



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2025 – 03:04 PM EDT

PDB ID : 3SOM  
Title : crystal structure of human MMACHC  
Authors : Krojer, T.; Froese, D.S.; von Delft, F.; Muniz, J.R.; Gileadi, C.; Vollmar, M.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Gravel, R.A.; Yue, W.W.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : 2011-06-30  
Resolution : 2.40 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

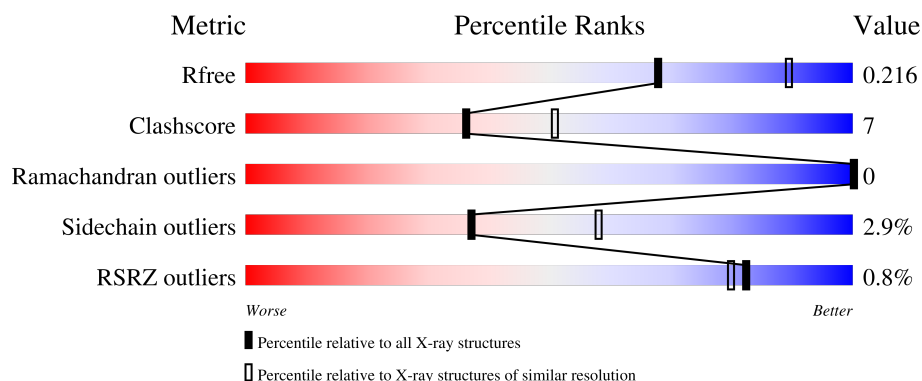
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	286	
1	B	286	
1	C	286	
1	D	286	

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Mol	Chain	Length	Quality of chain
1	E	286	
1	F	286	
1	G	286	
1	H	286	
1	I	286	
1	J	286	
1	K	286	
1	L	286	
1	M	286	
1	N	286	
1	O	286	
1	P	286	

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
5	5AD	A	401	X	-	-	-
5	5AD	B	401	X	-	-	-
5	5AD	C	401	X	-	-	-
5	5AD	D	401	X	-	-	-
5	5AD	E	401	X	-	-	-
5	5AD	F	401	X	-	-	-
5	5AD	G	283	X	-	-	-
5	5AD	G	401	X	-	-	-
5	5AD	H	401	X	-	-	-
5	5AD	I	283	X	-	-	-
5	5AD	I	401	X	-	-	-
5	5AD	J	401	X	-	-	-
5	5AD	K	401	X	-	-	-
5	5AD	L	401	X	-	-	-
5	5AD	M	401	X	-	-	-
5	5AD	N	401	X	-	-	-
5	5AD	O	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	5AD	P	401	X	-	-	-
6	EDO	P	284	-	-	X	-



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33236 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 Methylmalonic aciduria and homocystinuria type C protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	B	228	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	C	228	Total	C	N	O	S	Se	0	2	0
			1832	1190	318	316	6	2			
1	D	229	Total	C	N	O	S	Se	0	1	0
			1848	1200	320	320	6	2			
1	E	230	Total	C	N	O	S	Se	0	1	0
			1849	1201	321	319	6	2			
1	F	228	Total	C	N	O	S	Se	0	3	0
			1857	1203	324	322	6	2			
1	G	228	Total	C	N	O	S	Se	0	0	0
			1843	1195	322	319	5	2			
1	H	227	Total	C	N	O	S	Se	0	0	0
			1833	1190	317	319	5	2			
1	I	228	Total	C	N	O	S	Se	0	1	0
			1844	1196	321	319	6	2			
1	J	227	Total	C	N	O	S	Se	0	2	0
			1844	1196	321	319	5	3			
1	K	227	Total	C	N	O	S	Se	0	1	0
			1832	1189	318	318	5	2			
1	L	231	Total	C	N	O	S	Se	0	2	0
			1868	1213	325	322	6	2			
1	M	231	Total	C	N	O	S	Se	0	1	0
			1861	1206	321	326	6	2			
1	N	232	Total	C	N	O	S	Se	0	0	0
			1853	1204	324	318	5	2			
1	O	228	Total	C	N	O	S	Se	0	1	0
			1836	1194	316	318	6	2			
1	P	230	Total	C	N	O	S	Se	0	0	0
			1860	1208	322	323	5	2			

There are 64 discrepancies between the modelled and reference sequences:

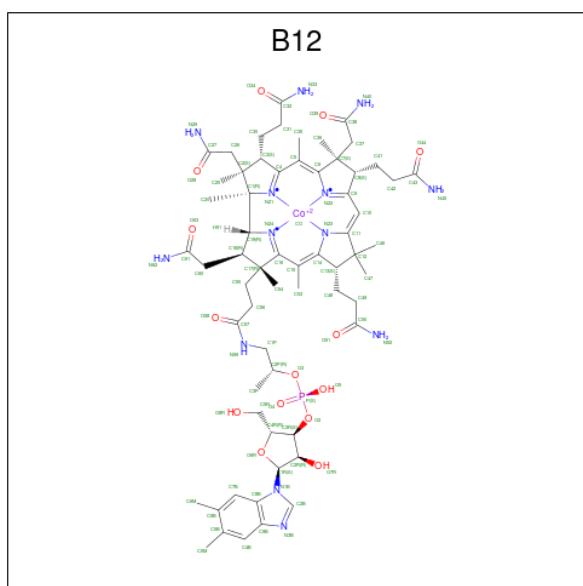
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q9Y4U1
A	-2	PHE	-	expression tag	UNP Q9Y4U1
A	-1	GLN	-	expression tag	UNP Q9Y4U1
A	0	SER	-	expression tag	UNP Q9Y4U1
B	-3	TYR	-	expression tag	UNP Q9Y4U1
B	-2	PHE	-	expression tag	UNP Q9Y4U1
B	-1	GLN	-	expression tag	UNP Q9Y4U1
B	0	SER	-	expression tag	UNP Q9Y4U1
C	-3	TYR	-	expression tag	UNP Q9Y4U1
C	-2	PHE	-	expression tag	UNP Q9Y4U1
C	-1	GLN	-	expression tag	UNP Q9Y4U1
C	0	SER	-	expression tag	UNP Q9Y4U1
D	-3	TYR	-	expression tag	UNP Q9Y4U1
D	-2	PHE	-	expression tag	UNP Q9Y4U1
D	-1	GLN	-	expression tag	UNP Q9Y4U1
D	0	SER	-	expression tag	UNP Q9Y4U1
E	-3	TYR	-	expression tag	UNP Q9Y4U1
E	-2	PHE	-	expression tag	UNP Q9Y4U1
E	-1	GLN	-	expression tag	UNP Q9Y4U1
E	0	SER	-	expression tag	UNP Q9Y4U1
F	-3	TYR	-	expression tag	UNP Q9Y4U1
F	-2	PHE	-	expression tag	UNP Q9Y4U1
F	-1	GLN	-	expression tag	UNP Q9Y4U1
F	0	SER	-	expression tag	UNP Q9Y4U1
G	-3	TYR	-	expression tag	UNP Q9Y4U1
G	-2	PHE	-	expression tag	UNP Q9Y4U1
G	-1	GLN	-	expression tag	UNP Q9Y4U1
G	0	SER	-	expression tag	UNP Q9Y4U1
H	-3	TYR	-	expression tag	UNP Q9Y4U1
H	-2	PHE	-	expression tag	UNP Q9Y4U1
H	-1	GLN	-	expression tag	UNP Q9Y4U1
H	0	SER	-	expression tag	UNP Q9Y4U1
I	-3	TYR	-	expression tag	UNP Q9Y4U1
I	-2	PHE	-	expression tag	UNP Q9Y4U1
I	-1	GLN	-	expression tag	UNP Q9Y4U1
I	0	SER	-	expression tag	UNP Q9Y4U1
J	-3	TYR	-	expression tag	UNP Q9Y4U1
J	-2	PHE	-	expression tag	UNP Q9Y4U1
J	-1	GLN	-	expression tag	UNP Q9Y4U1
J	0	SER	-	expression tag	UNP Q9Y4U1
K	-3	TYR	-	expression tag	UNP Q9Y4U1
K	-2	PHE	-	expression tag	UNP Q9Y4U1

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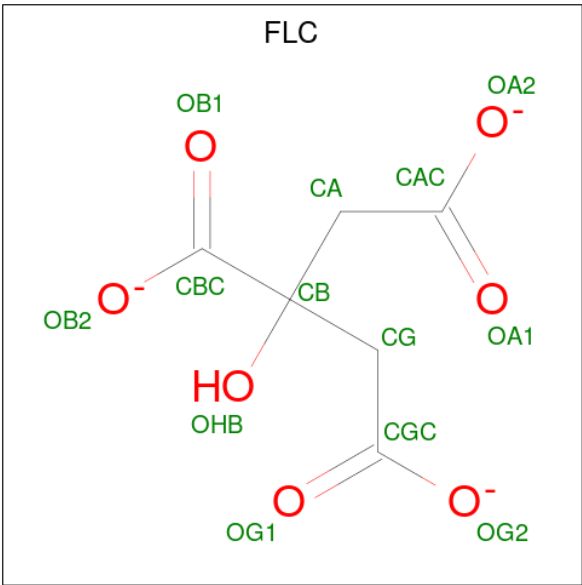
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLN	-	expression tag	UNP Q9Y4U1
K	0	SER	-	expression tag	UNP Q9Y4U1
L	-3	TYR	-	expression tag	UNP Q9Y4U1
L	-2	PHE	-	expression tag	UNP Q9Y4U1
L	-1	GLN	-	expression tag	UNP Q9Y4U1
L	0	SER	-	expression tag	UNP Q9Y4U1
M	-3	TYR	-	expression tag	UNP Q9Y4U1
M	-2	PHE	-	expression tag	UNP Q9Y4U1
M	-1	GLN	-	expression tag	UNP Q9Y4U1
M	0	SER	-	expression tag	UNP Q9Y4U1
N	-3	TYR	-	expression tag	UNP Q9Y4U1
N	-2	PHE	-	expression tag	UNP Q9Y4U1
N	-1	GLN	-	expression tag	UNP Q9Y4U1
N	0	SER	-	expression tag	UNP Q9Y4U1
O	-3	TYR	-	expression tag	UNP Q9Y4U1
O	-2	PHE	-	expression tag	UNP Q9Y4U1
O	-1	GLN	-	expression tag	UNP Q9Y4U1
O	0	SER	-	expression tag	UNP Q9Y4U1
P	-3	TYR	-	expression tag	UNP Q9Y4U1
P	-2	PHE	-	expression tag	UNP Q9Y4U1
P	-1	GLN	-	expression tag	UNP Q9Y4U1
P	0	SER	-	expression tag	UNP Q9Y4U1

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	E	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	F	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	G	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	H	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	I	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	J	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	K	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	L	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	M	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	N	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	O	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	P	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $\text{C}_6\text{H}_5\text{O}_7$ ).



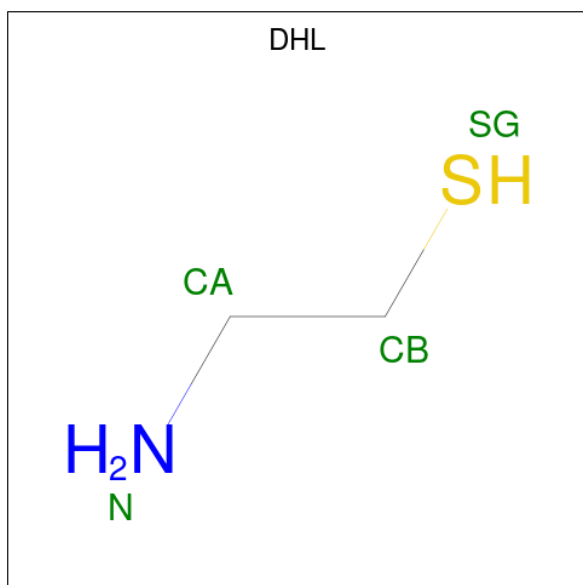
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		
3	I	1	Total	C	O	0	0
			13	6	7		
3	J	1	Total	C	O	0	0
			13	6	7		
3	K	1	Total	C	O	0	0
			13	6	7		
3	L	1	Total	C	O	0	0
			13	6	7		
3	M	1	Total	C	O	0	0
			13	6	7		
3	N	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			13	6	7		
3	P	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 2-AMINO-ETHANETHIOL (three-letter code: DHL) (formula: C<sub>2</sub>H<sub>7</sub>NS).



