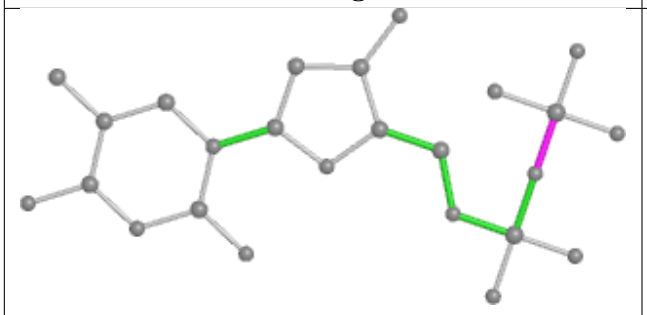

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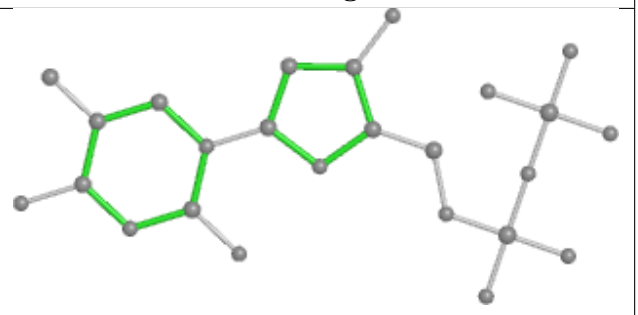
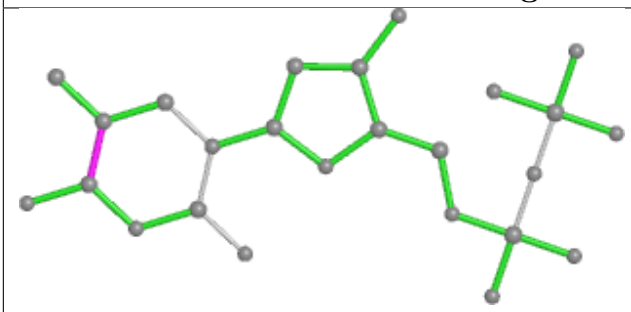


Rings

Ligand TYD H 303



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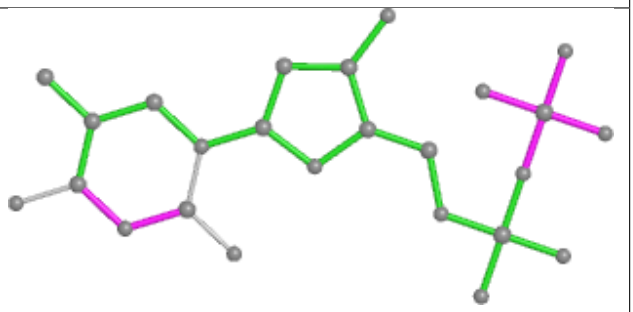

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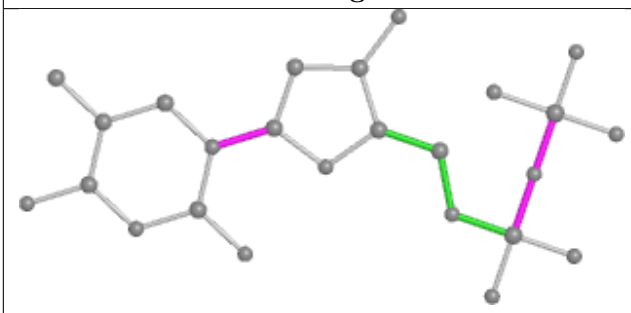

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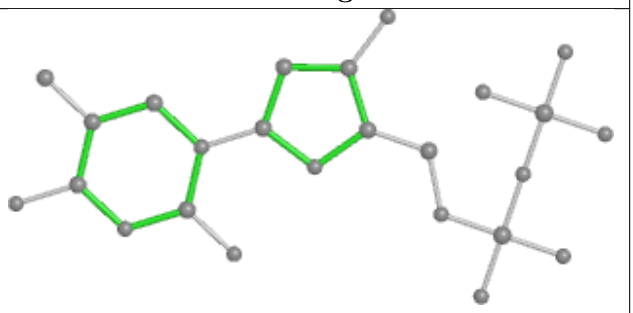
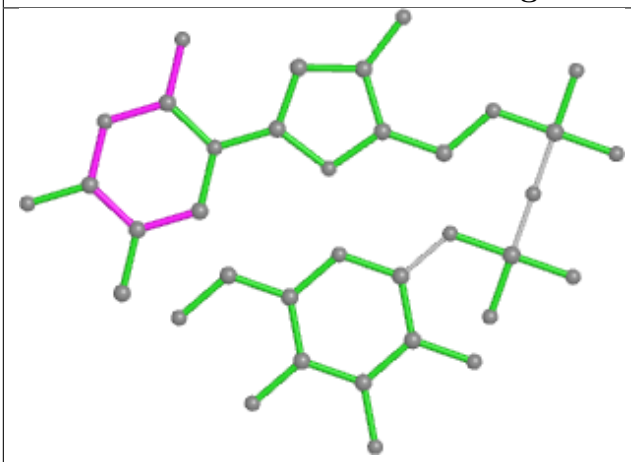


Rings

Ligand DAU H 301



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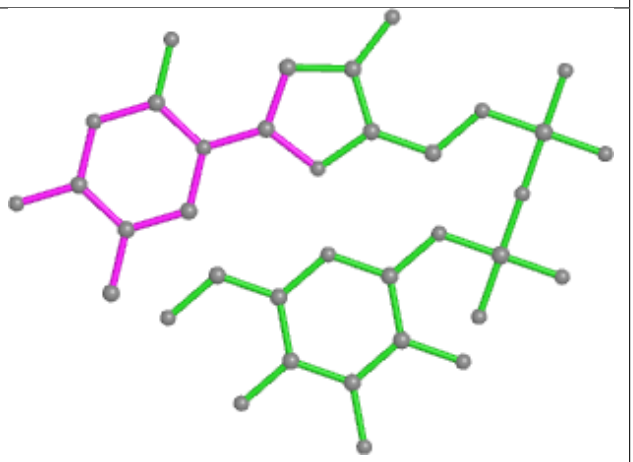

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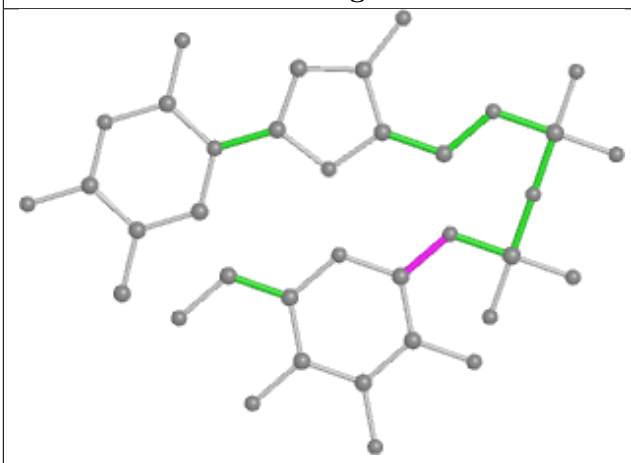

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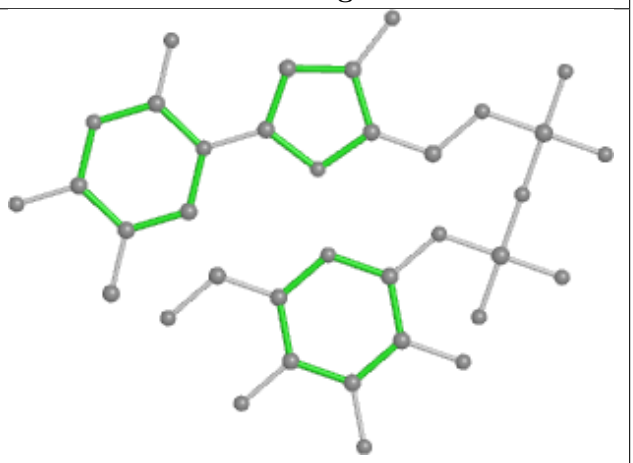
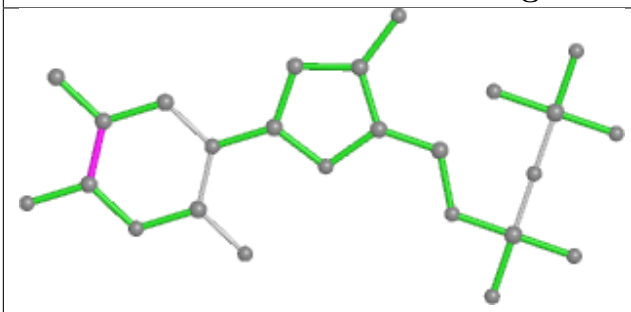


Rings

Ligand TYD C 303



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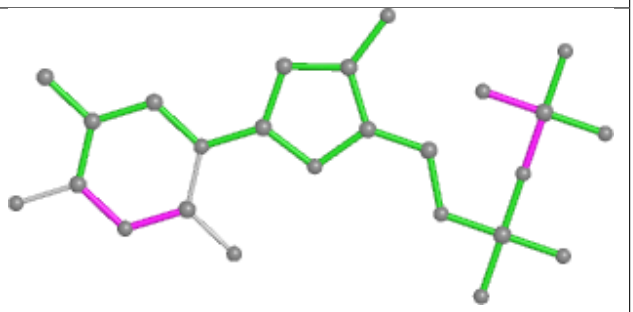

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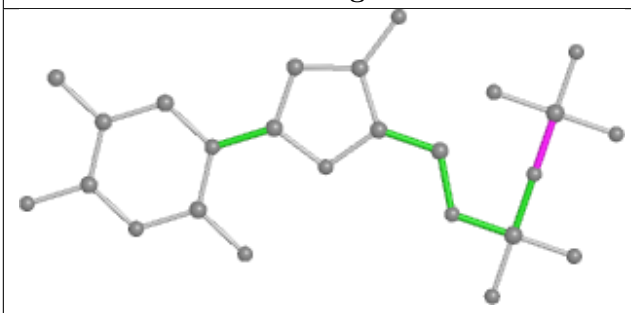

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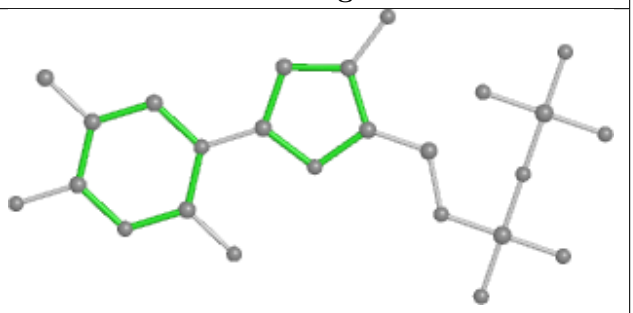
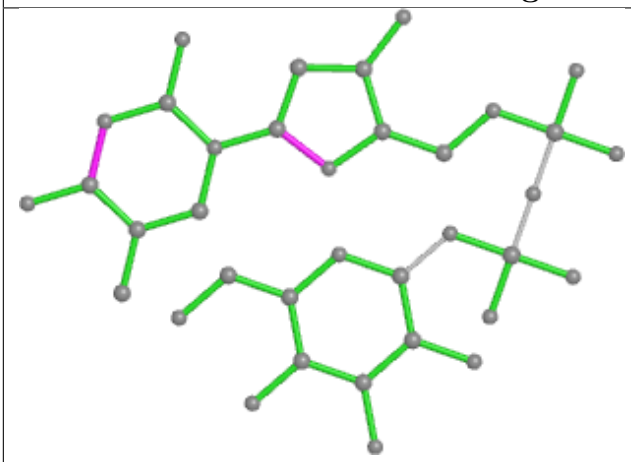


Rings

Ligand DAU B 301



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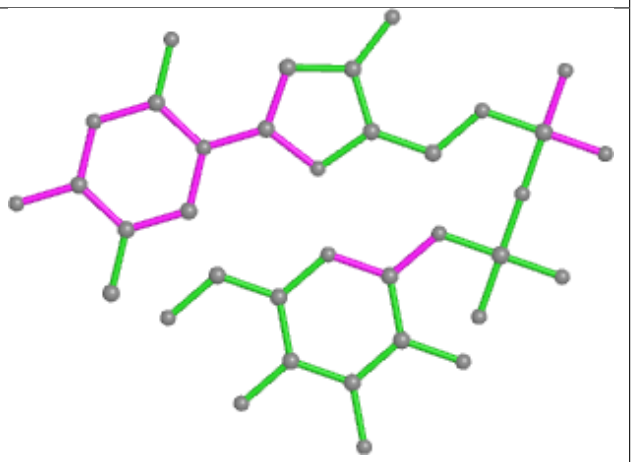

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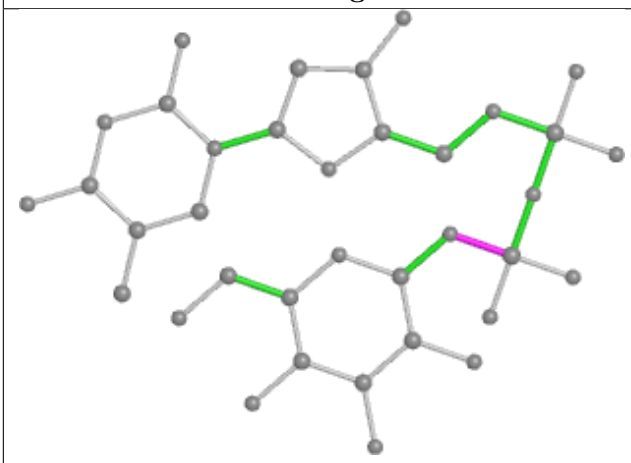