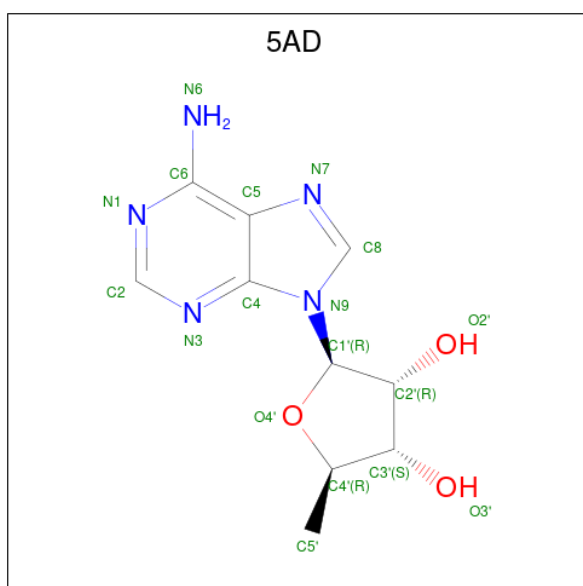
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			4	2	1	1		
4	C	1	Total	C	N	S	0	0
			4	2	1	1		
4	D	1	Total	C	N	S	0	0
			4	2	1	1		
4	F	1	Total	C	N	S	0	0
			4	2	1	1		
4	G	1	Total	C	N	S	0	0
			4	2	1	1		
4	H	1	Total	C	N	S	0	0
			4	2	1	1		
4	I	1	Total	C	N	S	0	0
			4	2	1	1		
4	J	1	Total	C	N	S	0	0
			4	2	1	1		
4	K	1	Total	C	N	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	S	0	0
			4	2	1	1		
4	M	1	Total	C	N	S	0	0
			4	2	1	1		
4	N	1	Total	C	N	S	0	0
			4	2	1	1		
4	O	1	Total	C	N	S	0	0
			4	2	1	1		
4	P	1	Total	C	N	S	0	0
			4	2	1	1		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



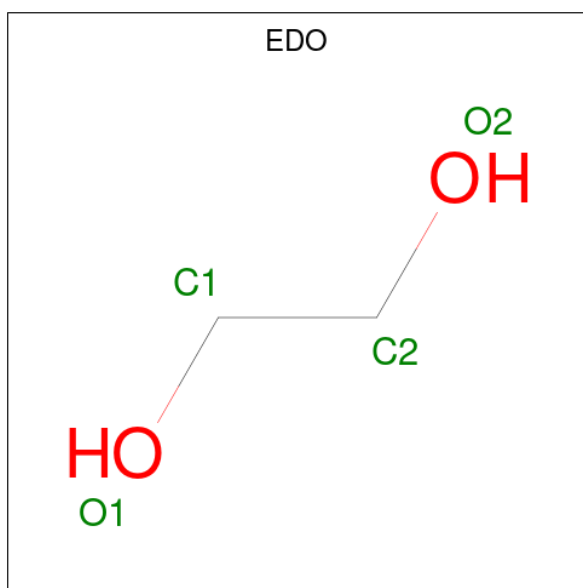
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		
5	E	1	Total	C	N	O	0	0
			18	10	5	3		
5	F	1	Total	C	N	O	0	0
			18	10	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	H	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	J	1	Total	C	N	O	0	0
			18	10	5	3		
5	K	1	Total	C	N	O	0	0
			18	10	5	3		
5	L	1	Total	C	N	O	0	0
			18	10	5	3		
5	M	1	Total	C	N	O	0	0
			18	10	5	3		
5	N	1	Total	C	N	O	0	0
			18	10	5	3		
5	O	1	Total	C	N	O	0	0
			18	10	5	3		
5	P	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





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

- Molecule 7 is water.

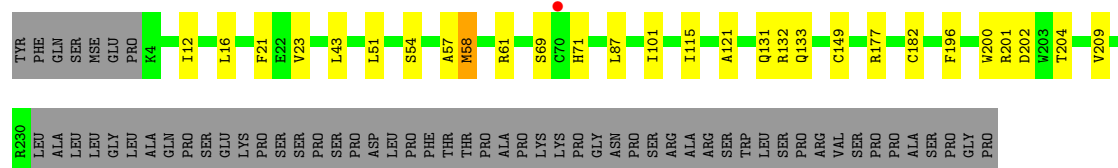
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	63	Total O 63 63	0	0
7	C	63	Total O 63 63	0	0
7	D	79	Total O 79 79	0	0
7	E	105	Total O 105 105	0	0
7	F	111	Total O 111 111	0	0
7	G	125	Total O 125 125	0	0
7	H	124	Total O 124 124	0	0
7	I	122	Total O 122 122	0	0
7	J	111	Total O 111 111	0	0
7	K	100	Total O 100 100	0	0
7	L	130	Total O 130 130	0	0
7	M	125	Total O 125 125	0	0
7	N	100	Total O 100 100	0	0
7	O	124	Total O 124 124	0	0
7	P	94	Total O 94 94	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.

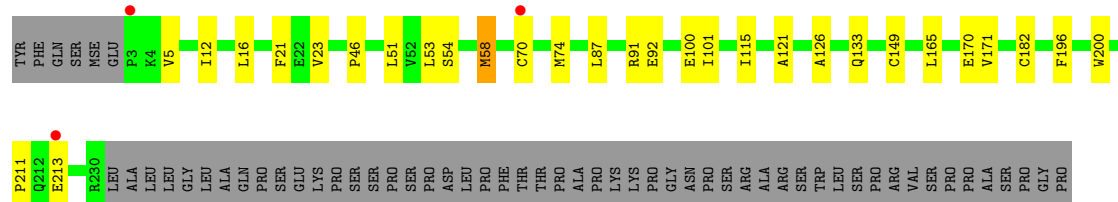
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain A: 



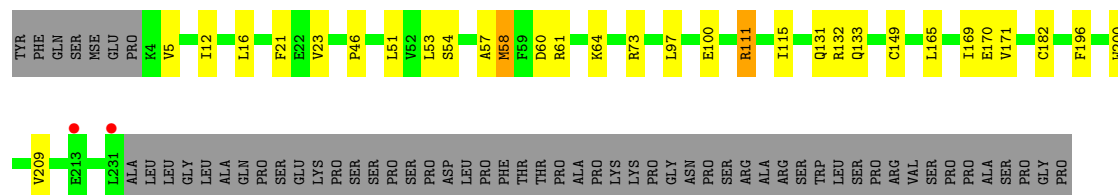
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain B: 



- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

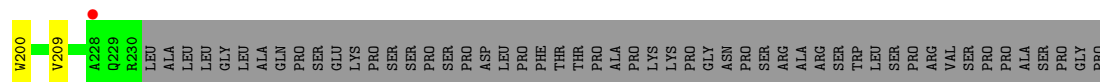
Chain C: 



- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

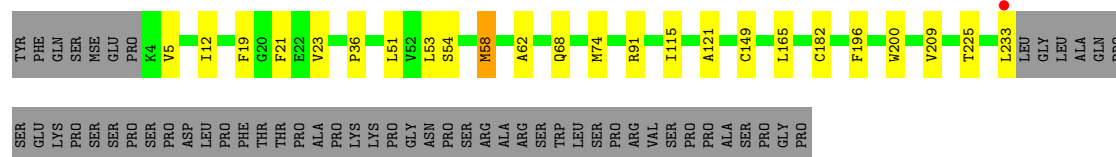
Chain D: 





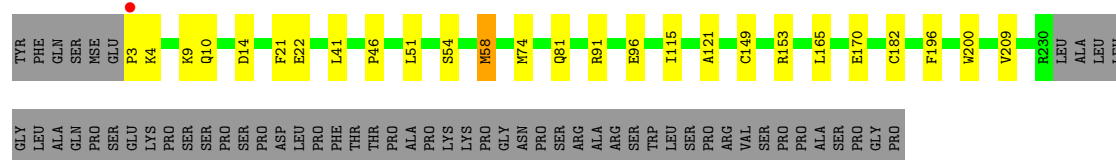
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain E: 72% 8% 20%



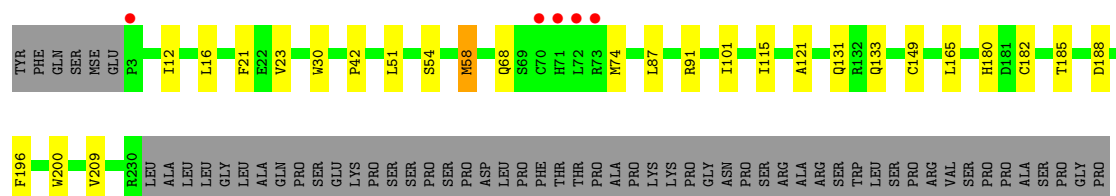
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain F: 71% 9% 20%



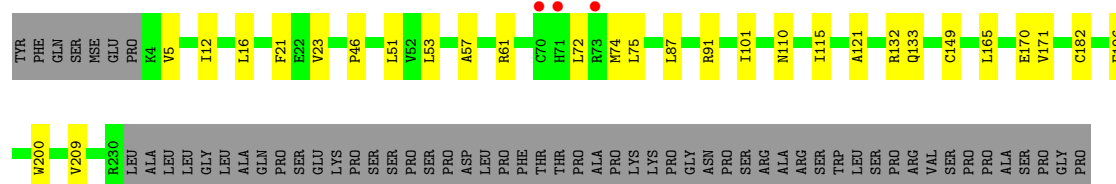
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain G: 2% 70% 9% 20%



- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

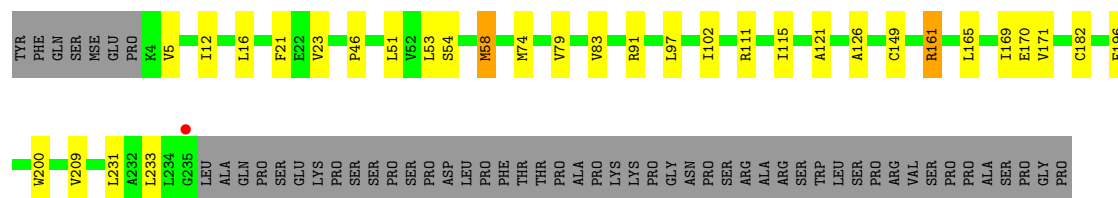
Chain H: 69% 10% 21%



- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

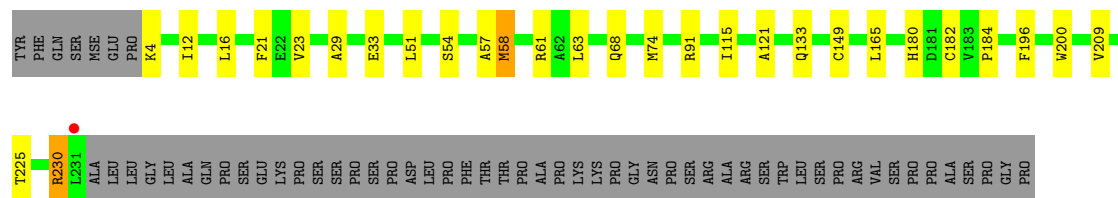
Chain I: 69% 10% 20%





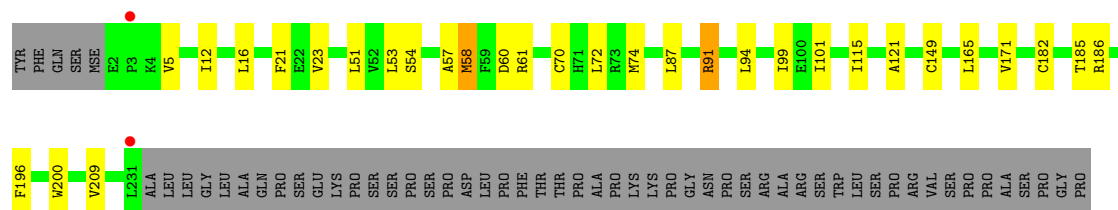
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain O: 70% 9% 20%



- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain P: 70% 10% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.66Å 71.96Å 300.06Å 88.53° 85.25° 83.76°	Depositor
Resolution (Å)	19.86 – 2.40 19.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.86-2.40) 98.6 (19.86-2.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.182 , 0.206 0.190 , 0.216	Depositor DCC
$R_{free}$ test set	11473 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, B12, 5AD, DHL, FLC

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	0.47	0/1898	0.63	0/2592
1	B	0.45	0/1899	0.64	0/2595
1	C	0.46	0/1899	0.64	0/2598
1	D	0.47	0/1913	0.64	0/2616
1	E	0.47	0/1913	0.65	0/2615
1	F	0.50	0/1928	0.67	0/2635
1	G	0.48	0/1905	0.64	0/2603
1	H	0.48	0/1894	0.65	0/2588
1	I	0.46	0/1909	0.64	0/2609
1	J	0.48	0/1911	0.66	0/2610
1	K	0.49	0/1899	0.66	0/2596
1	L	0.49	0/1936	0.68	0/2646
1	M	0.49	0/1926	0.66	0/2635
1	N	0.48	0/1914	0.67	0/2618
1	O	0.49	0/1900	0.67	0/2596
1	P	0.48	0/1922	0.65	0/2626
All	All	0.48	0/30566	0.65	0/41778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1837	0	1791	15	0
1	B	1837	0	1792	15	0
1	C	1832	0	1779	18	0
1	D	1848	0	1798	20	0
1	E	1849	0	1802	18	0
1	F	1857	0	1813	19	0
1	G	1843	0	1797	21	0
1	H	1833	0	1782	22	0
1	I	1844	0	1796	22	0
1	J	1844	0	1804	16	0
1	K	1832	0	1783	21	0
1	L	1868	0	1826	17	0
1	M	1861	0	1800	19	0
1	N	1853	0	1806	21	0
1	O	1836	0	1786	23	0
1	P	1860	0	1817	22	0
2	A	91	0	88	14	0
2	B	91	0	88	13	0
2	C	91	0	88	15	0
2	D	91	0	88	12	0
2	E	91	0	88	14	0
2	F	91	0	88	13	0
2	G	91	0	88	15	0
2	H	91	0	88	13	0
2	I	91	0	88	14	0
2	J	91	0	88	12	0
2	K	91	0	88	12	0
2	L	91	0	88	13	0
2	M	91	0	88	12	0
2	N	91	0	88	13	0
2	O	91	0	88	15	0
2	P	91	0	88	16	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	G	13	0	5	0	0
3	H	13	0	5	0	0
3	I	13	0	5	0	0
3	J	13	0	5	0	0
3	K	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	13	0	5	0	0
3	M	13	0	5	0	0
3	N	13	0	5	0	0
3	O	13	0	5	0	0
3	P	13	0	5	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	1	0
4	H	4	0	6	0	0
4	I	4	0	7	3	0
4	J	4	0	7	1	0
4	K	4	0	7	3	0
4	L	4	0	6	0	0
4	M	4	0	6	0	0
4	N	4	0	7	1	0
4	O	4	0	6	1	0
4	P	4	0	6	0	0
5	A	18	0	13	3	0
5	B	18	0	13	3	0
5	C	18	0	13	4	0
5	D	18	0	13	3	0
5	E	18	0	13	3	0
5	F	18	0	13	3	0
5	G	36	0	26	4	0
5	H	18	0	13	4	0
5	I	36	0	26	4	0
5	J	18	0	13	3	0
5	K	18	0	13	3	0
5	L	18	0	13	3	0
5	M	18	0	13	3	0
5	N	18	0	13	4	0
5	O	18	0	13	3	0
5	P	18	0	13	3	0
6	E	4	0	6	2	0
6	P	8	0	12	7	0
7	A	70	0	0	0	0
7	B	63	0	0	1	0
7	C	63	0	0	0	0
7	D	79	0	0	0	0
7	E	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	111	0	0	0	0
7	G	125	0	0	1	0
7	H	124	0	0	0	0
7	I	122	0	0	2	0
7	J	111	0	0	0	0
7	K	100	0	0	0	0
7	L	130	0	0	0	0
7	M	125	0	0	3	0
7	N	100	0	0	0	0
7	O	124	0	0	1	0
7	P	94	0	0	0	0
All	All	33236	0	30600	442	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 7.