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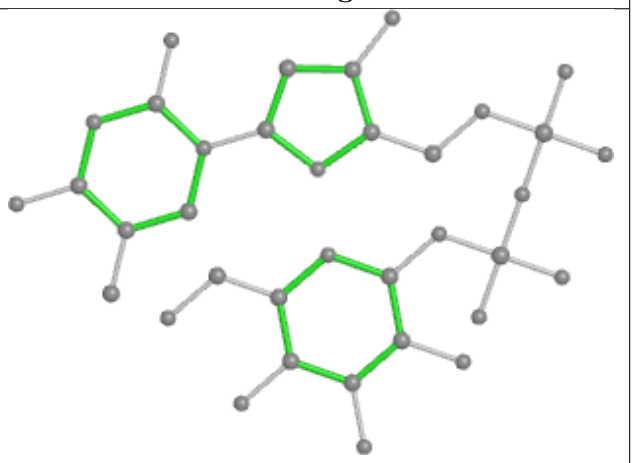

Rings

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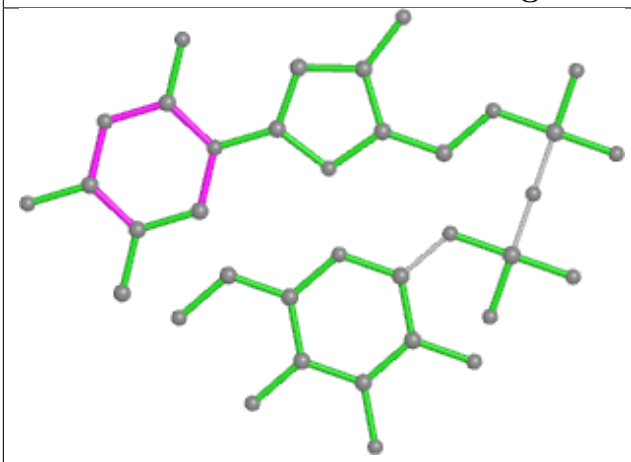

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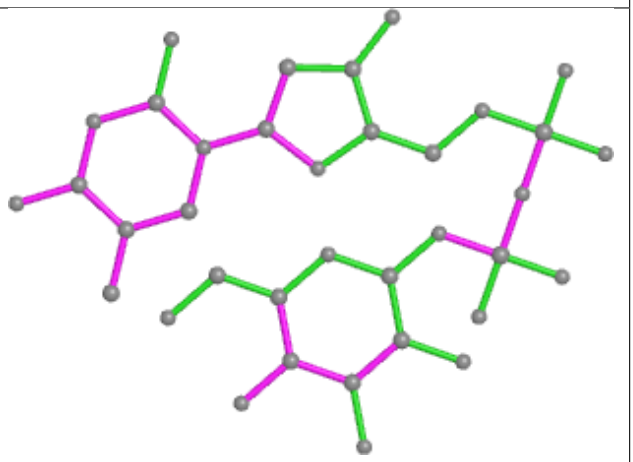
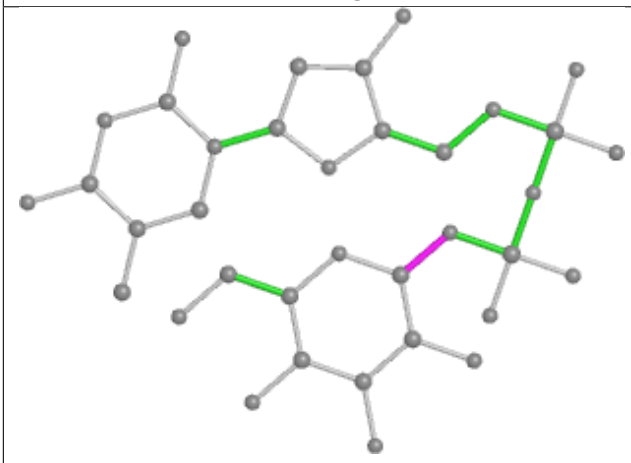


Bond angles



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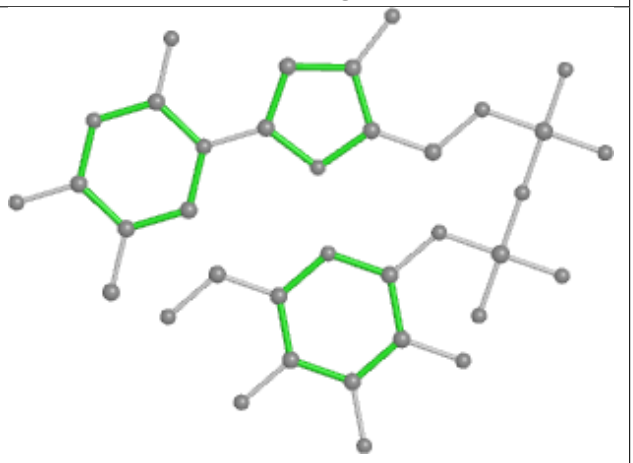
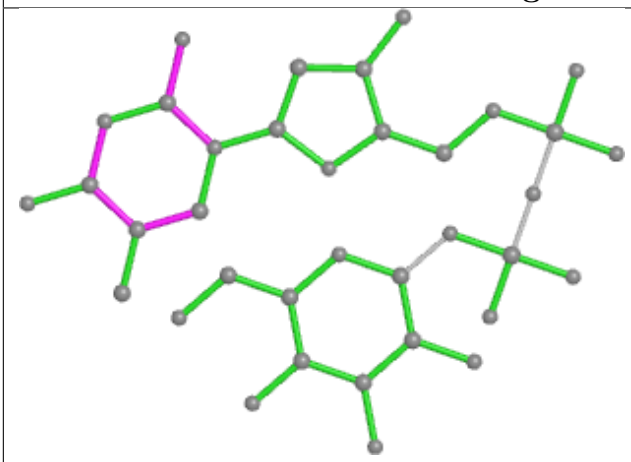


Rings

Ligand DAU E 302



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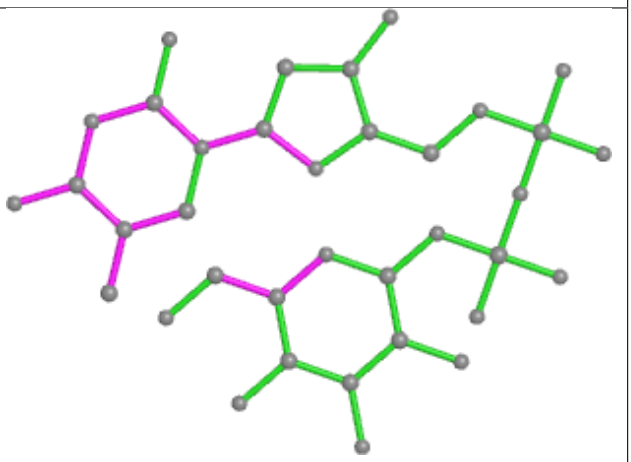
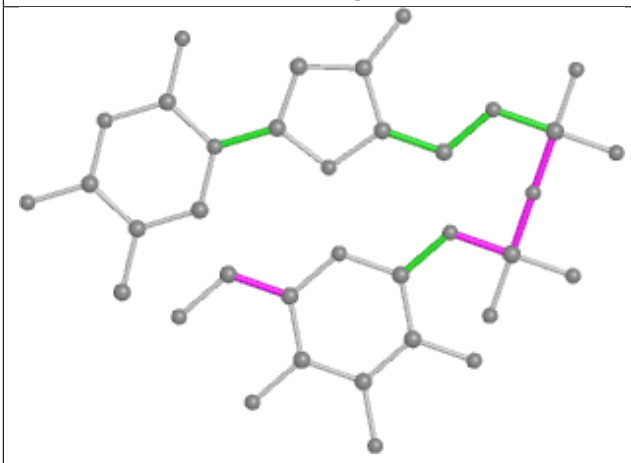


Bond angles



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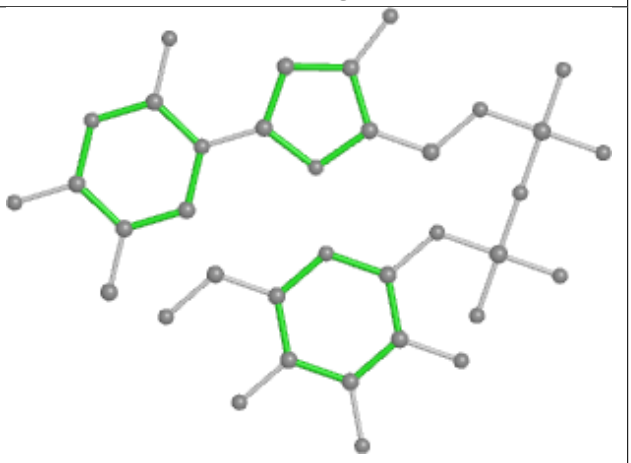
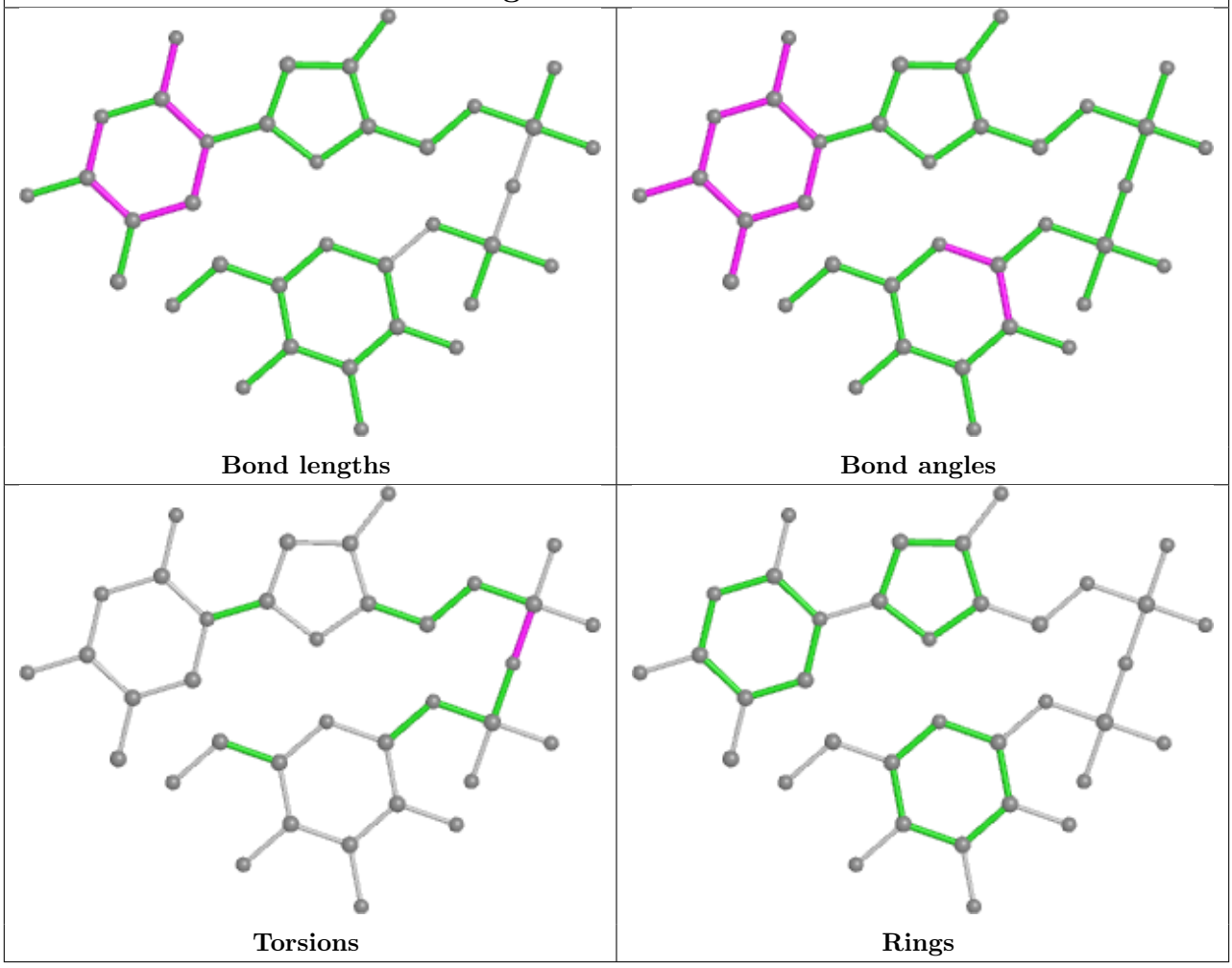