The worst 5 of 442 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:D:182:CYS:SG	4:D:601:DHL:SG	2.33	1.26
2:A:301:B12:H362	2:A:301:B12:H351	1.37	1.06
2:P:301:B12:H362	2:P:301:B12:H351	1.37	1.05
2:D:301:B12:H362	2:D:301:B12:H351	1.39	1.03
2:G:301:B12:H362	2:G:301:B12:H351	1.37	1.03

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	225/286 (79%)	222 (99%)	3 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	226/286 (79%)	222 (98%)	4 (2%)	0	100	100
1	C	228/286 (80%)	226 (99%)	2 (1%)	0	100	100
1	D	228/286 (80%)	224 (98%)	4 (2%)	0	100	100
1	E	229/286 (80%)	227 (99%)	2 (1%)	0	100	100
1	F	229/286 (80%)	225 (98%)	4 (2%)	0	100	100
1	G	226/286 (79%)	223 (99%)	3 (1%)	0	100	100
1	H	225/286 (79%)	224 (100%)	1 (0%)	0	100	100
1	I	227/286 (79%)	223 (98%)	4 (2%)	0	100	100
1	J	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	K	226/286 (79%)	224 (99%)	2 (1%)	0	100	100
1	L	231/286 (81%)	228 (99%)	3 (1%)	0	100	100
1	M	230/286 (80%)	228 (99%)	2 (1%)	0	100	100
1	N	230/286 (80%)	229 (100%)	1 (0%)	0	100	100
1	O	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	P	228/286 (80%)	227 (100%)	1 (0%)	0	100	100
All	All	3642/4576 (80%)	3600 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	193/243 (79%)	187 (97%)	6 (3%)	35	56
1	B	193/243 (79%)	187 (97%)	6 (3%)	35	56
1	C	192/243 (79%)	184 (96%)	8 (4%)	25	43
1	D	194/243 (80%)	187 (96%)	7 (4%)	30	49
1	E	193/243 (79%)	187 (97%)	6 (3%)	35	56
1	F	197/243 (81%)	192 (98%)	5 (2%)	42	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	194/243 (80%)	189 (97%)	5 (3%)	41	62
1	H	192/243 (79%)	186 (97%)	6 (3%)	35	56
1	I	194/243 (80%)	189 (97%)	5 (3%)	41	62
1	J	195/243 (80%)	189 (97%)	6 (3%)	35	56
1	K	192/243 (79%)	189 (98%)	3 (2%)	58	76
1	L	196/243 (81%)	190 (97%)	6 (3%)	35	56
1	M	195/243 (80%)	193 (99%)	2 (1%)	73	86
1	N	192/243 (79%)	186 (97%)	6 (3%)	35	56
1	O	192/243 (79%)	185 (96%)	7 (4%)	30	49
1	P	196/243 (81%)	189 (96%)	7 (4%)	30	49
All	All	3100/3888 (80%)	3009 (97%)	91 (3%)	37	58

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	70	CYS
1	N	58	MSE
1	J	115	ILE
1	L	91	ARG
1	N	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	199	HIS
1	I	212	GLN
1	P	98	GLN
1	M	68	GLN
1	M	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

67 ligands are modelled in this entry.

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	$\# Z  > 2$
3	FLC	O	501	-	12,12,12	1.45	3 (25%)	17,17,17	1.34	2 (11%)
3	FLC	F	501	-	12,12,12	1.61	3 (25%)	17,17,17	1.23	2 (11%)
5	5AD	P	401	2	16,20,20	0.97	1 (6%)	14,30,30	1.60	4 (28%)
4	DHL	G	601	1	2,3,3	0.48	0	1,2,2	0.19	0
5	5AD	C	401	2	16,20,20	1.01	1 (6%)	14,30,30	1.56	3 (21%)
4	DHL	L	601	-	2,3,3	1.77	1 (50%)	1,2,2	0.69	0
3	FLC	N	501	-	12,12,12	1.34	2 (16%)	17,17,17	1.37	2 (11%)
5	5AD	L	401	2	16,20,20	1.00	1 (6%)	14,30,30	1.66	3 (21%)
2	B12	B	301	5	91,101,101	1.52	11 (12%)	140,166,166	1.99	20 (14%)
3	FLC	D	501	-	12,12,12	1.80	2 (16%)	17,17,17	1.38	3 (17%)
4	DHL	F	601	1	2,3,3	0.84	0	1,2,2	0.06	0
5	5AD	M	401	2	16,20,20	0.92	1 (6%)	14,30,30	1.63	3 (21%)
5	5AD	B	401	2	16,20,20	0.93	1 (6%)	14,30,30	1.76	4 (28%)
5	5AD	K	401	2	16,20,20	1.05	1 (6%)	14,30,30	1.61	3 (21%)
6	EDO	P	283	-	3,3,3	0.52	0	2,2,2	0.16	0
2	B12	L	301	5	91,101,101	1.50	8 (8%)	140,166,166	1.98	18 (12%)
3	FLC	J	501	-	12,12,12	1.67	4 (33%)	17,17,17	1.26	2 (11%)
5	5AD	I	401	2	16,20,20	1.06	1 (6%)	14,30,30	1.65	4 (28%)
2	B12	C	301	5	91,101,101	1.54	10 (10%)	140,166,166	2.03	22 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FLC	I	501	-	12,12,12	1.62	4 (33%)	17,17,17	1.42	2 (11%)
4	DHL	I	601	-	2,3,3	0.67	0	1,2,2	0.67	0
2	B12	P	301	5	91,101,101	1.52	11 (12%)	140,166,166	2.00	20 (14%)
3	FLC	H	501	-	12,12,12	1.38	3 (25%)	17,17,17	1.41	2 (11%)
2	B12	N	301	5	91,101,101	1.54	10 (10%)	140,166,166	1.99	21 (15%)
6	EDO	P	284	-	3,3,3	0.37	0	2,2,2	0.19	0
2	B12	M	301	5	91,101,101	1.49	8 (8%)	140,166,166	2.00	21 (15%)
3	FLC	E	501	-	12,12,12	1.57	3 (25%)	17,17,17	1.33	2 (11%)
2	B12	I	301	5	91,101,101	1.54	11 (12%)	140,166,166	1.98	22 (15%)
3	FLC	M	501	-	12,12,12	1.63	3 (25%)	17,17,17	1.47	2 (11%)
4	DHL	J	601	-	2,3,3	1.62	1 (50%)	1,2,2	0.77	0
6	EDO	E	283	-	3,3,3	0.50	0	2,2,2	0.17	0
3	FLC	K	501	-	12,12,12	1.64	3 (25%)	17,17,17	1.44	2 (11%)
2	B12	J	301	5	91,101,101	1.54	11 (12%)	140,166,166	1.95	21 (15%)
3	FLC	A	501	-	12,12,12	1.49	3 (25%)	17,17,17	1.35	3 (17%)
3	FLC	B	501	-	12,12,12	1.47	4 (33%)	17,17,17	1.49	4 (23%)
4	DHL	O	601	1	2,3,3	0.72	0	1,2,2	0.08	0
5	5AD	F	401	2	16,20,20	0.95	1 (6%)	14,30,30	1.63	3 (21%)
4	DHL	D	601	-	2,3,3	1.26	0	1,2,2	0.34	0
5	5AD	G	401	2	16,20,20	1.02	1 (6%)	14,30,30	1.73	3 (21%)
4	DHL	A	601	1	2,3,3	1.04	0	1,2,2	0.17	0
2	B12	F	301	5	91,101,101	1.51	9 (9%)	140,166,166	1.97	22 (15%)
5	5AD	H	401	2	16,20,20	0.96	1 (6%)	14,30,30	1.86	5 (35%)
2	B12	E	301	5	91,101,101	1.55	10 (10%)	140,166,166	1.98	22 (15%)
2	B12	G	301	5	91,101,101	1.51	10 (10%)	140,166,166	1.96	20 (14%)
4	DHL	N	601	-	2,3,3	0.45	0	1,2,2	0.80	0
5	5AD	A	401	2	16,20,20	0.97	1 (6%)	14,30,30	1.57	3 (21%)
2	B12	K	301	5	91,101,101	1.51	10 (10%)	140,166,166	2.01	21 (15%)
4	DHL	K	601	-	2,3,3	1.34	0	1,2,2	0.02	0
3	FLC	L	501	-	12,12,12	1.51	2 (16%)	17,17,17	1.43	3 (17%)
4	DHL	M	601	-	2,3,3	1.13	0	1,2,2	0.03	0
4	DHL	H	601	1	2,3,3	0.64	0	1,2,2	1.53	0
4	DHL	P	601	-	2,3,3	0.89	0	1,2,2	0.13	0
5	5AD	G	283	-	16,20,20	1.29	2 (12%)	14,30,30	1.67	3 (21%)
5	5AD	N	401	2	16,20,20	0.94	1 (6%)	14,30,30	1.70	3 (21%)
2	B12	O	301	5	91,101,101	1.50	10 (10%)	140,166,166	1.96	21 (15%)
5	5AD	D	401	2	16,20,20	1.07	1 (6%)	14,30,30	1.65	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	B12	A	301	5	91,101,101	1.53	10 (10%)	140,166,166	1.98	20 (14%)
5	5AD	I	283	-	16,20,20	1.18	2 (12%)	14,30,30	1.54	2 (14%)
5	5AD	J	401	2	16,20,20	0.96	1 (6%)	14,30,30	1.77	5 (35%)
2	B12	D	301	5	91,101,101	1.50	10 (10%)	140,166,166	1.98	21 (15%)
5	5AD	E	401	2	16,20,20	1.02	1 (6%)	14,30,30	1.84	4 (28%)
3	FLC	G	501	-	12,12,12	1.52	4 (33%)	17,17,17	1.35	3 (17%)
2	B12	H	301	5	91,101,101	1.51	11 (12%)	140,166,166	2.01	19 (13%)
3	FLC	P	501	-	12,12,12	1.46	2 (16%)	17,17,17	1.47	3 (17%)
3	FLC	C	501	-	12,12,12	1.51	3 (25%)	17,17,17	1.42	2 (11%)
4	DHL	C	601	-	2,3,3	0.61	0	1,2,2	0.42	0
5	5AD	O	401	2	16,20,20	0.99	1 (6%)	14,30,30	1.83	4 (28%)