Rings

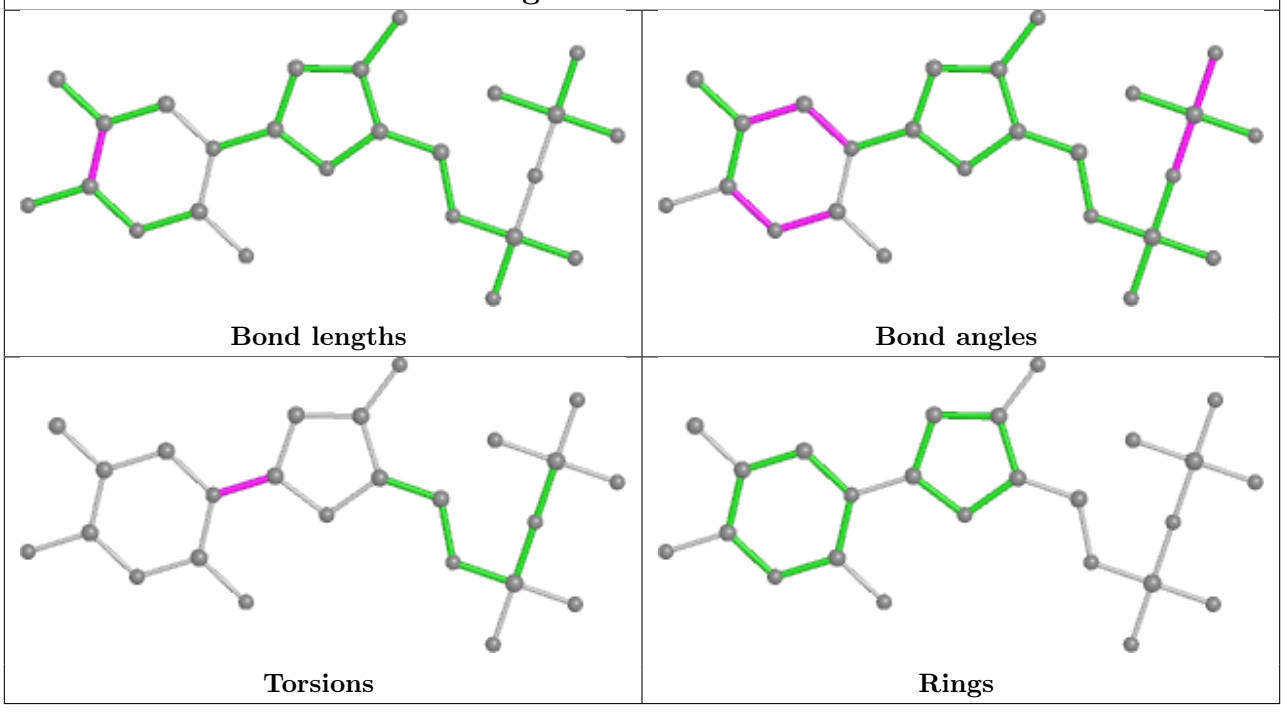
Ligand DAU F 302



Bond lengths | Bond angles

Torsions | Rings

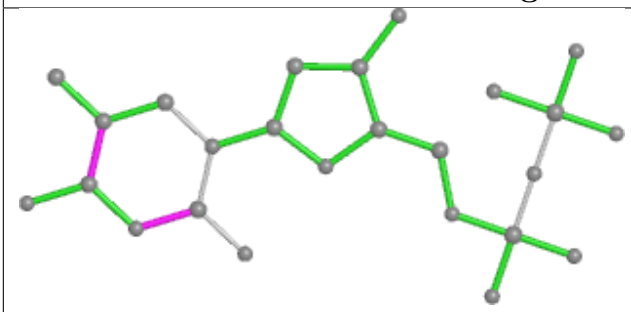
Ligand TYD A 303



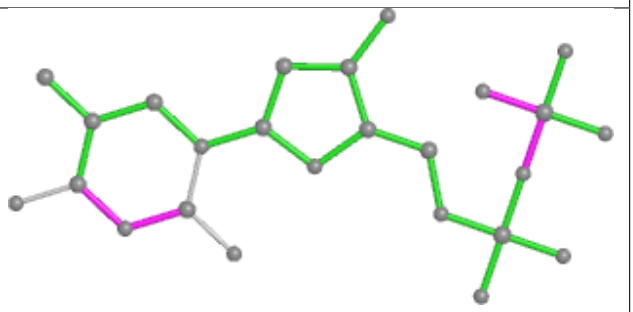
Bond lengths | Bond angles

Torsions | Rings

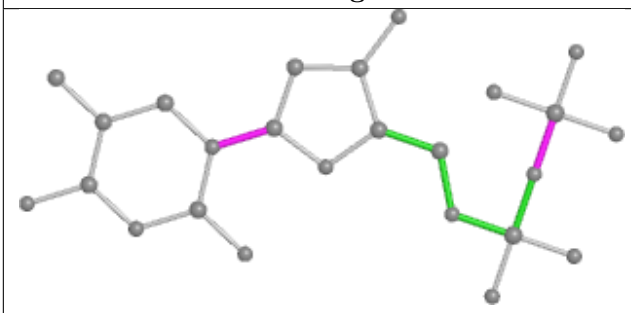
Ligand TYD G 303



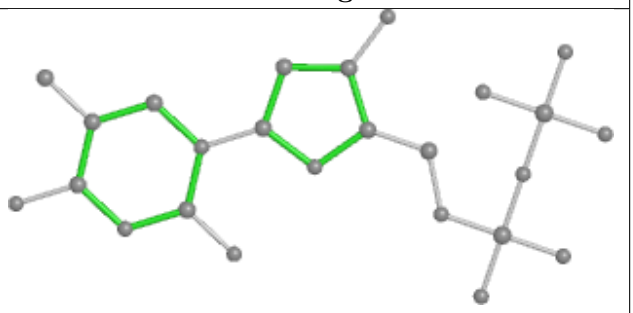
Bond lengths



Bond angles

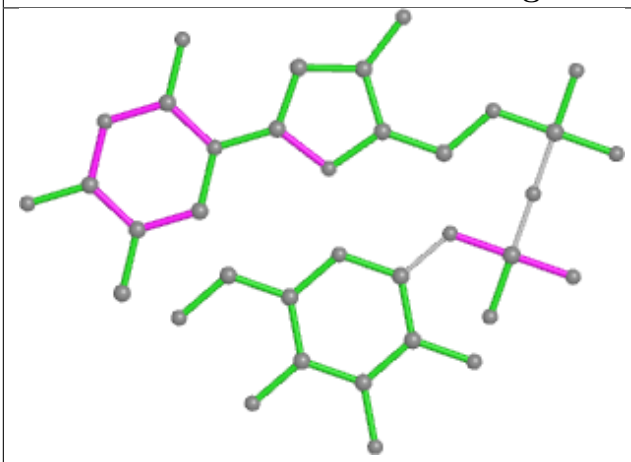


Torsions

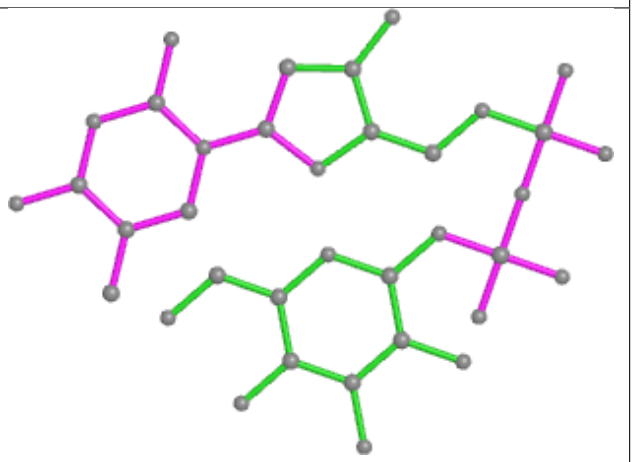


Rings

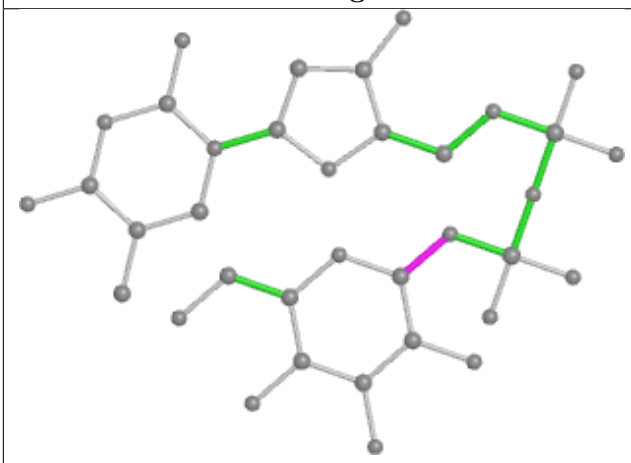
Ligand DAU E 301



Bond lengths



Bond angles



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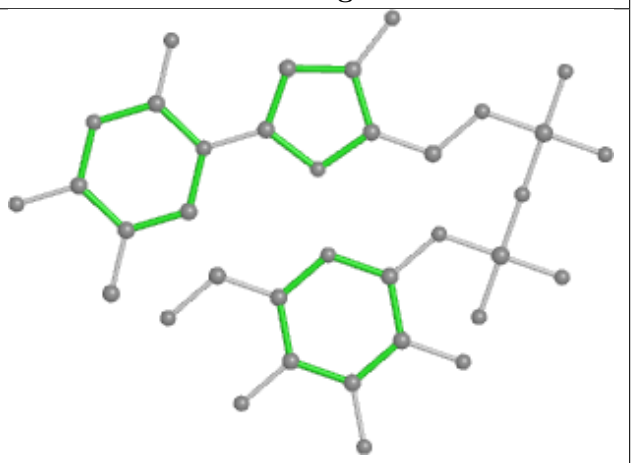
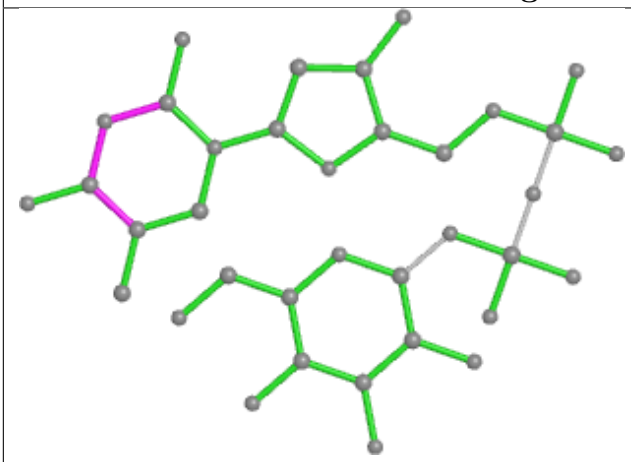
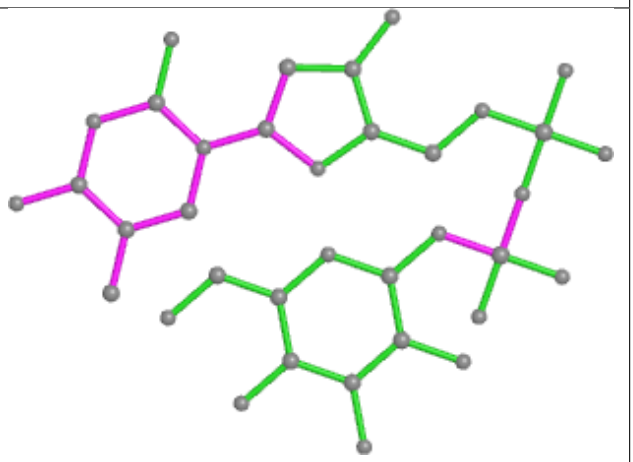