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
3	FLC	O	501	-	-	0/16/16/16	-
3	FLC	F	501	-	-	0/16/16/16	-
5	5AD	P	401	2	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	C	401	2	1/1/4/4	0/0/20/20	0/3/3/3
4	DHL	G	601	1	-	1/1/1/1	-
4	DHL	L	601	-	-	0/1/1/1	-
3	FLC	N	501	-	-	0/16/16/16	-
5	5AD	L	401	2	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	B	301	5	-	6/52/223/223	0/3/11/11
3	FLC	D	501	-	-	0/16/16/16	-
4	DHL	F	601	1	-	1/1/1/1	-
5	5AD	M	401	2	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	B	401	2	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	K	401	2	1/1/4/4	0/0/20/20	0/3/3/3
6	EDO	P	283	-	-	1/1/1/1	-
2	B12	L	301	5	-	8/52/223/223	0/3/11/11
3	FLC	J	501	-	-	0/16/16/16	-
5	5AD	I	401	2	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	C	301	5	-	6/52/223/223	0/3/11/11
3	FLC	I	501	-	-	0/16/16/16	-
4	DHL	I	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B12	P	301	5	-	7/52/223/223	0/3/11/11
3	FLC	H	501	-	-	0/16/16/16	-
2	B12	N	301	5	-	7/52/223/223	0/3/11/11
6	EDO	P	284	-	-	0/1/1/1	-
2	B12	M	301	5	-	7/52/223/223	0/3/11/11
3	FLC	E	501	-	-	0/16/16/16	-
2	B12	I	301	5	-	7/52/223/223	0/3/11/11
3	FLC	M	501	-	-	0/16/16/16	-
4	DHL	J	601	-	-	0/1/1/1	-
6	EDO	E	283	-	-	1/1/1/1	-
3	FLC	K	501	-	-	0/16/16/16	-
2	B12	J	301	5	-	8/52/223/223	0/3/11/11
5	5AD	F	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	A	501	-	-	0/16/16/16	-
3	FLC	B	501	-	-	0/16/16/16	-
4	DHL	O	601	1	-	1/1/1/1	-
5	5AD	G	401	2	1/1/4/4	0/0/20/20	0/3/3/3
4	DHL	D	601	-	-	1/1/1/1	-
4	DHL	A	601	1	-	0/1/1/1	-
2	B12	F	301	5	-	7/52/223/223	0/3/11/11
5	5AD	H	401	2	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	E	301	5	-	7/52/223/223	0/3/11/11
2	B12	G	301	5	-	7/52/223/223	0/3/11/11
5	5AD	A	401	2	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	G	283	-	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	K	301	5	-	6/52/223/223	0/3/11/11
4	DHL	K	601	-	-	0/1/1/1	-
3	FLC	L	501	-	-	0/16/16/16	-
4	DHL	M	601	-	-	0/1/1/1	-
4	DHL	H	601	1	-	1/1/1/1	-
5	5AD	N	401	2	1/1/4/4	0/0/20/20	0/3/3/3
4	DHL	N	601	-	-	1/1/1/1	-
4	DHL	P	601	-	-	1/1/1/1	-
5	5AD	D	401	2	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	O	301	5	-	6/52/223/223	0/3/11/11
2	B12	A	301	5	-	7/52/223/223	0/3/11/11
5	5AD	I	283	-	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	J	401	2	1/1/4/4	0/0/20/20	0/3/3/3
5	5AD	E	401	2	1/1/4/4	0/0/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B12	D	301	5	-	8/52/223/223	0/3/11/11
3	FLC	G	501	-	-	0/16/16/16	-
2	B12	H	301	5	-	7/52/223/223	0/3/11/11
3	FLC	P	501	-	-	0/16/16/16	-
3	FLC	C	501	-	-	0/16/16/16	-
4	DHL	C	601	-	-	0/1/1/1	-
5	5AD	O	401	2	1/1/4/4	0/0/20/20	0/3/3/3

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	B12	C19-N24	-7.89	1.39	1.49
2	E	301	B12	C19-N24	-7.73	1.39	1.49
2	A	301	B12	C19-N24	-7.61	1.39	1.49
2	C	301	B12	C19-N24	-7.58	1.39	1.49
2	H	301	B12	C19-N24	-7.49	1.39	1.49

The worst 5 of 433 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	B12	C20-C1-C19	-8.93	100.75	109.35
2	K	301	B12	C20-C1-C19	-8.41	101.25	109.35
2	H	301	B12	C20-C1-C19	-8.38	101.28	109.35
2	B	301	B12	C20-C1-C19	-8.27	101.39	109.35
2	C	301	B12	C2-C1-C19	8.18	131.34	118.61

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	401	5AD	C4'
5	B	401	5AD	C4'
5	C	401	5AD	C4'
5	D	401	5AD	C4'
5	E	401	5AD	C4'

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	B12	C1P-C2P-O3-P
2	D	301	B12	C1P-C2P-O3-P
2	E	301	B12	C1P-C2P-O3-P

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Mol	Chain	Res	Type	Atoms
2	F	301	B12	C1P-C2P-O3-P
2	K	301	B12	C1P-C2P-O3-P

There are no ring outliers.

44 monomers are involved in 241 short contacts:

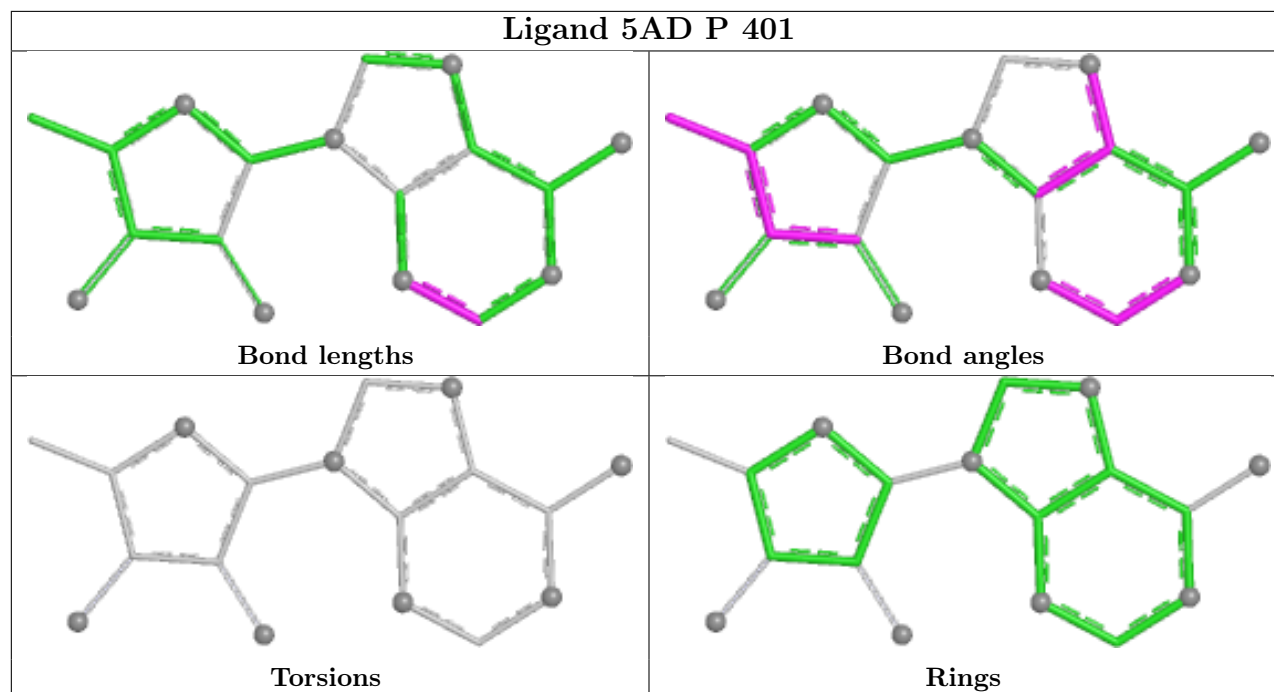
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	401	5AD	3	0
4	G	601	DHL	1	0
5	C	401	5AD	4	0
5	L	401	5AD	3	0
2	B	301	B12	13	0
5	M	401	5AD	3	0
5	B	401	5AD	3	0
5	K	401	5AD	3	0
6	P	283	EDO	2	0
2	L	301	B12	13	0
5	I	401	5AD	3	0
2	C	301	B12	15	0
4	I	601	DHL	3	0
2	P	301	B12	16	0
2	N	301	B12	13	0
6	P	284	EDO	5	0
2	M	301	B12	12	0
2	I	301	B12	14	0
4	J	601	DHL	1	0
6	E	283	EDO	2	0
2	J	301	B12	12	0
4	O	601	DHL	1	0
5	F	401	5AD	3	0
4	D	601	DHL	2	0
5	G	401	5AD	3	0
2	F	301	B12	13	0
5	H	401	5AD	4	0
2	E	301	B12	14	0
2	G	301	B12	15	0
4	N	601	DHL	1	0
5	A	401	5AD	3	0
2	K	301	B12	12	0
4	K	601	DHL	3	0
5	G	283	5AD	1	0
5	N	401	5AD	4	0

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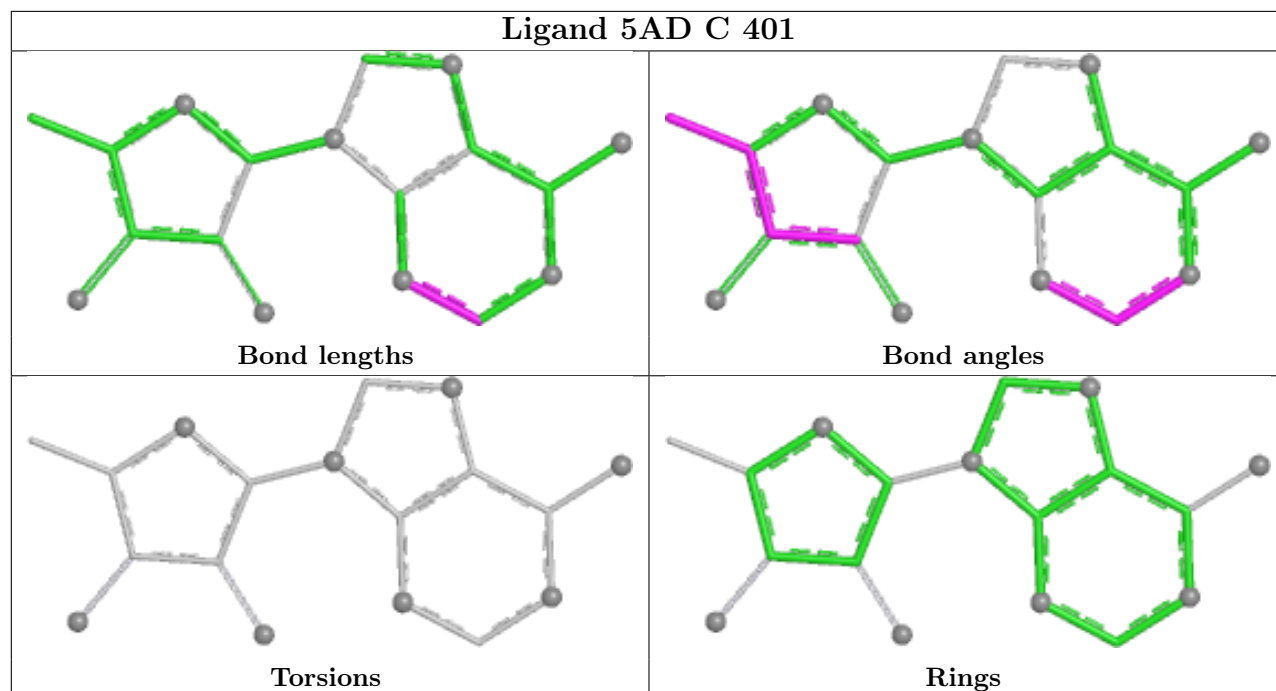
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	301	B12	15	0
5	D	401	5AD	3	0
2	A	301	B12	14	0
5	I	283	5AD	1	0
5	J	401	5AD	3	0
2	D	301	B12	12	0
5	E	401	5AD	3	0
2	H	301	B12	13	0
5	O	401	5AD	3	0

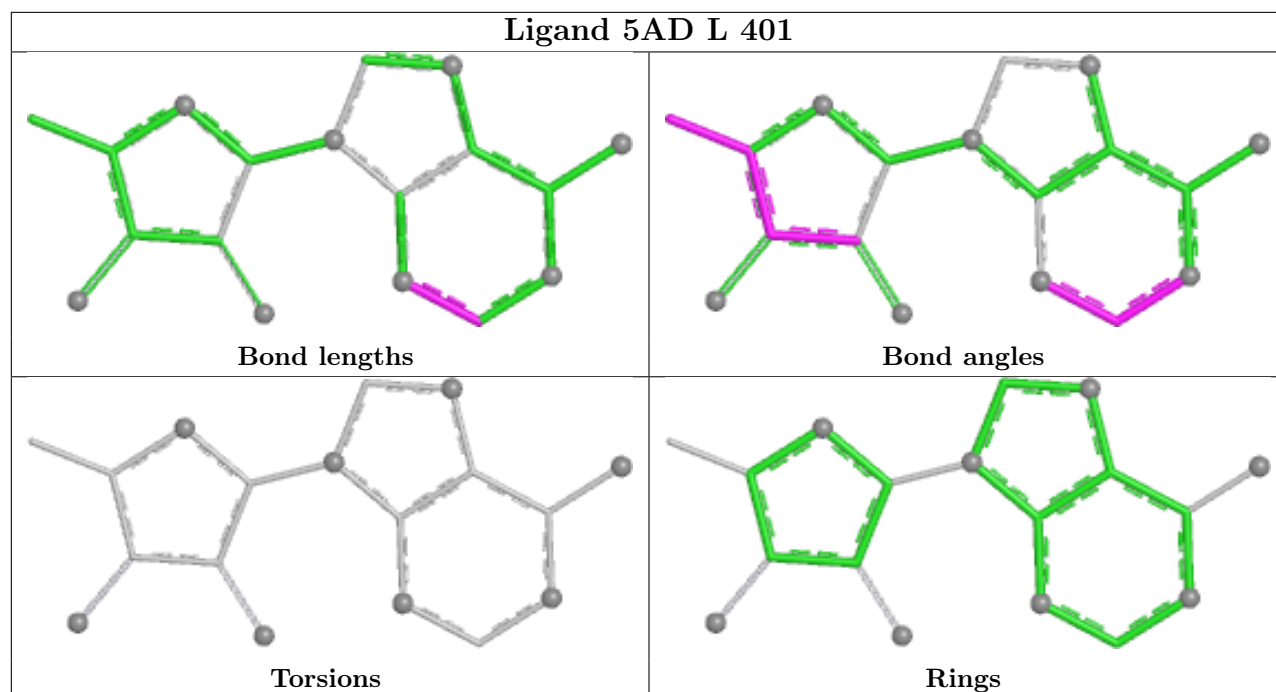
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

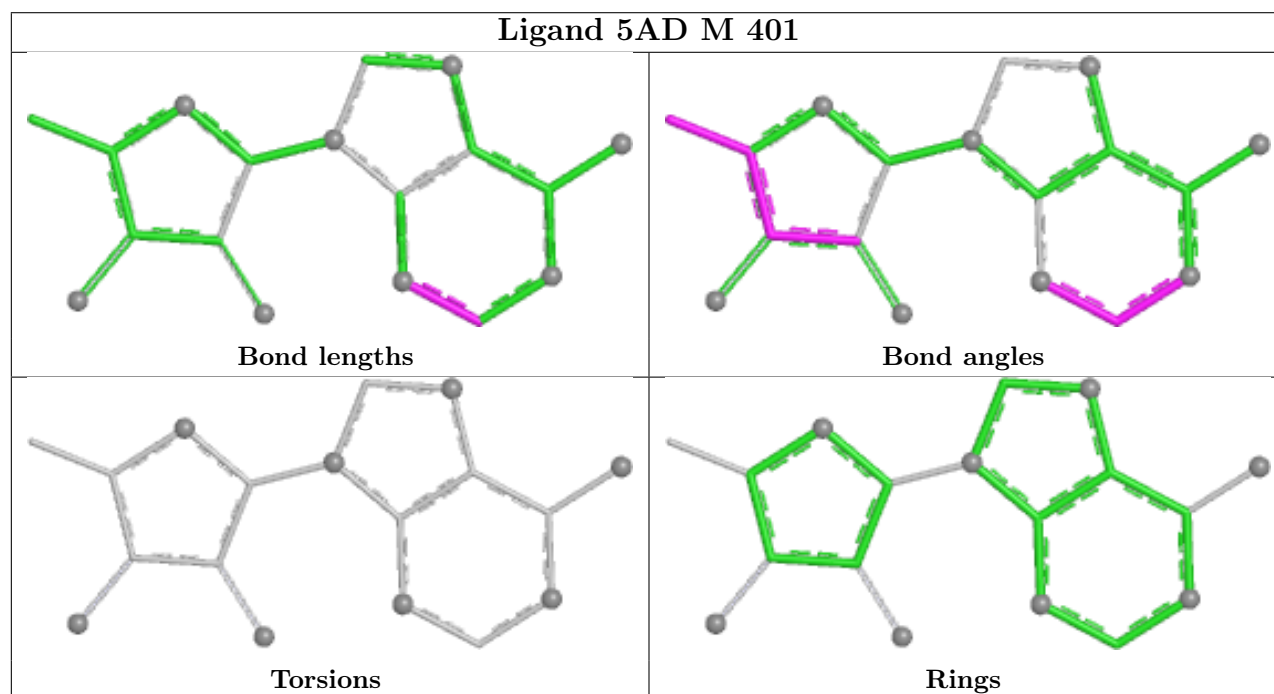
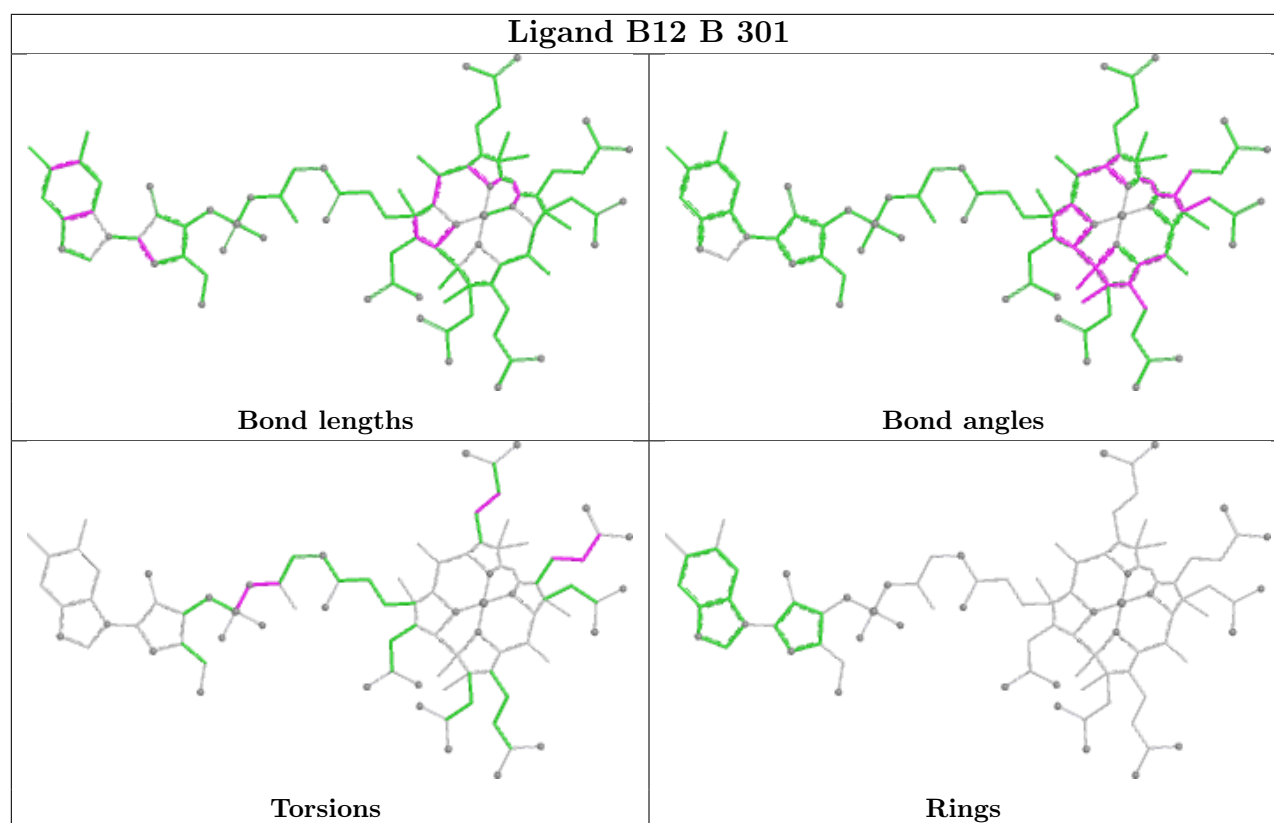