Rings

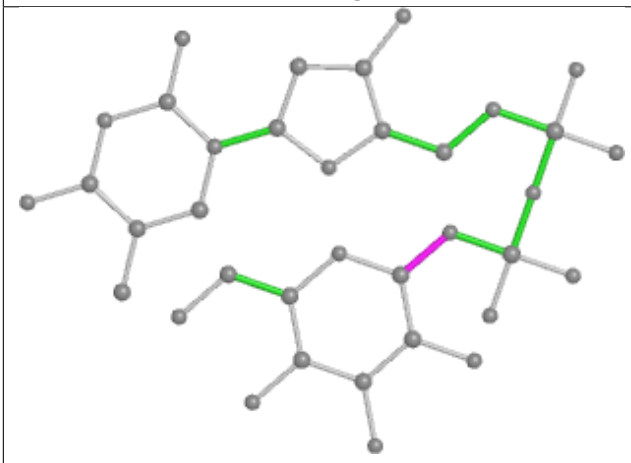
Ligand DAU D 301



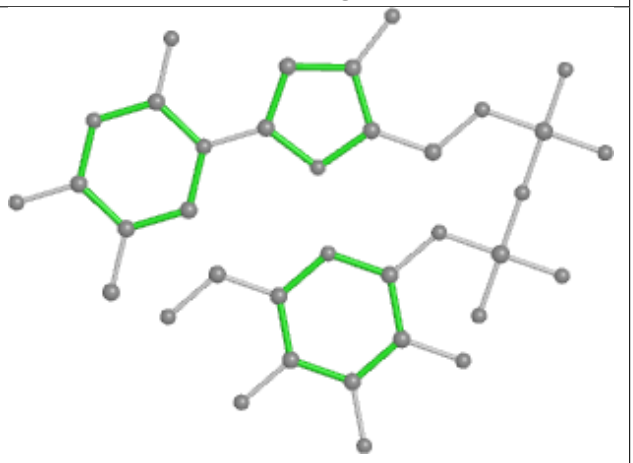
Bond lengths



Bond angles

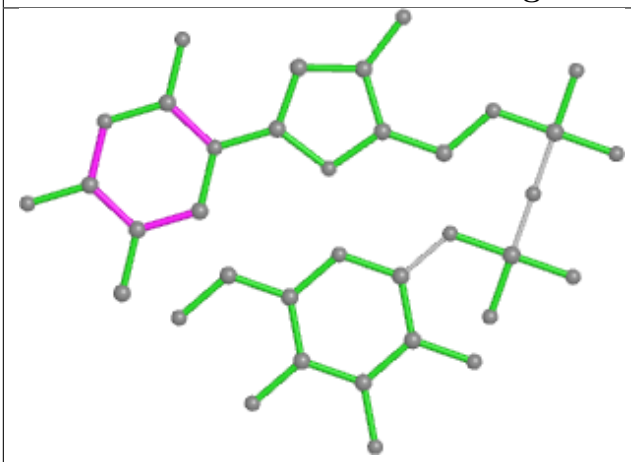


Torsions

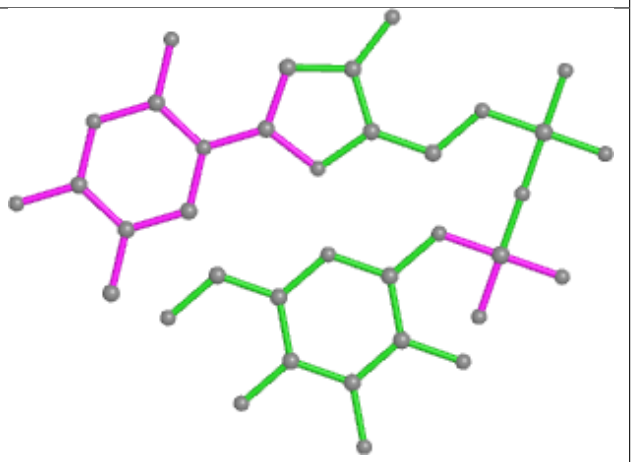


Rings

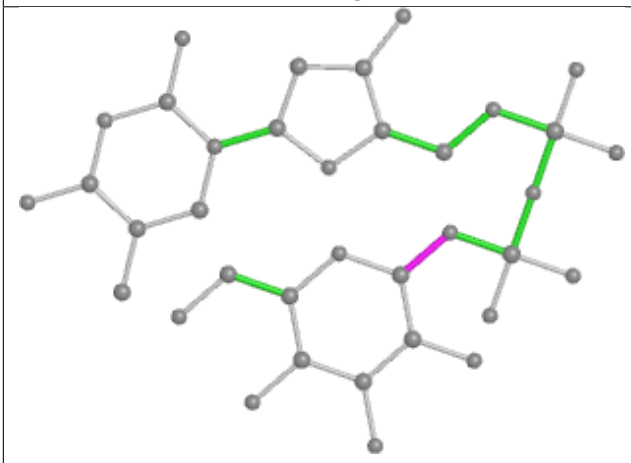
Ligand DAU F 301



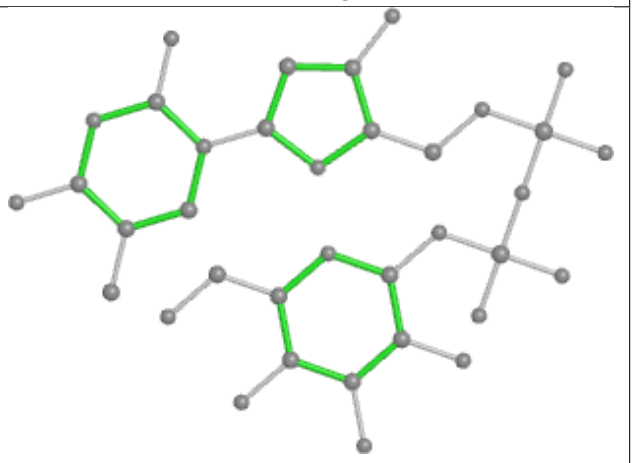
Bond lengths



Bond angles

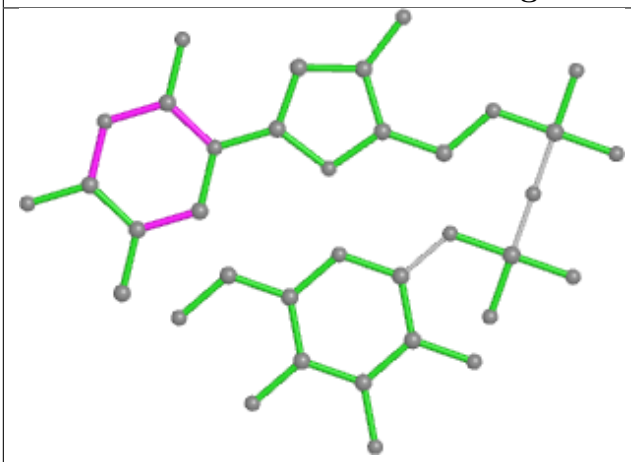


Torsions

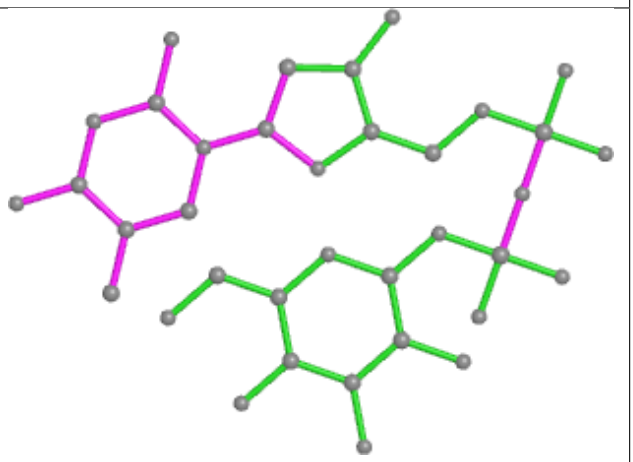


Rings

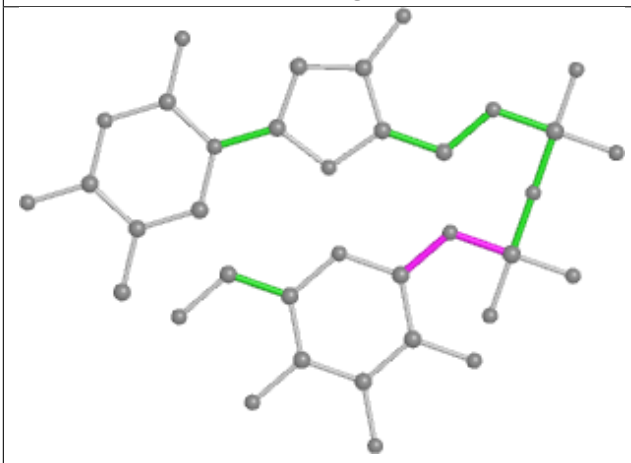
Ligand DAU G 301



Bond lengths



Bond angles



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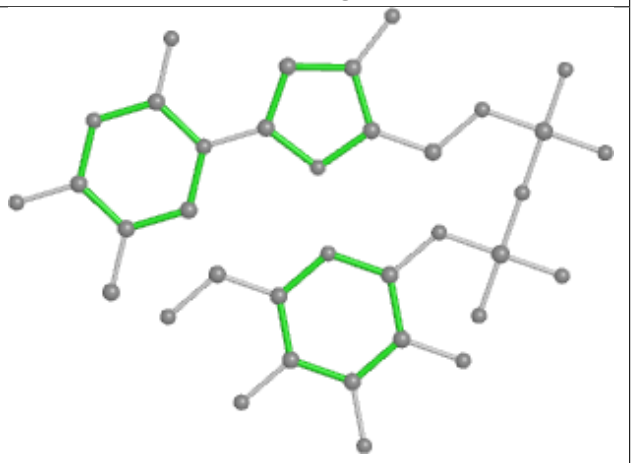
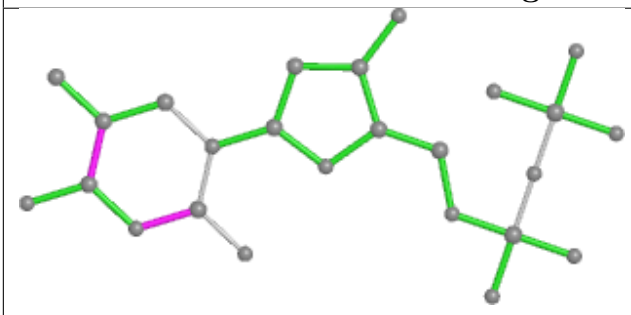
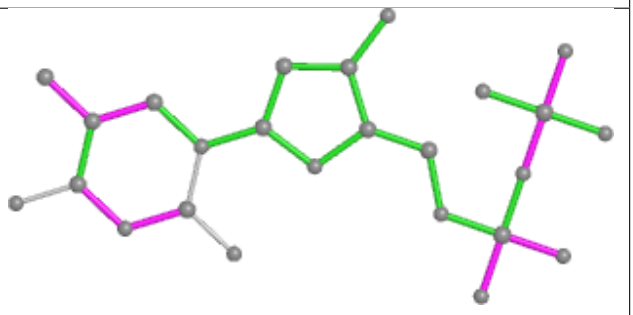


Rings

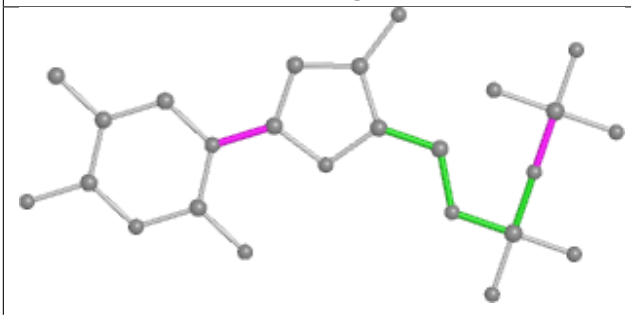
Ligand TYD B 304



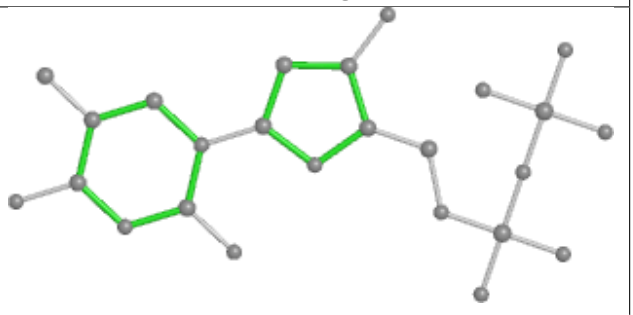
Bond lengths



Bond angles

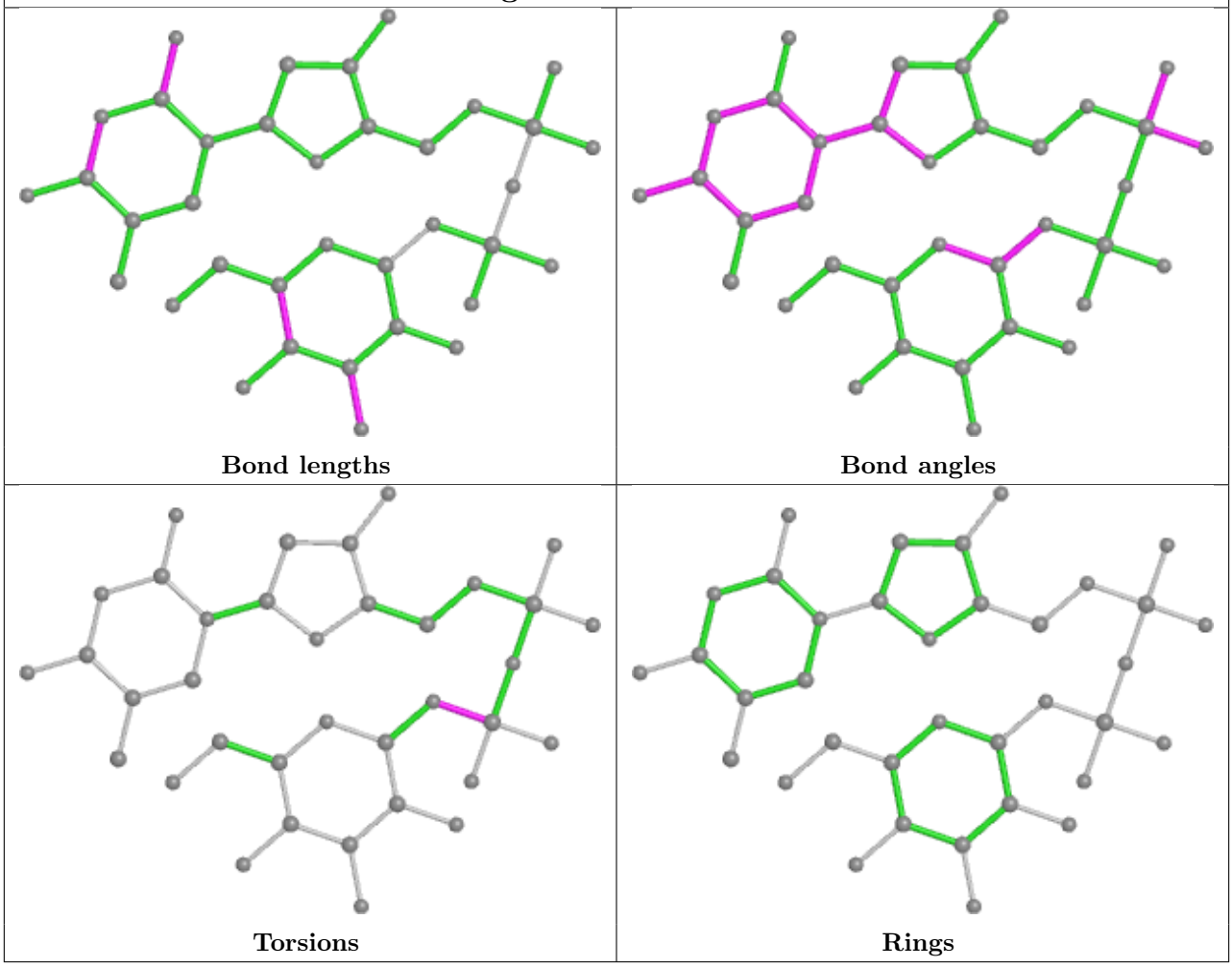


Torsions



Rings

Ligand DAU A 301



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	283/296 (95%)	-0.19	3 (1%)	80	81	10, 18, 41, 70	0
1	B	286/296 (96%)	-0.23	3 (1%)	82	82	9, 17, 37, 69	0
1	C	286/296 (96%)	-0.02	8 (2%)	53	52	14, 23, 50, 88	0
1	D	286/296 (96%)	0.14	9 (3%)	49	47	14, 28, 50, 84	0
1	E	286/296 (96%)	0.04	16 (5%)	24	23	13, 22, 54, 72	0
1	F	284/296 (95%)	0.20	19 (6%)	17	17	14, 25, 51, 77	0
1	G	284/296 (95%)	-0.06	12 (4%)	36	34	13, 23, 43, 59	0
1	H	279/296 (94%)	0.72	34 (12%)	4	4	15, 35, 63, 102	0
All	All	2274/2368 (96%)	0.07	104 (4%)	32	31	9, 23, 51, 102	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	ARG	6.8
1	E	149	ALA	6.4
1	C	190	ALA	6.0
1	H	186	LEU	5.5
1	B	190	ALA	5.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