## Ligand 5AD C 401

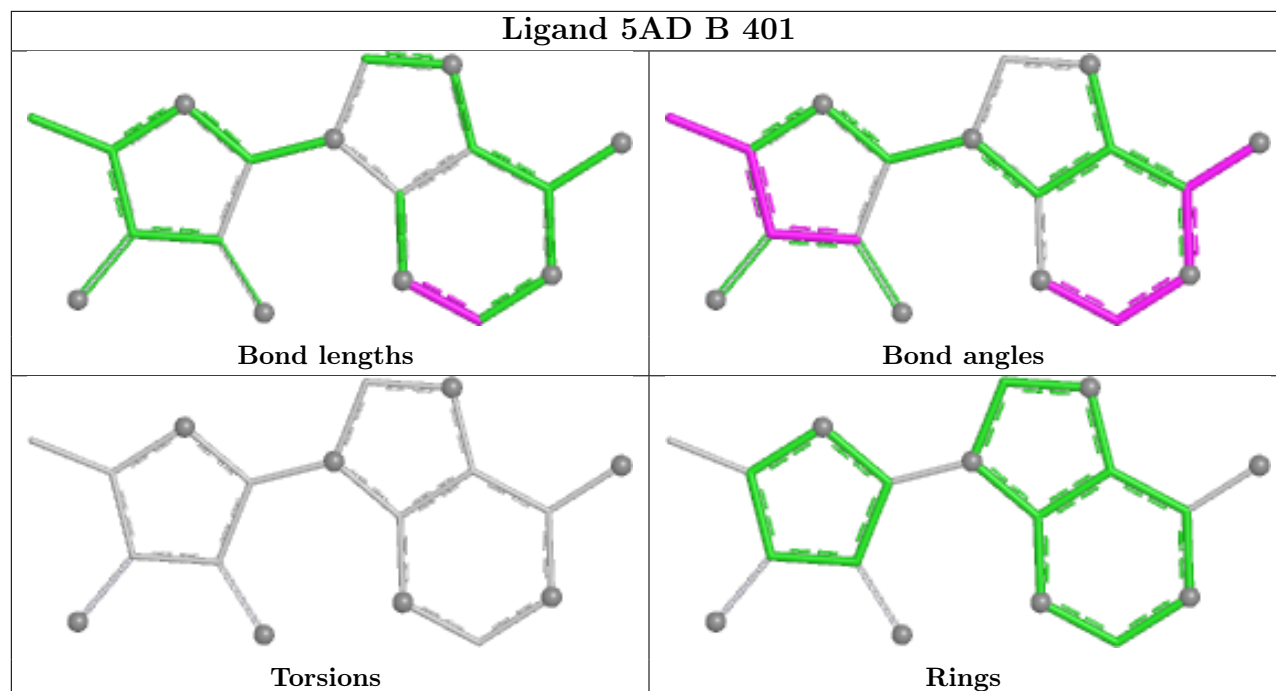


## Ligand 5AD L 401

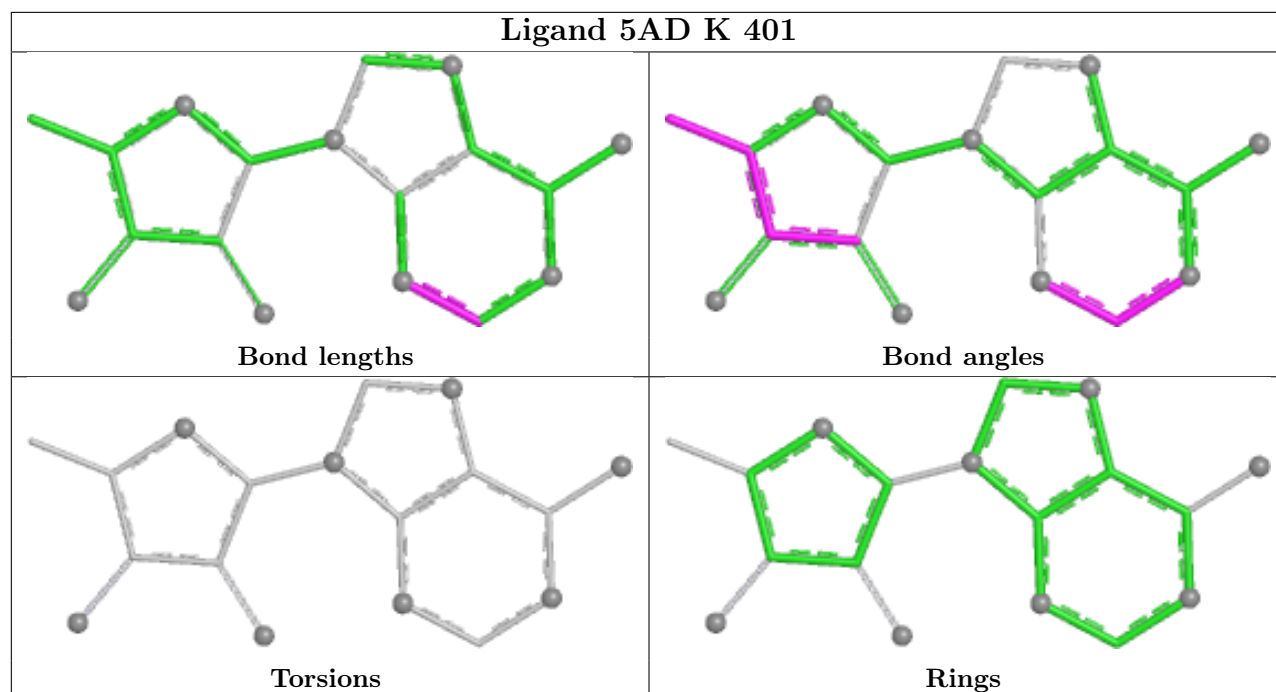


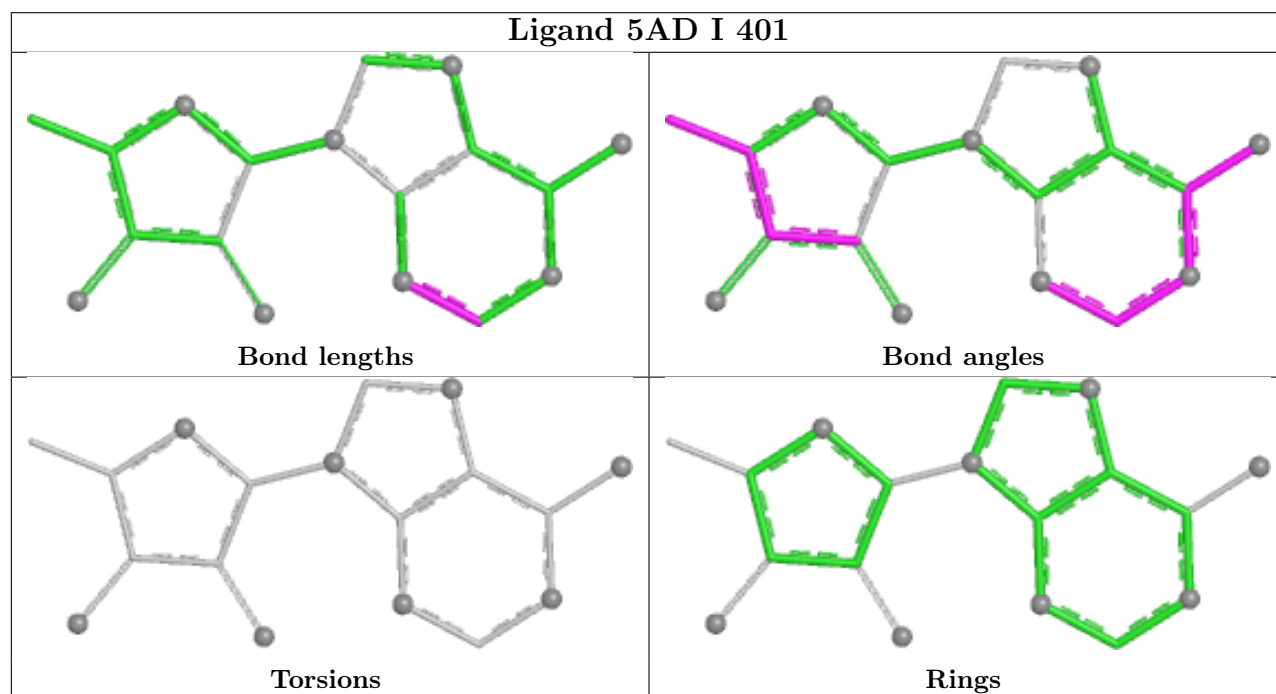
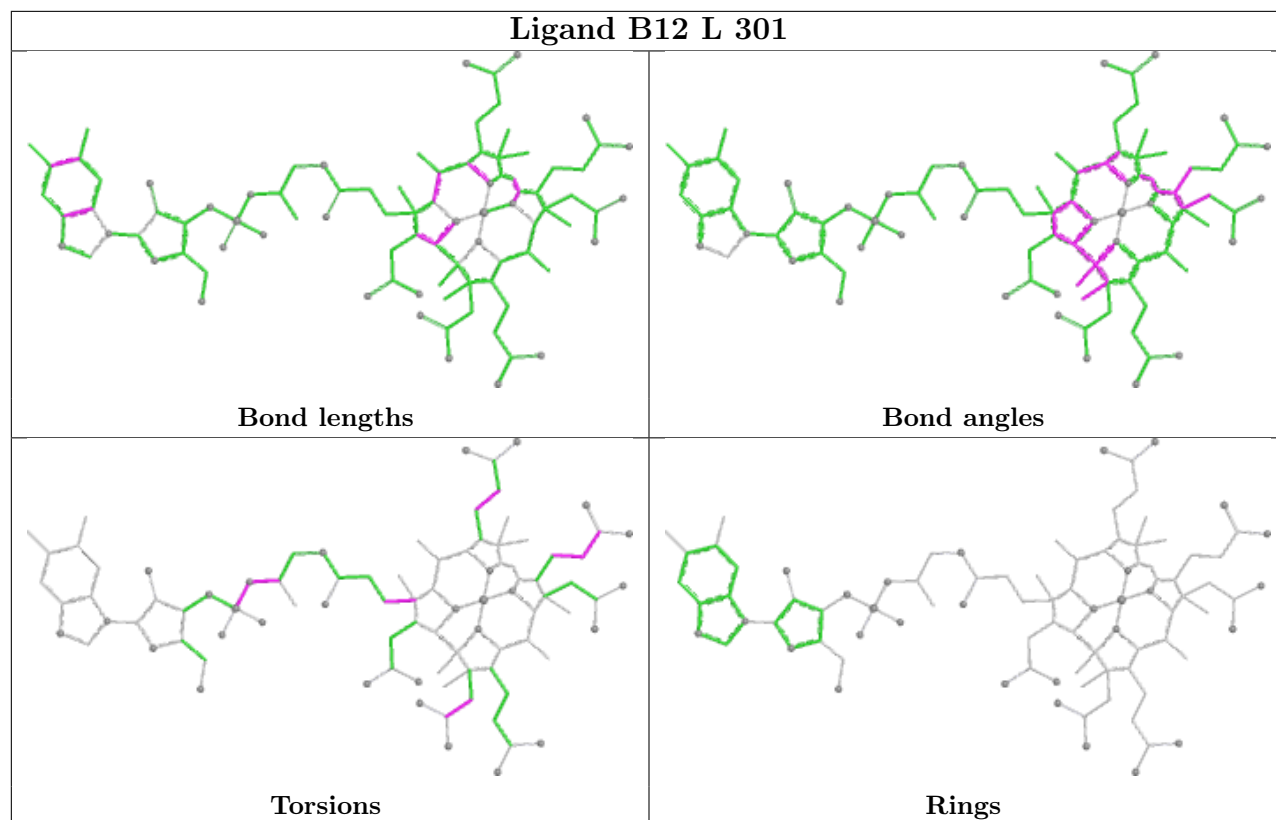


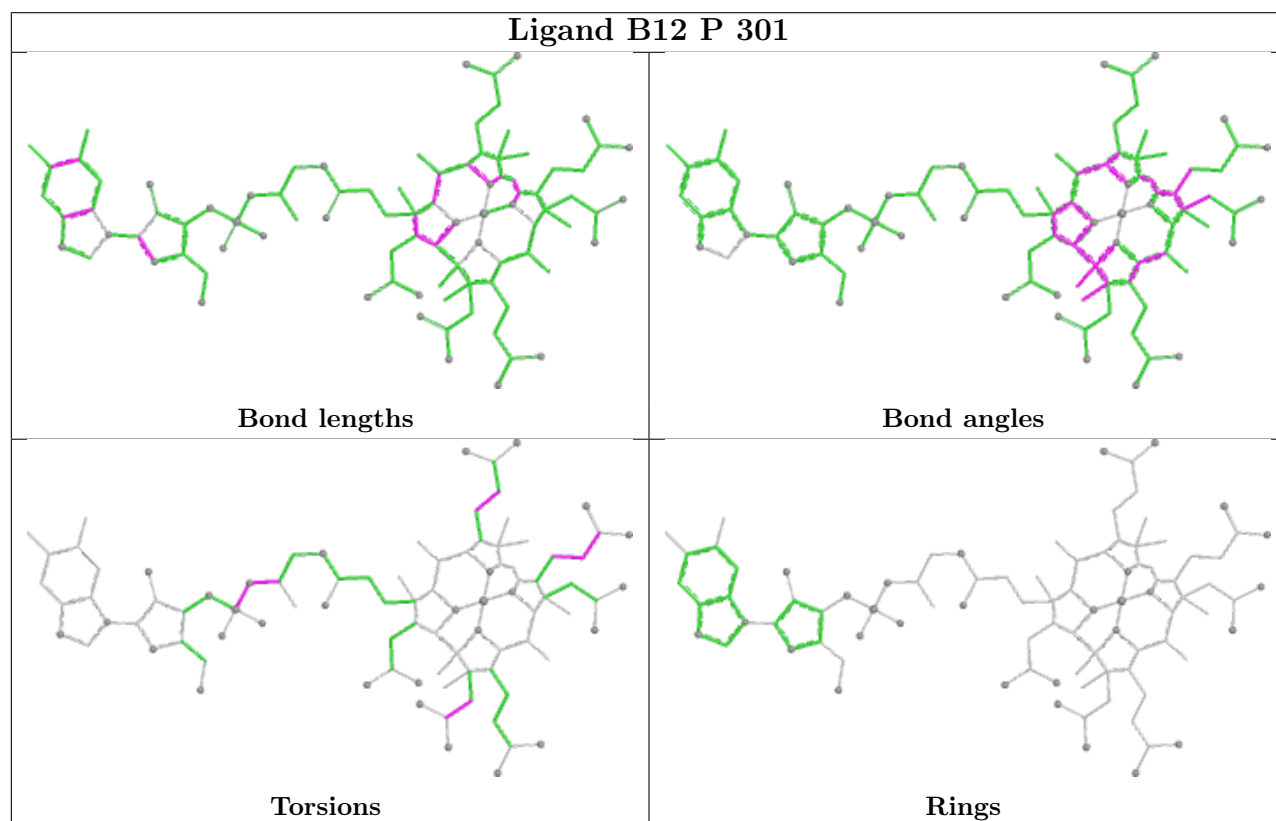
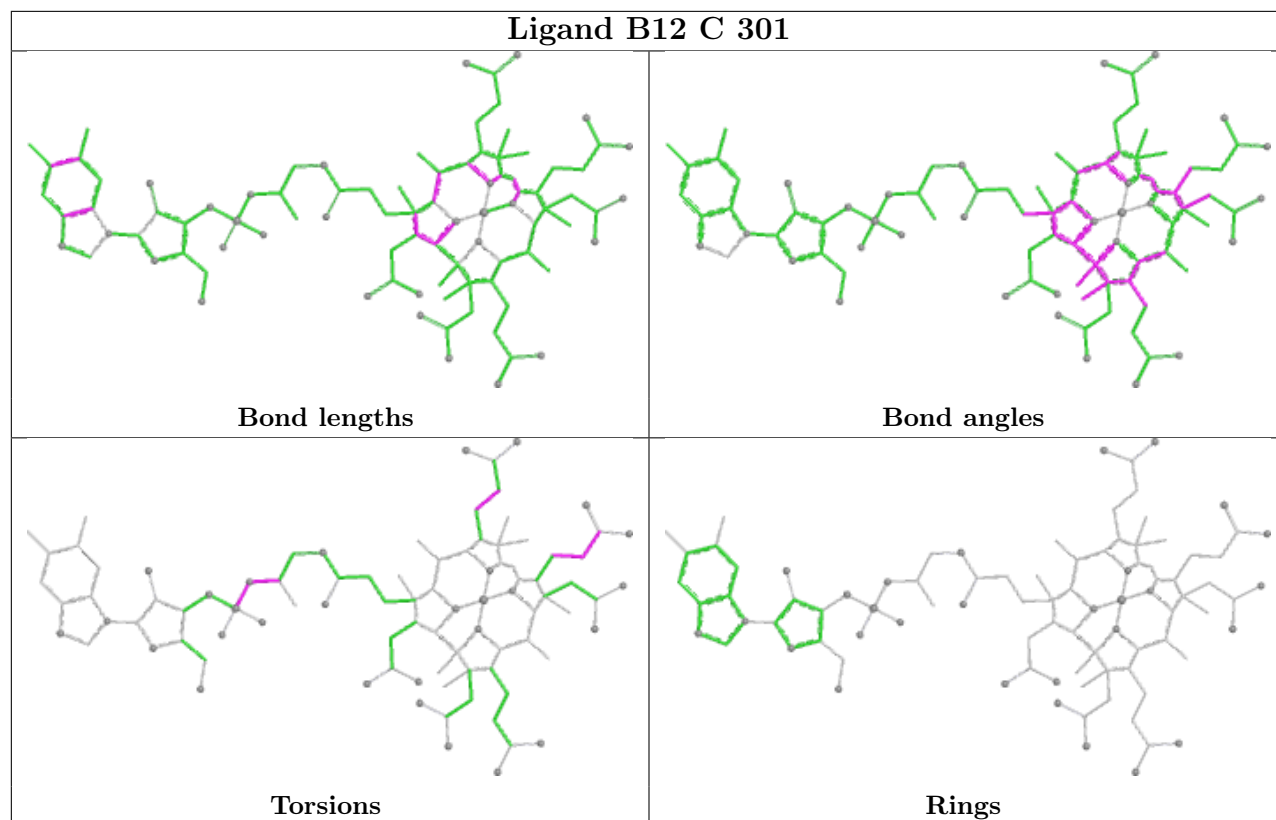
## Ligand 5AD B 401