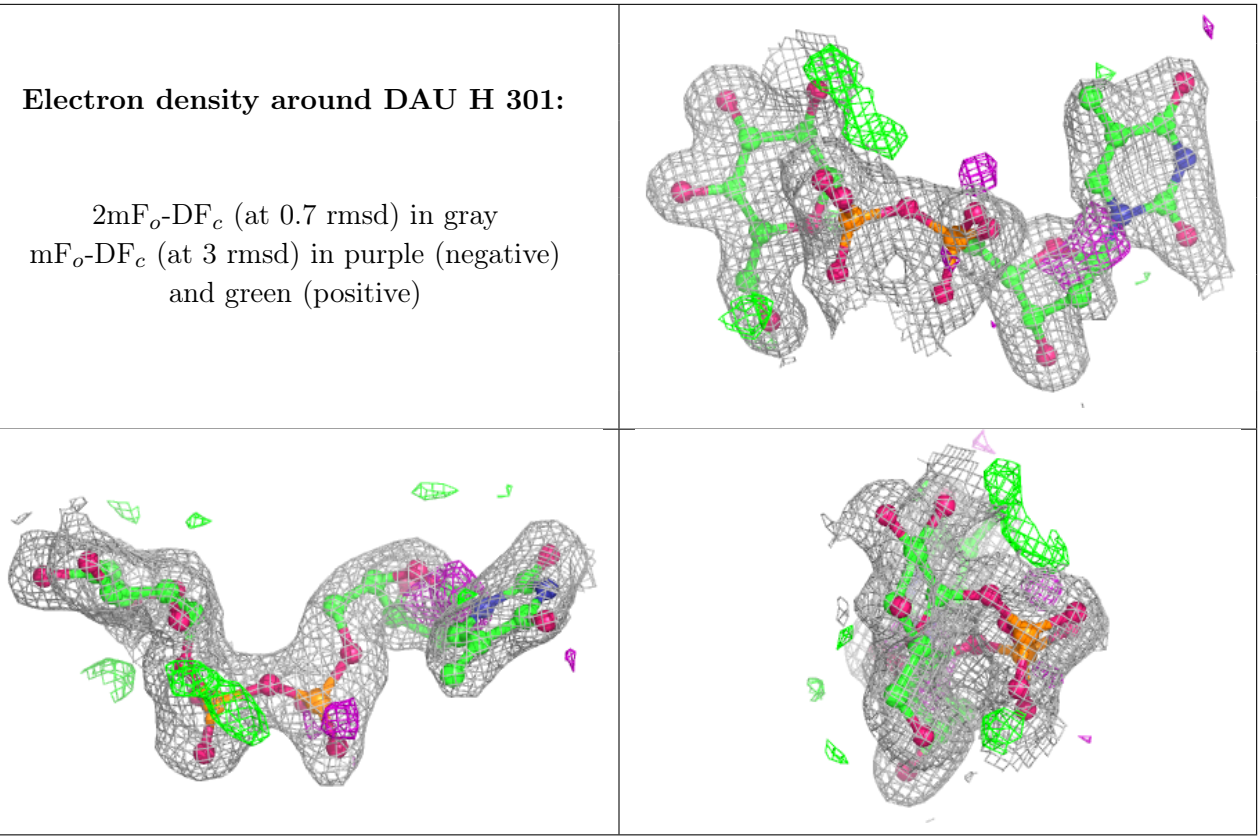
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	DAU	H	301	36/36	0.93	0.12	21,30,39,43	0
4	TYD	H	303	25/25	0.94	0.11	29,33,38,41	0
3	MG	H	302	1/1	0.95	0.07	30,30,30,30	0
3	MG	B	303	1/1	0.95	0.07	34,34,34,34	0
4	TYD	C	303	25/25	0.96	0.09	23,26,32,35	0
2	DAU	C	301	36/36	0.96	0.09	19,22,27,28	0
6	EDO	A	305	4/4	0.96	0.10	23,24,26,29	0
7	NA	B	305	1/1	0.96	0.20	32,32,32,32	0
4	TYD	B	304	25/25	0.97	0.07	16,19,22,27	0
2	DAU	D	301	36/36	0.97	0.07	19,23,26,30	0
4	TYD	D	303	25/25	0.97	0.08	24,27,32,36	0
4	TYD	G	303	25/25	0.97	0.07	24,28,33,34	0
2	DAU	E	302	36/36	0.97	0.09	20,28,50,57	0
2	DAU	F	302	36/36	0.97	0.08	20,24,40,42	0
4	TYD	A	303	25/25	0.97	0.08	18,20,25,29	0
2	DAU	A	301	36/36	0.98	0.07	12,15,18,20	0
2	DAU	F	301	36/36	0.98	0.07	17,21,26,27	0
2	DAU	B	301	36/36	0.98	0.08	9,12,15,16	0
2	DAU	G	301	36/36	0.98	0.07	13,16,19,21	0
2	DAU	E	301	36/36	0.98	0.06	12,16,18,19	0
3	MG	F	303	1/1	0.99	0.09	18,18,18,18	0
3	MG	A	302	1/1	0.99	0.06	12,12,12,12	0
3	MG	C	302	1/1	0.99	0.07	20,20,20,20	0
3	MG	D	302	1/1	0.99	0.06	17,17,17,17	0
3	MG	E	303	1/1	0.99	0.03	17,17,17,17	0
7	NA	C	304	1/1	0.99	0.08	17,17,17,17	0
3	MG	G	302	1/1	1.00	0.06	14,14,14,14	0
3	MG	B	302	1/1	1.00	0.06	10,10,10,10	0
5	CL	A	304	1/1	1.00	0.06	19,19,19,19	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.

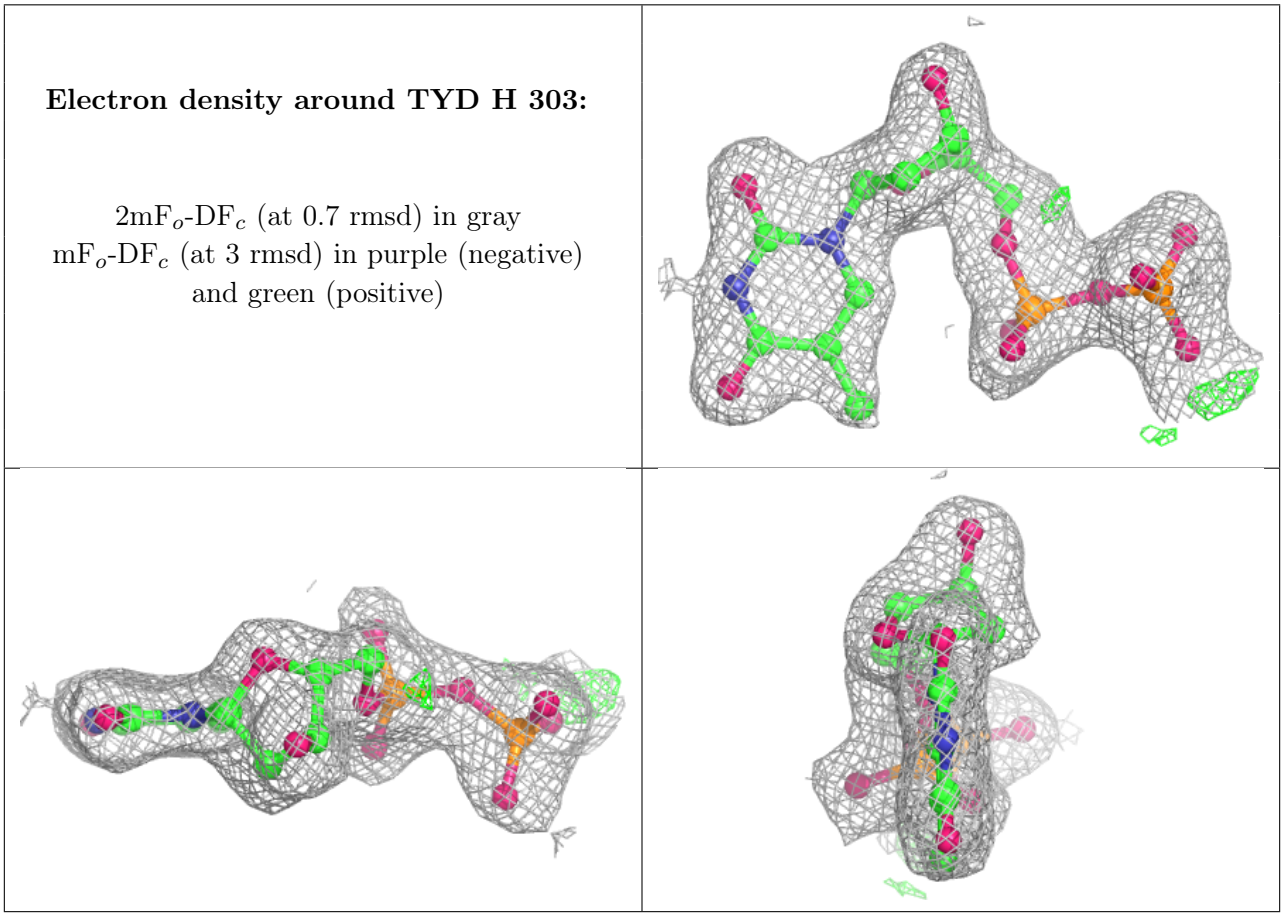
Electron density around DAU H 301:

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



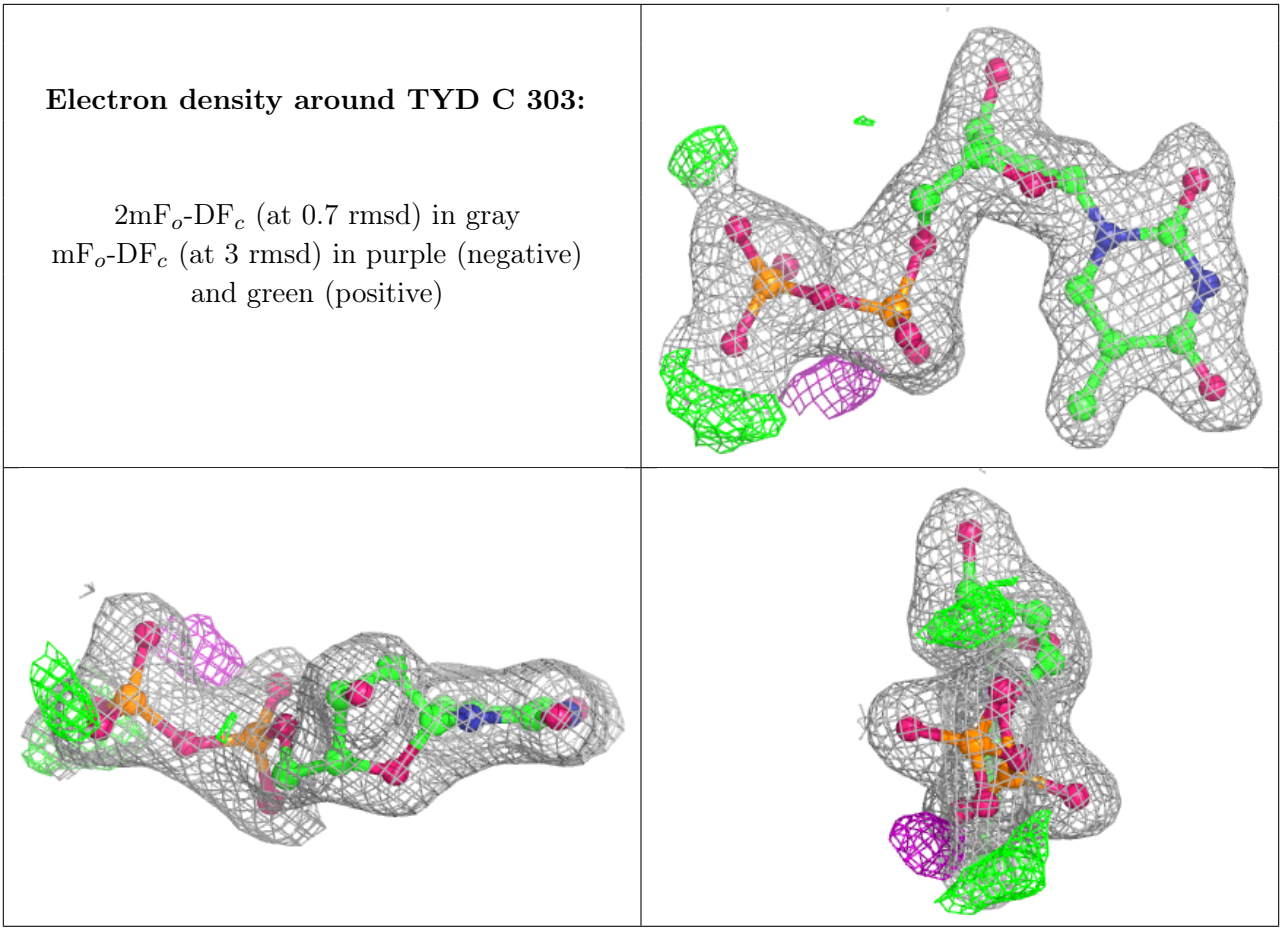
Electron density around TYD H 303:

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



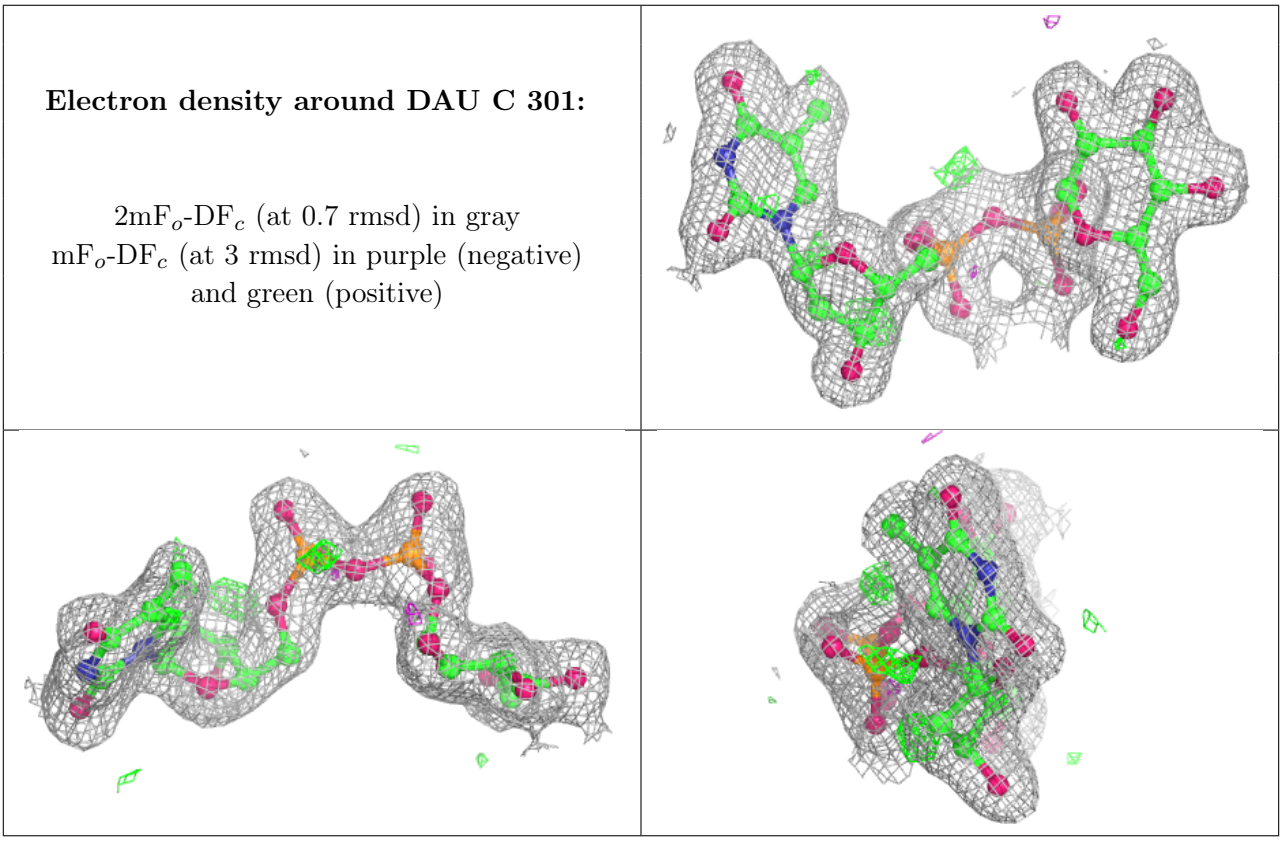
Electron density around TYD C 303:

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



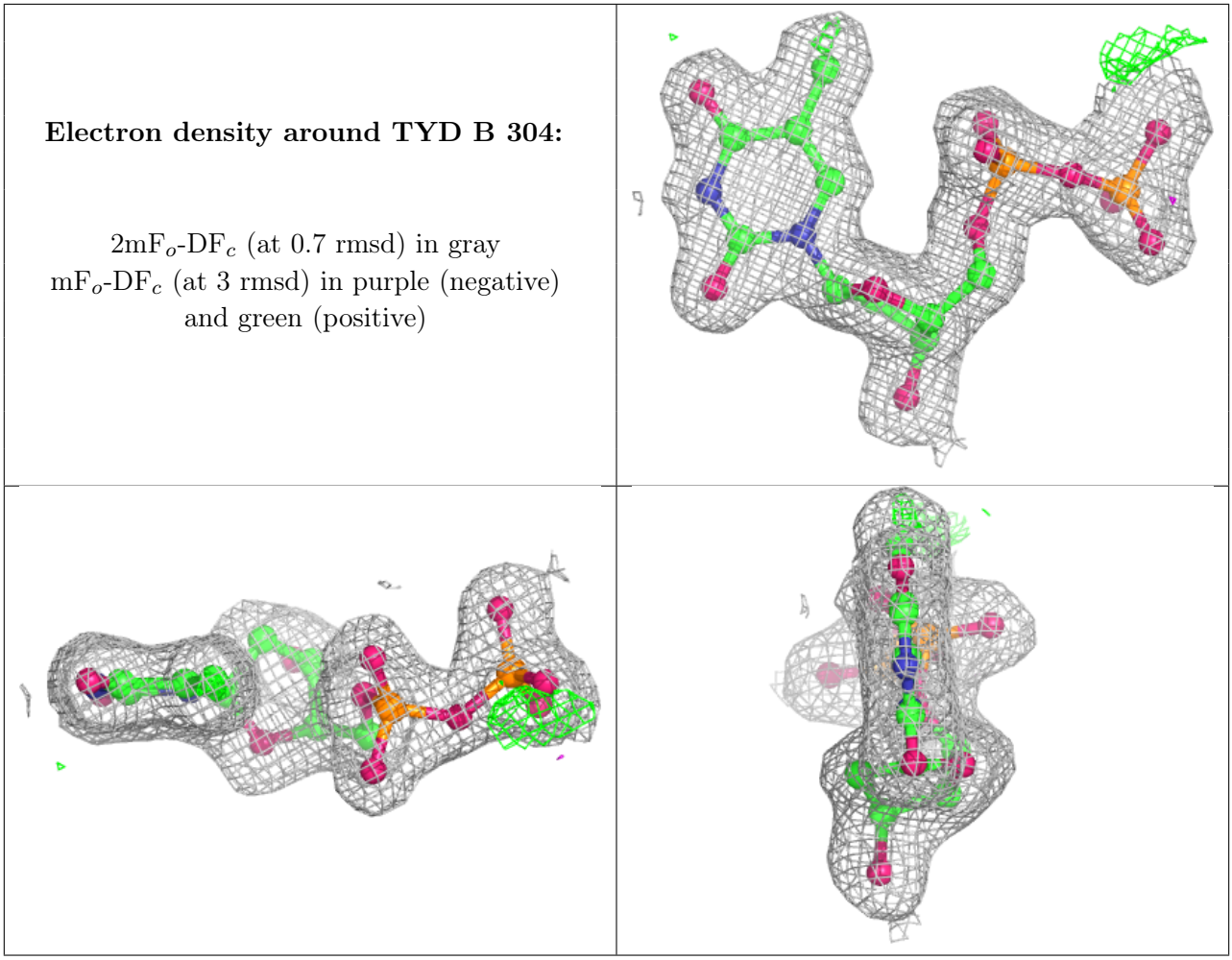
Electron density around DAU C 301:

$2mF_o$-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 304:

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



Electron density around DAU D 301:

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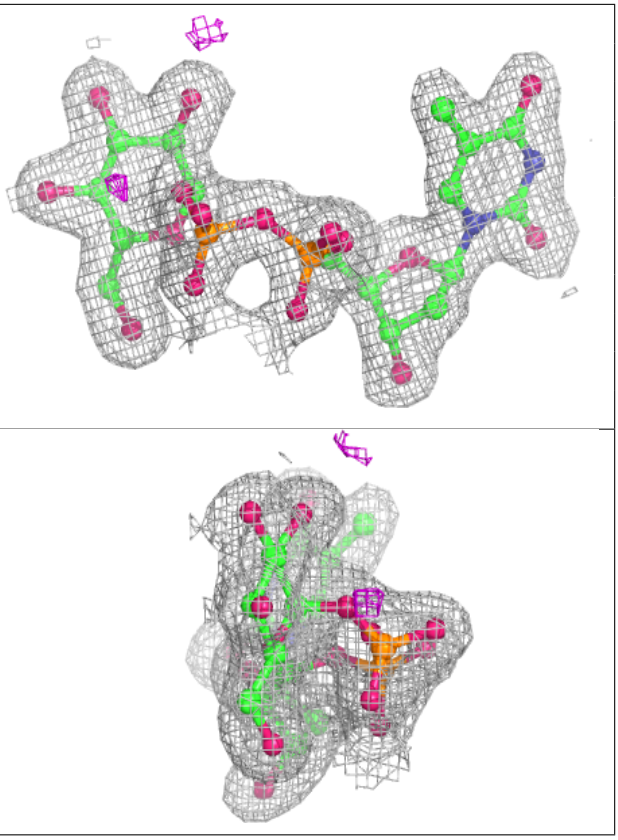
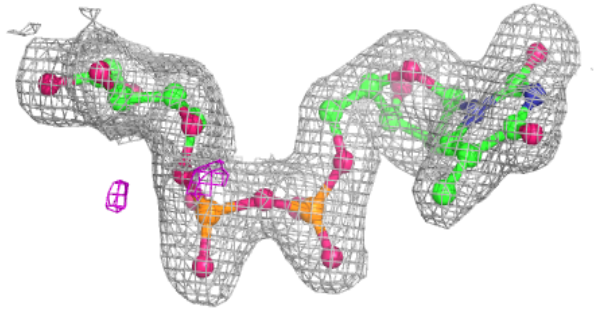
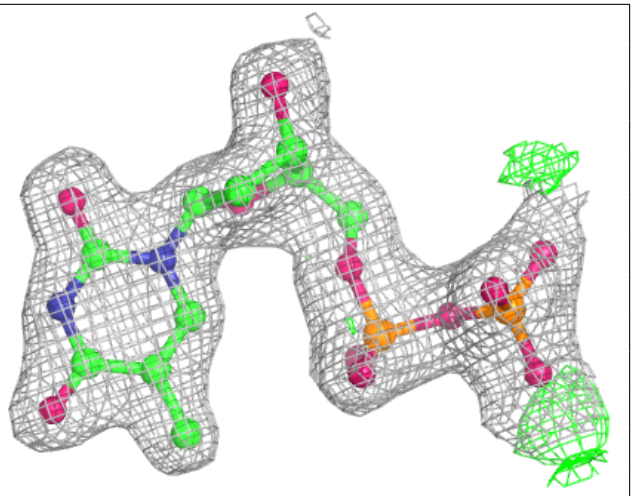
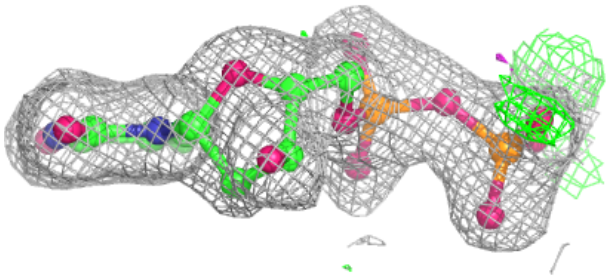


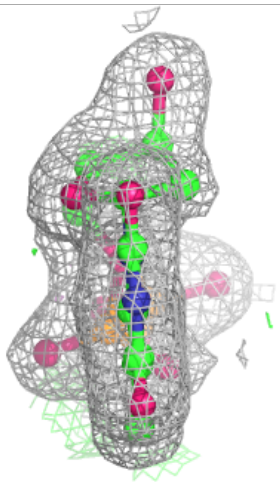


Electron density around TYD D 303:

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

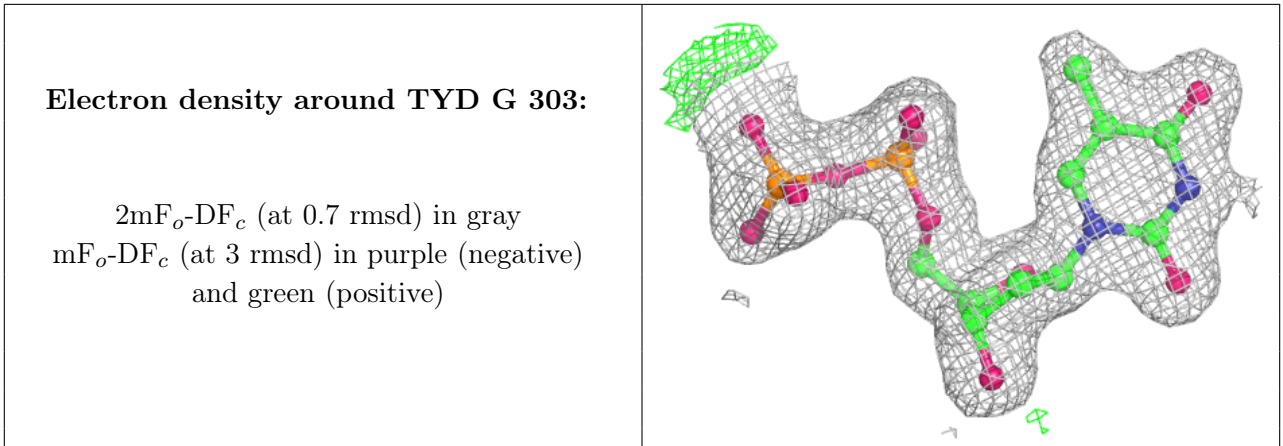






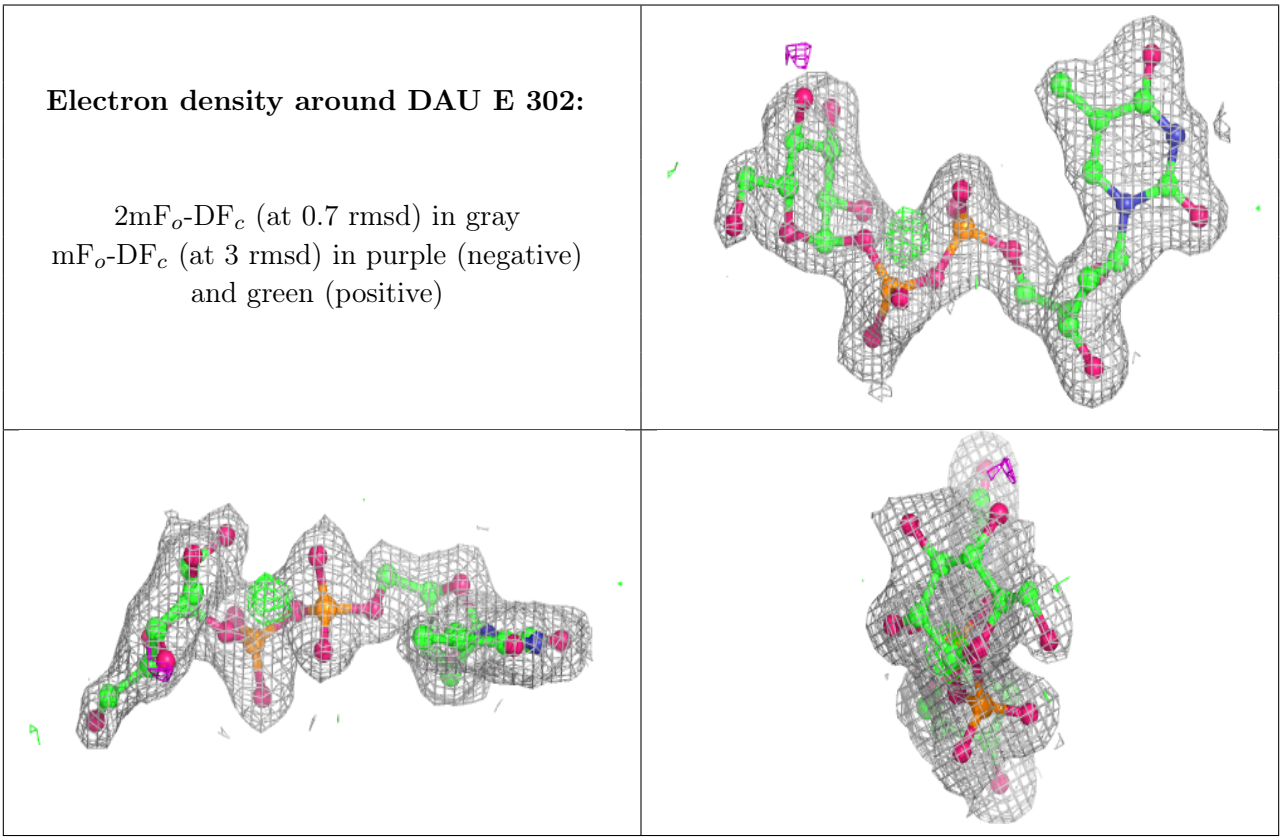
Electron density around TYD G 303:

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



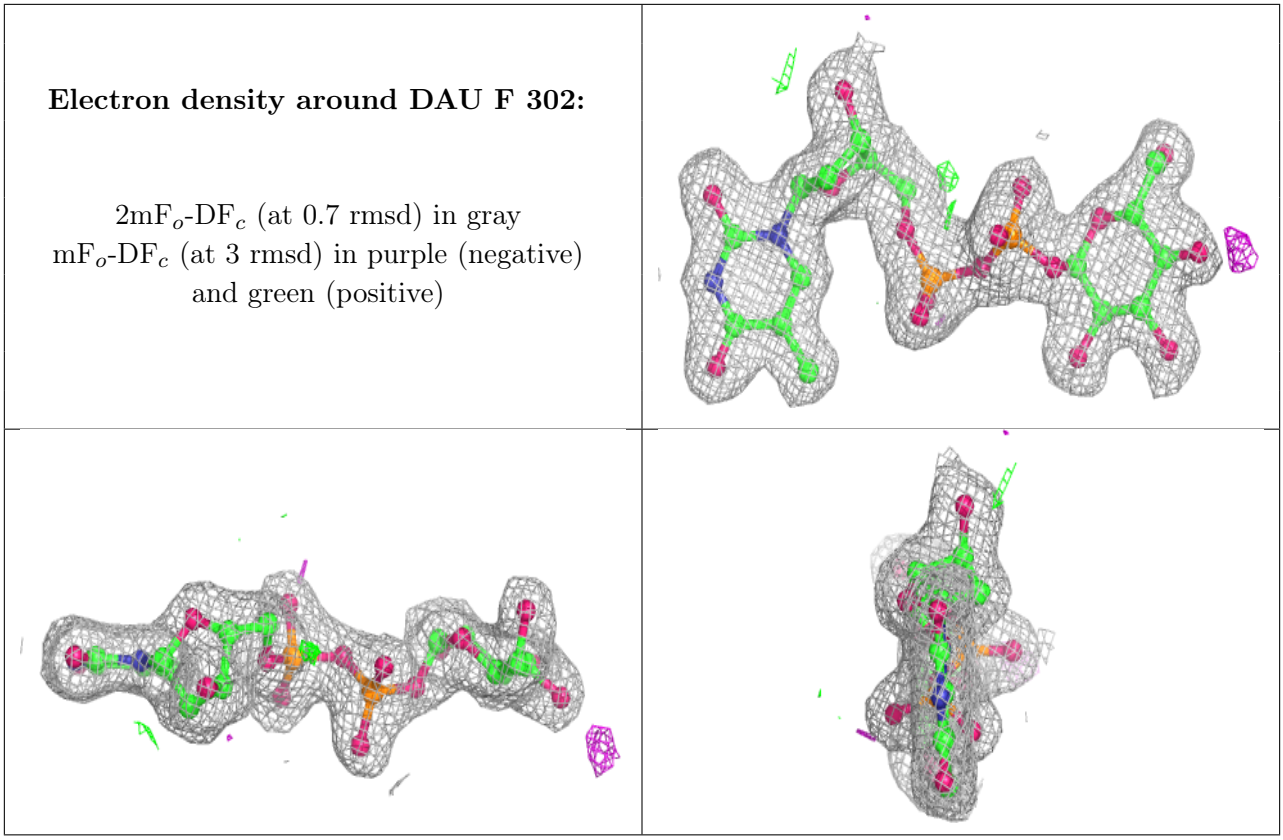
Electron density around DAU E 302:

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



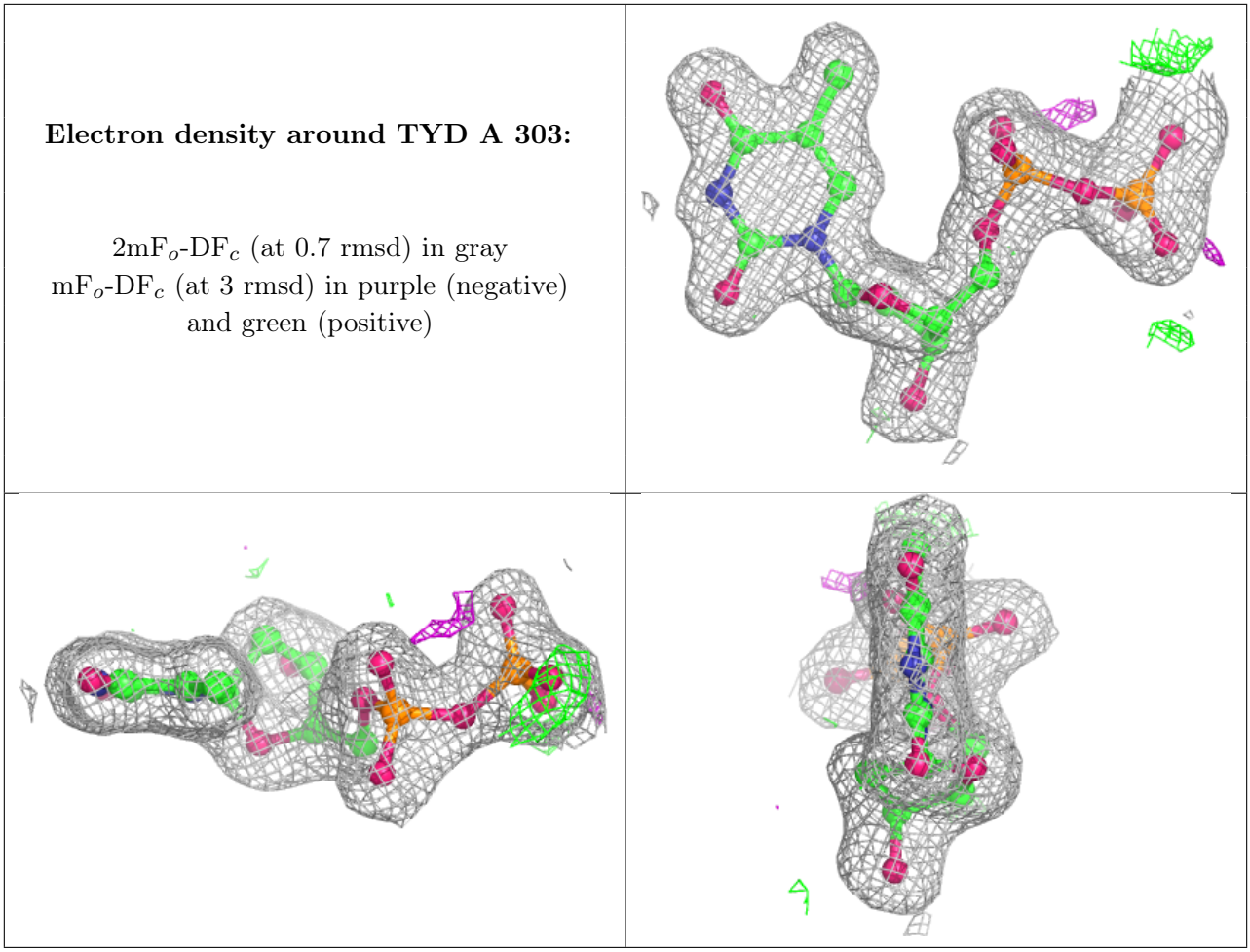
Electron density around DAU F 302:

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



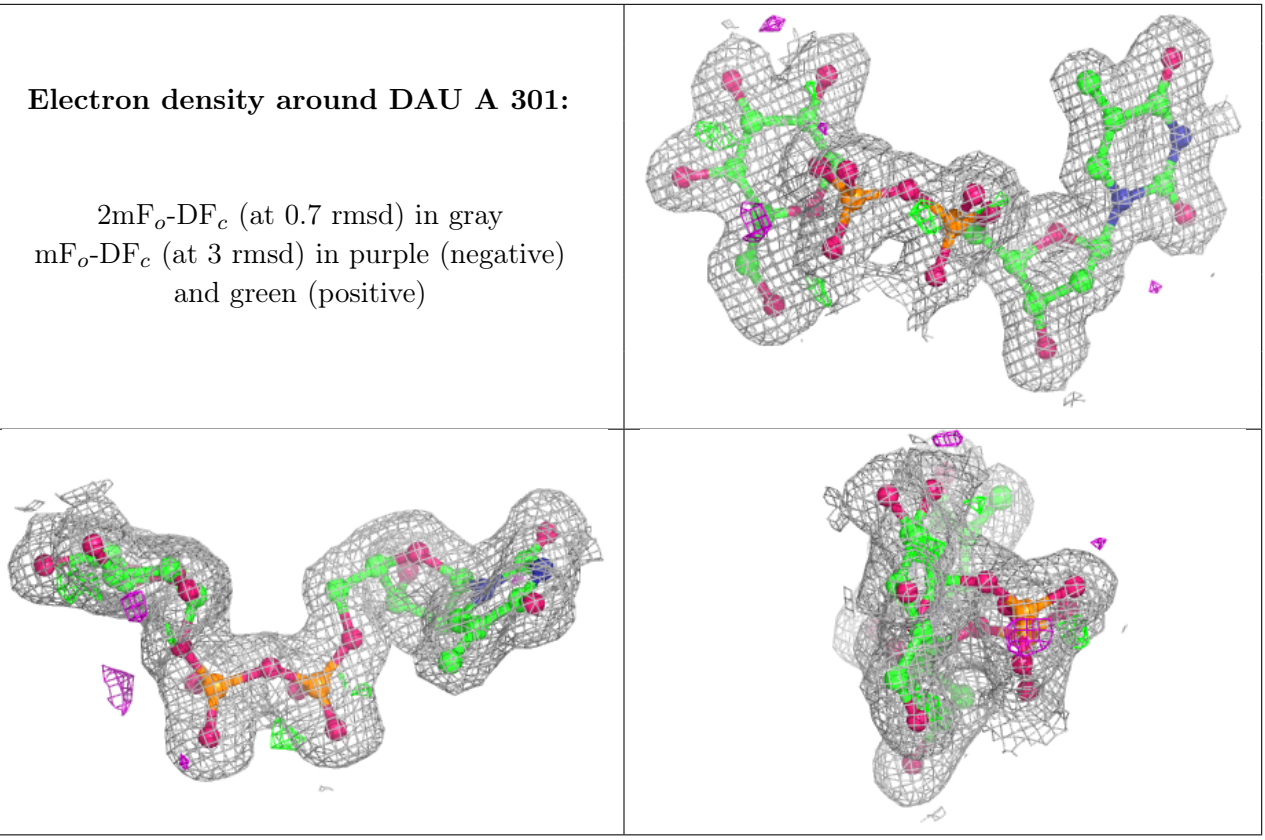
Electron density around TYD A 303:

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



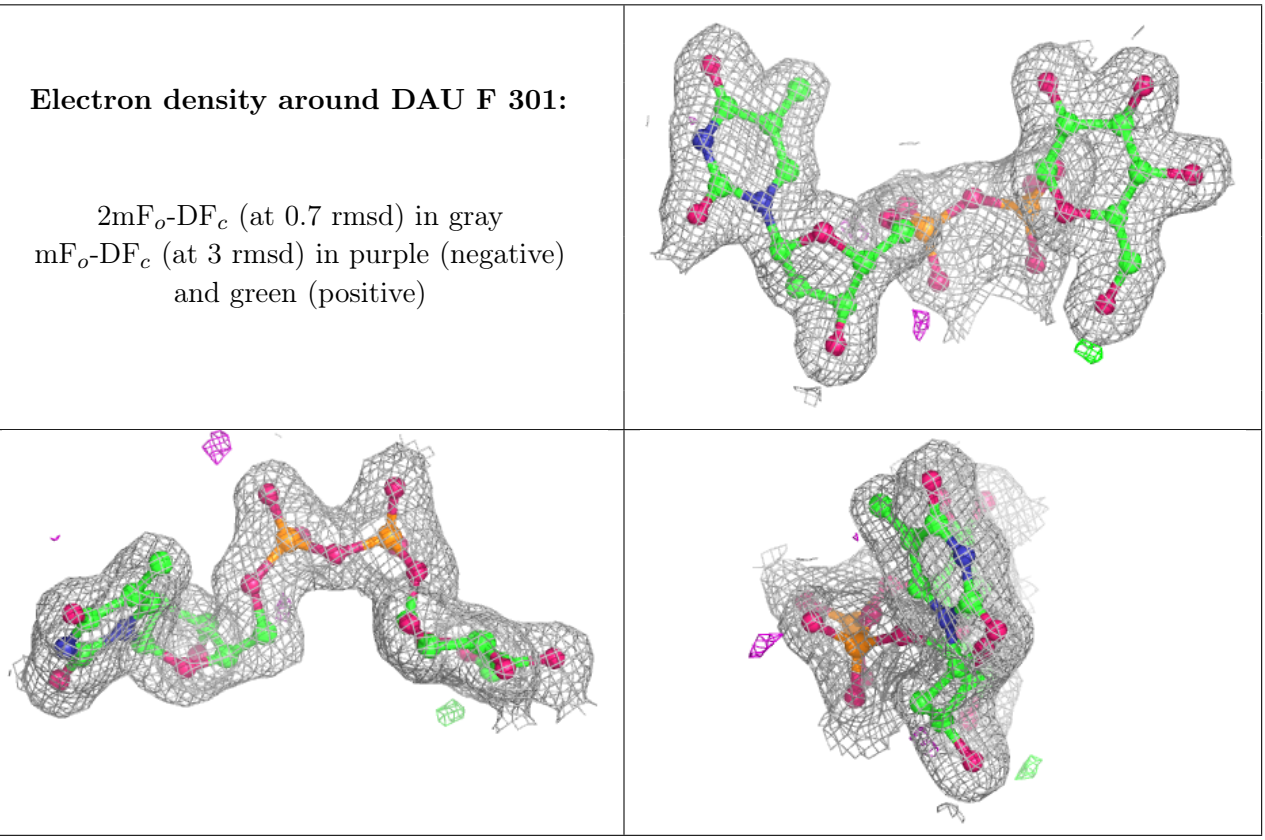
Electron density around DAU A 301:

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



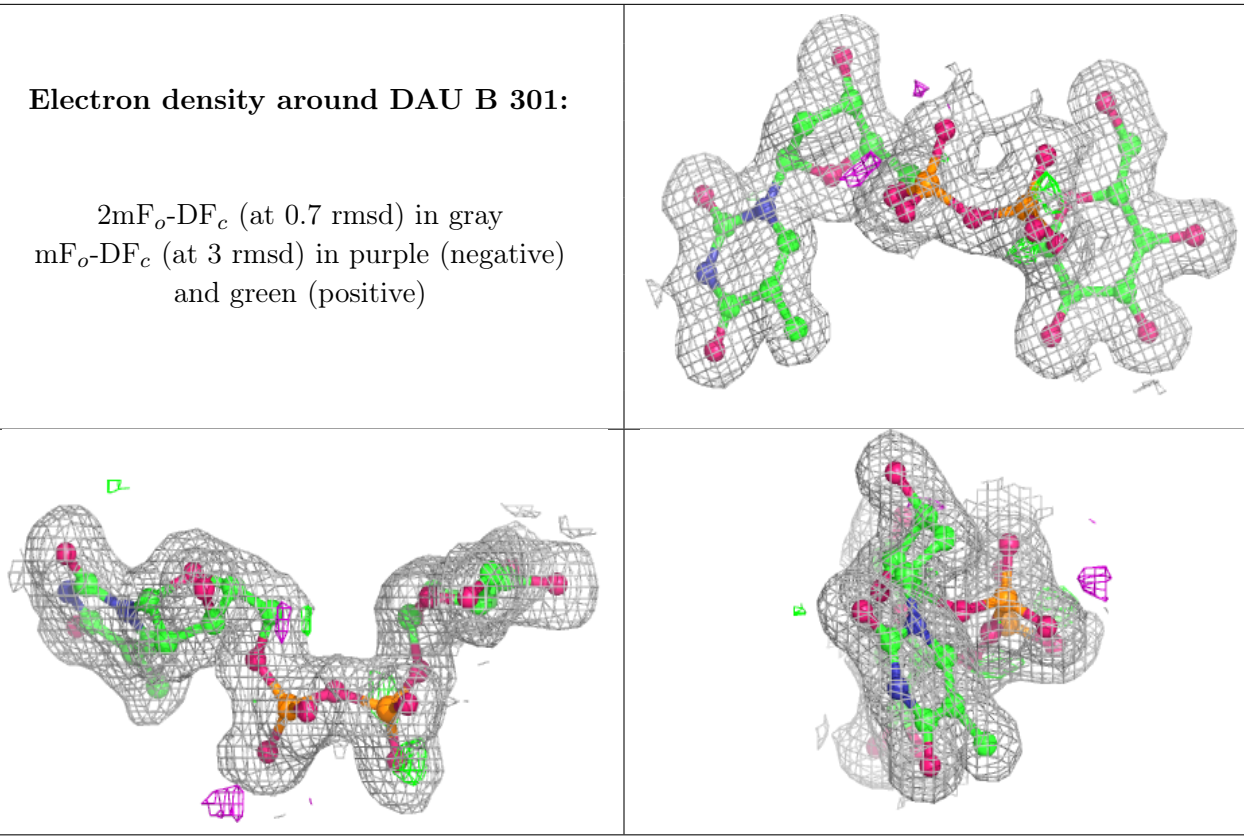
Electron density around DAU F 301:

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



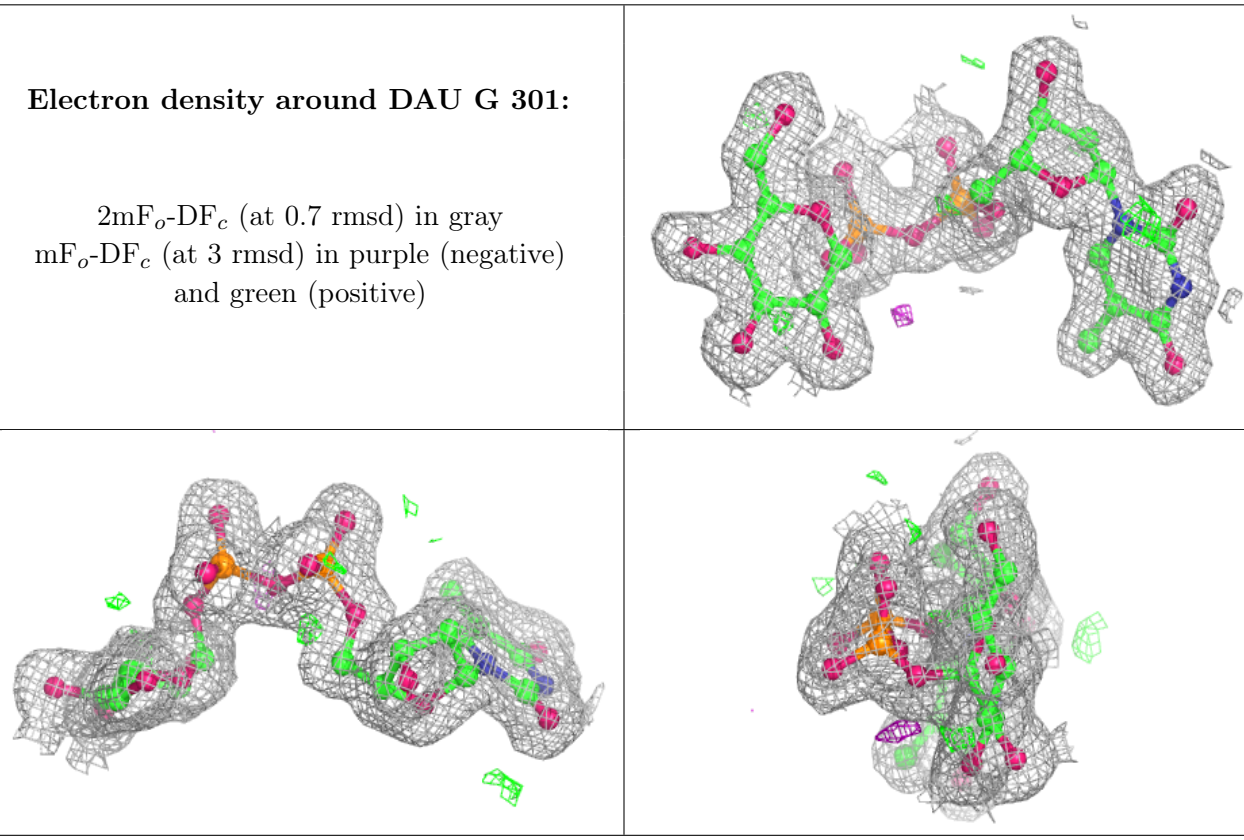
Electron density around DAU B 301:

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



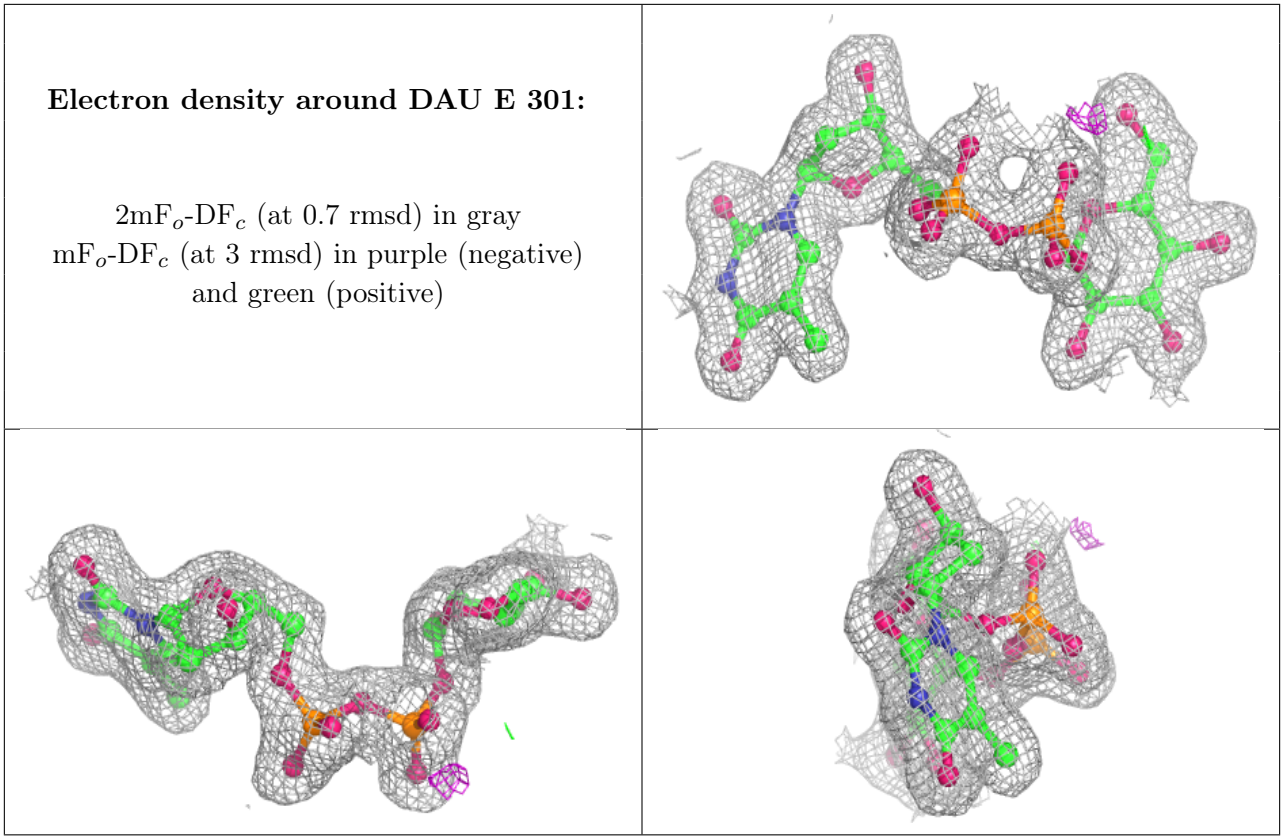
Electron density around DAU G 301:

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



Electron density around DAU E 301:

$2mF_o$-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.