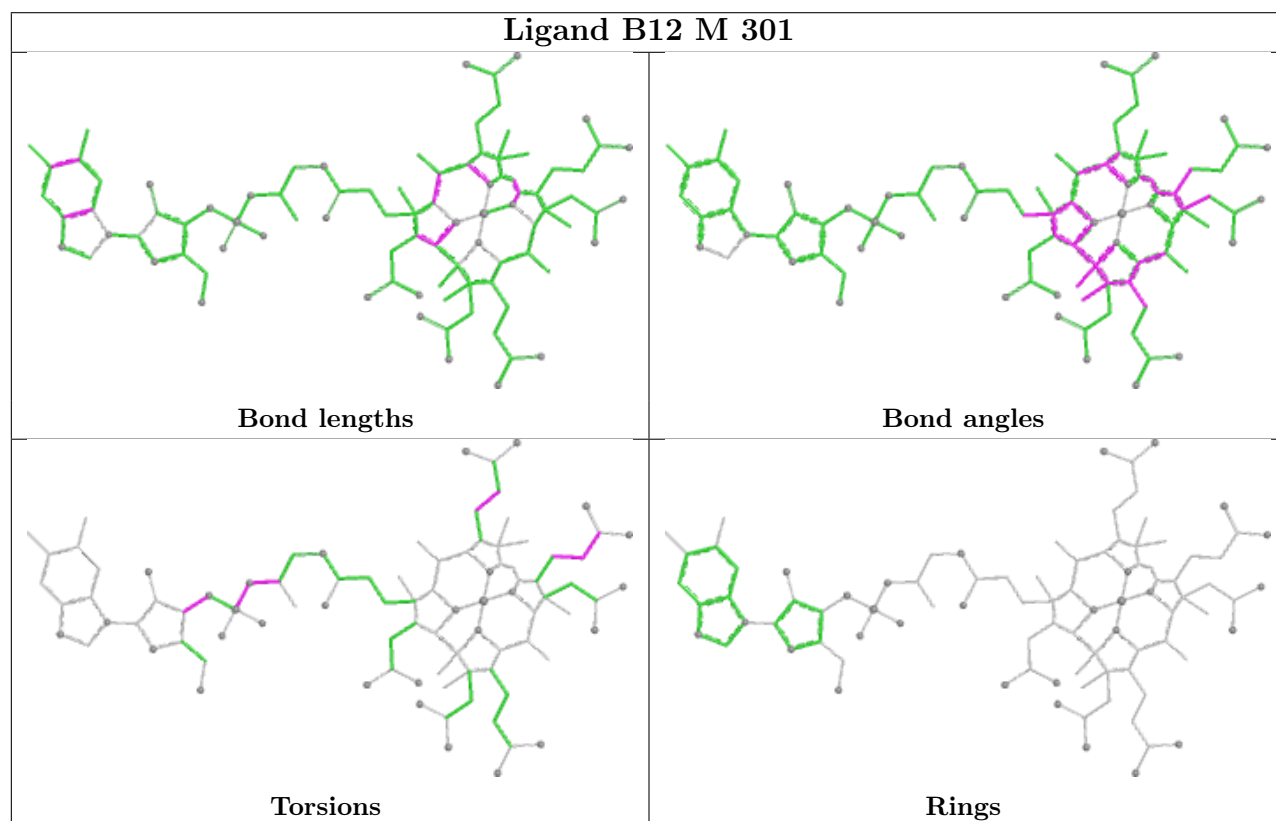
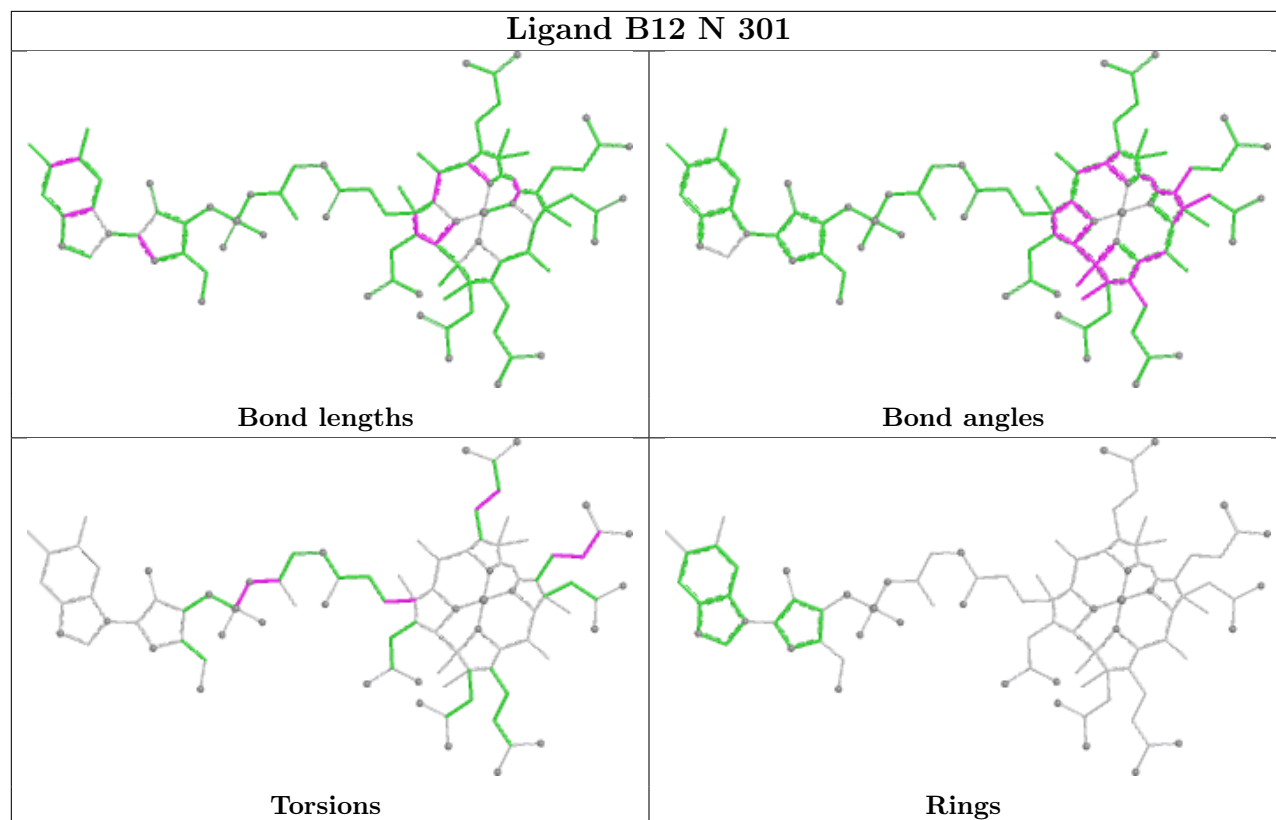
## Ligand 5AD K 401

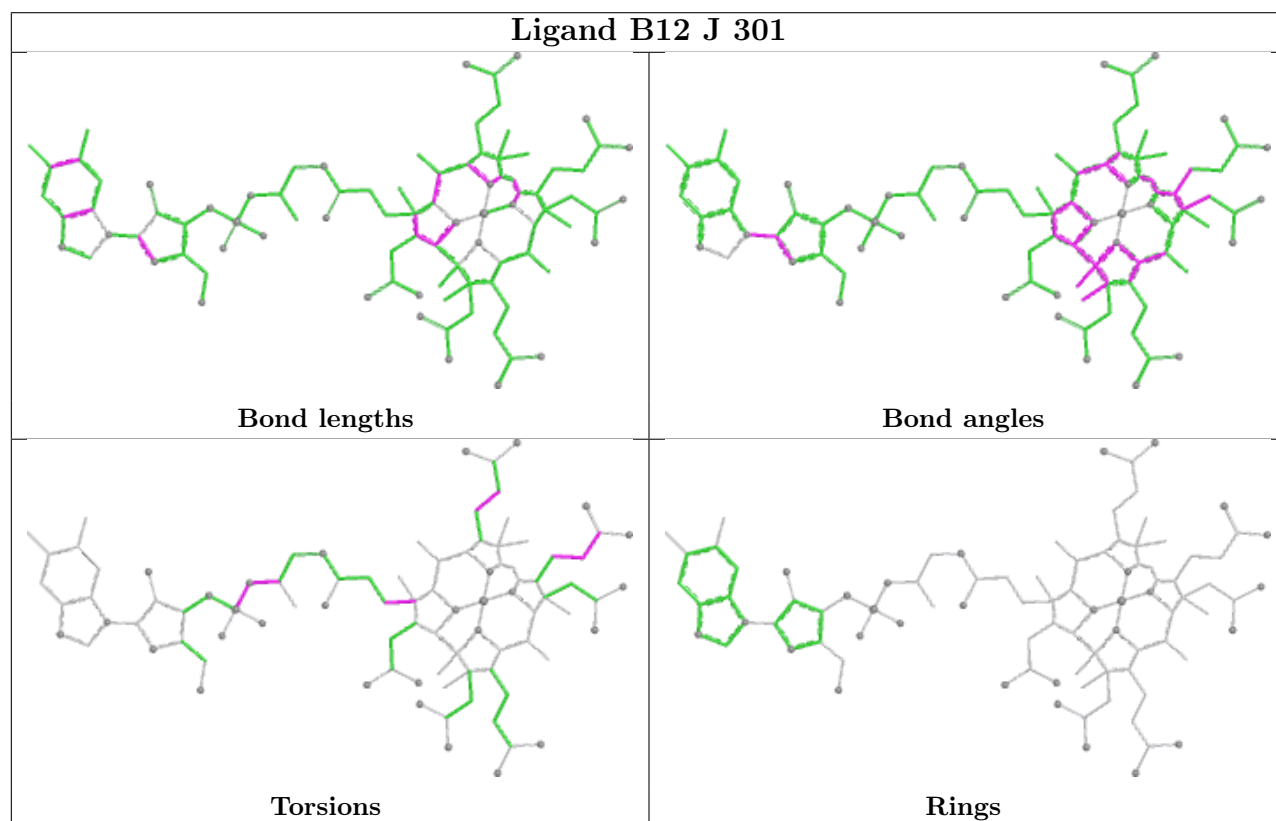
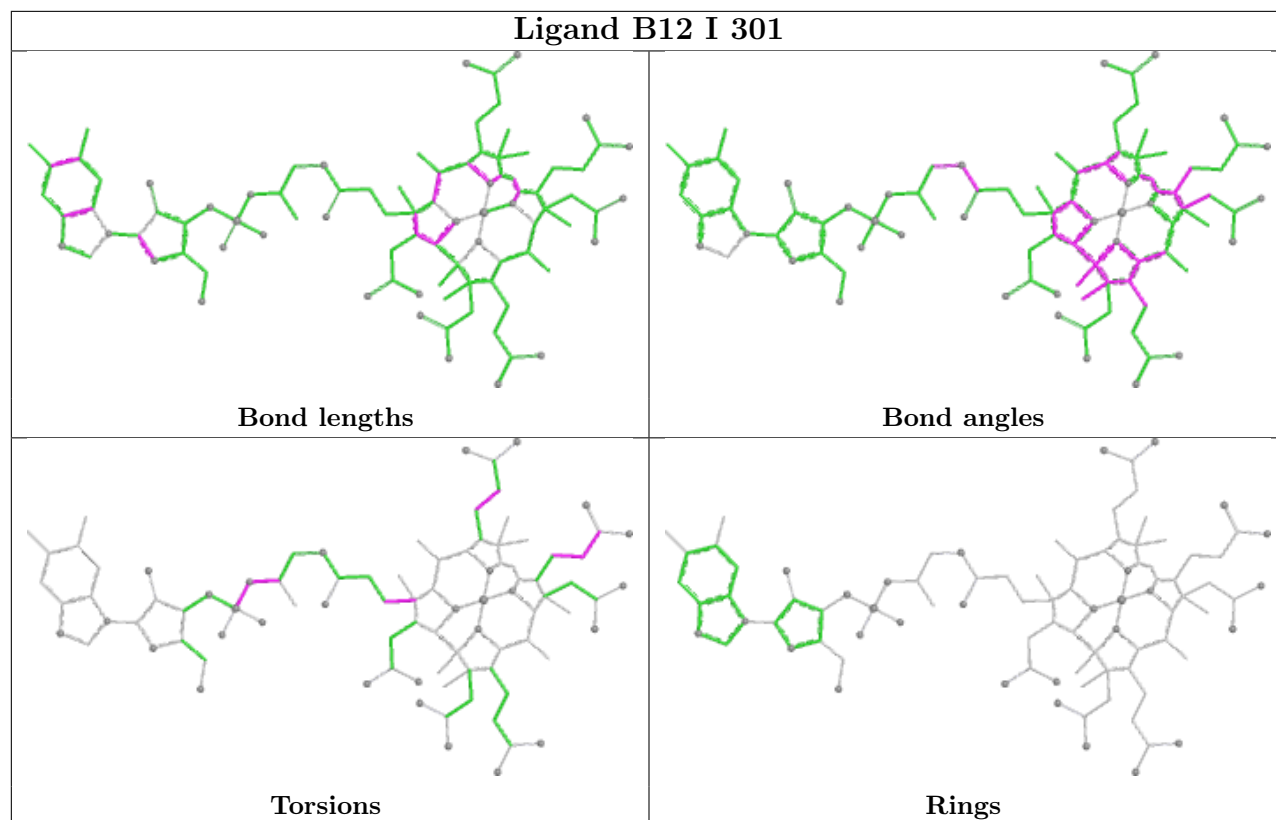




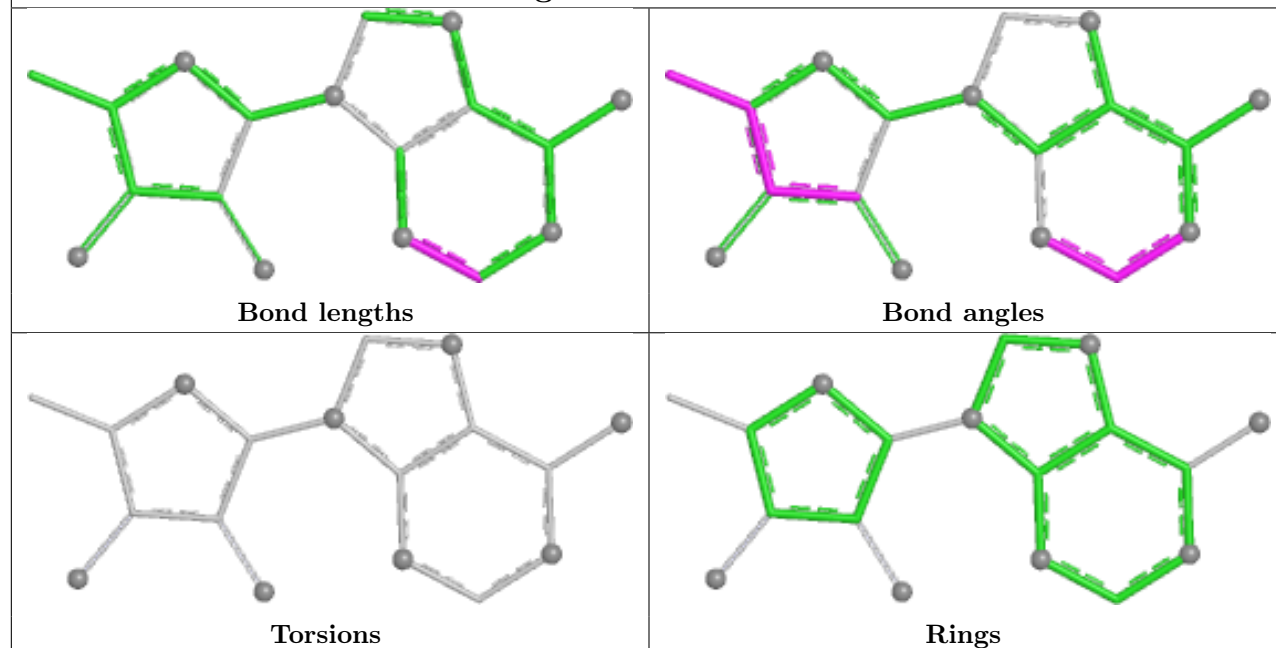




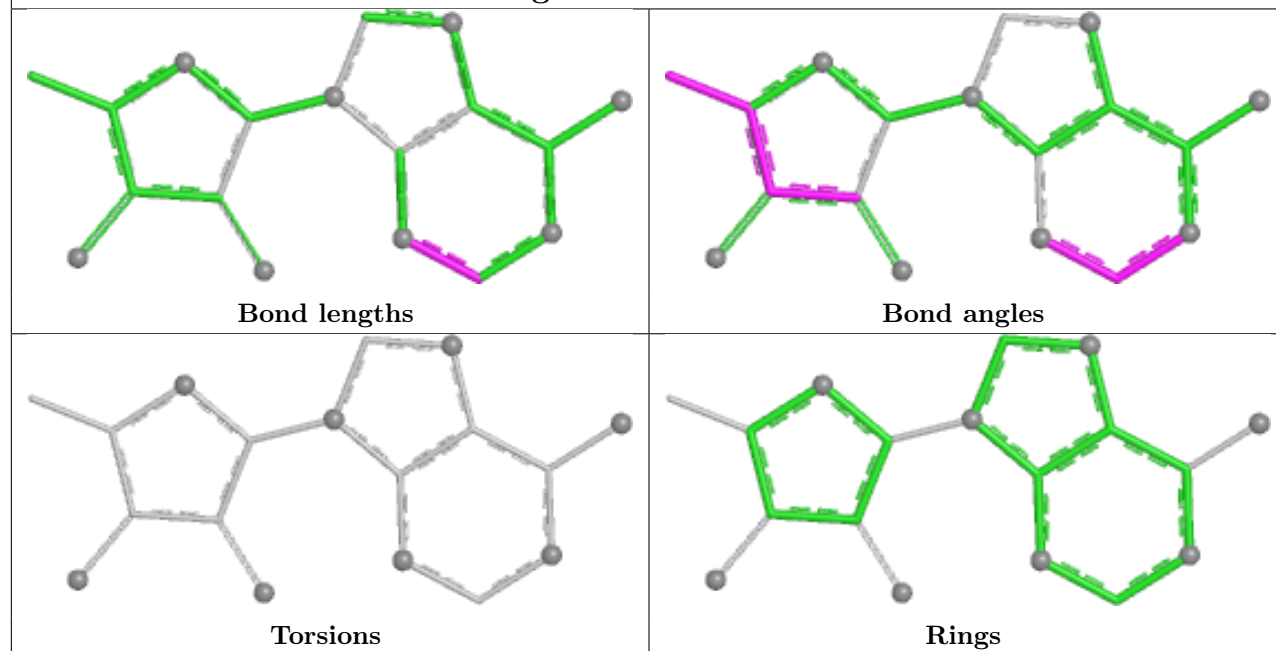


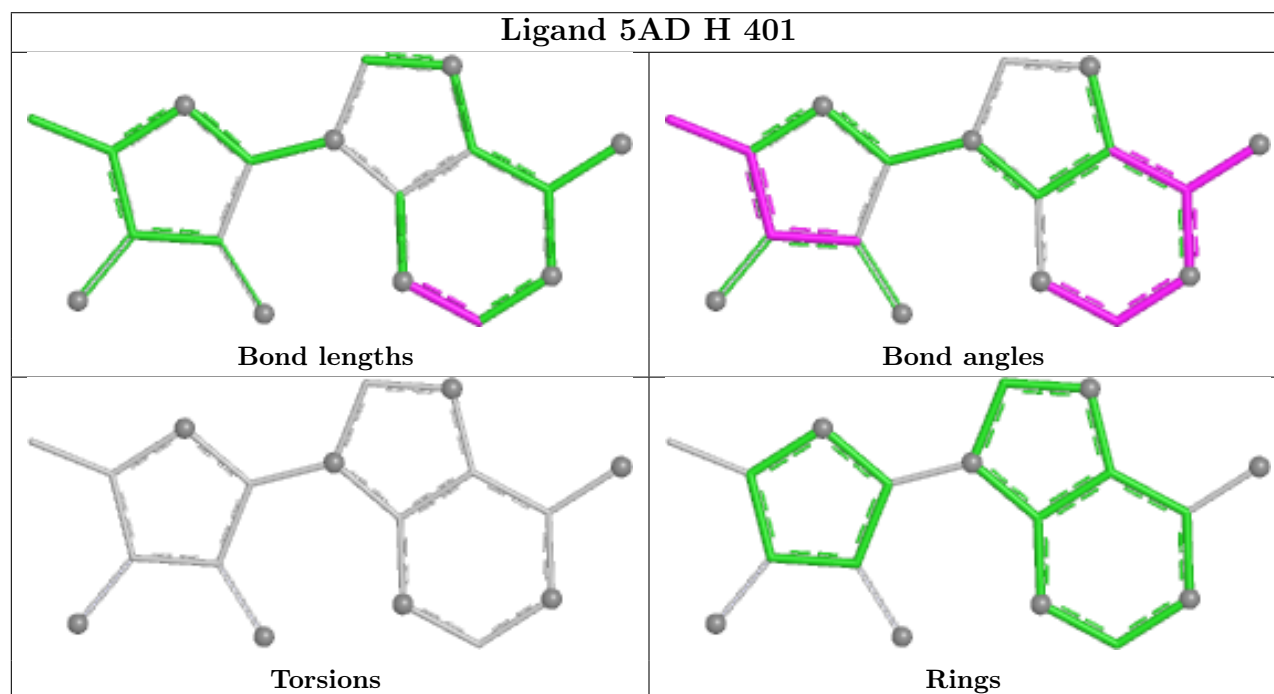
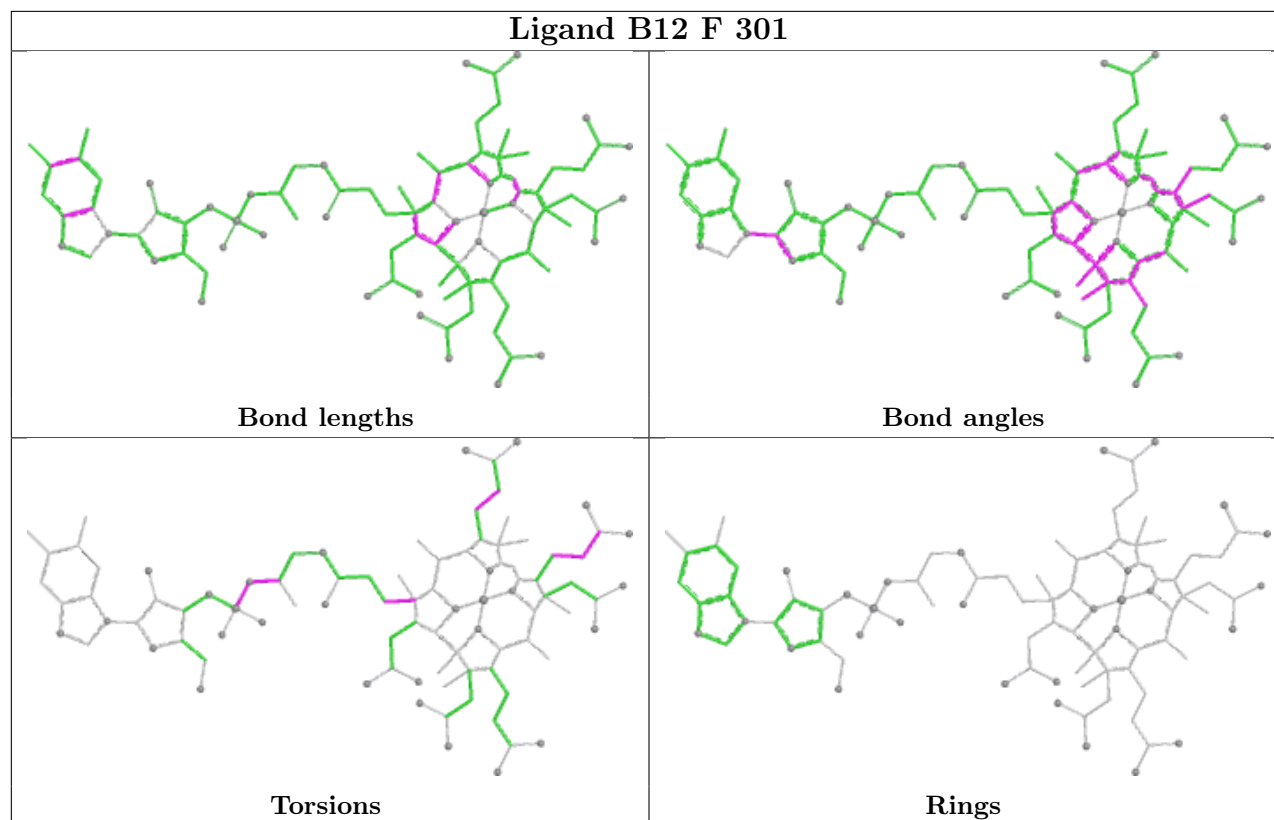


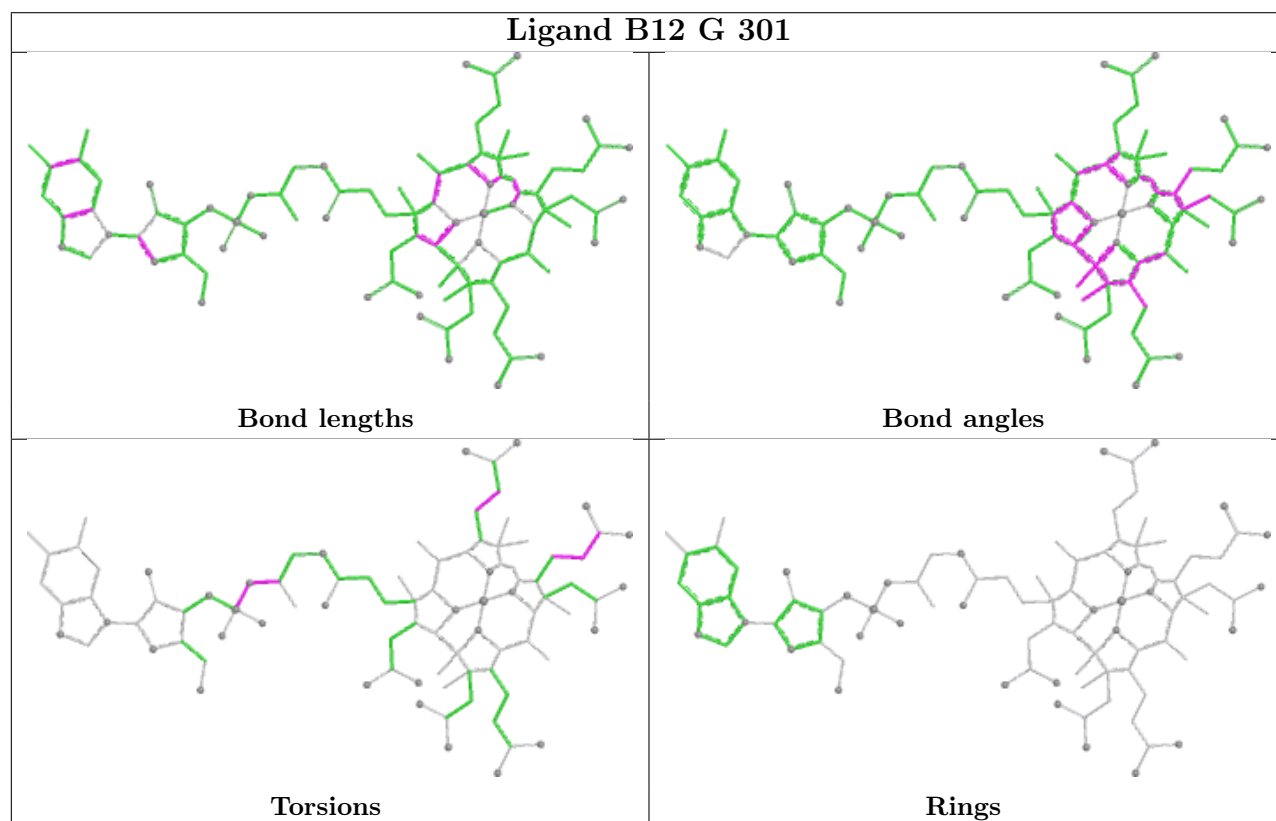
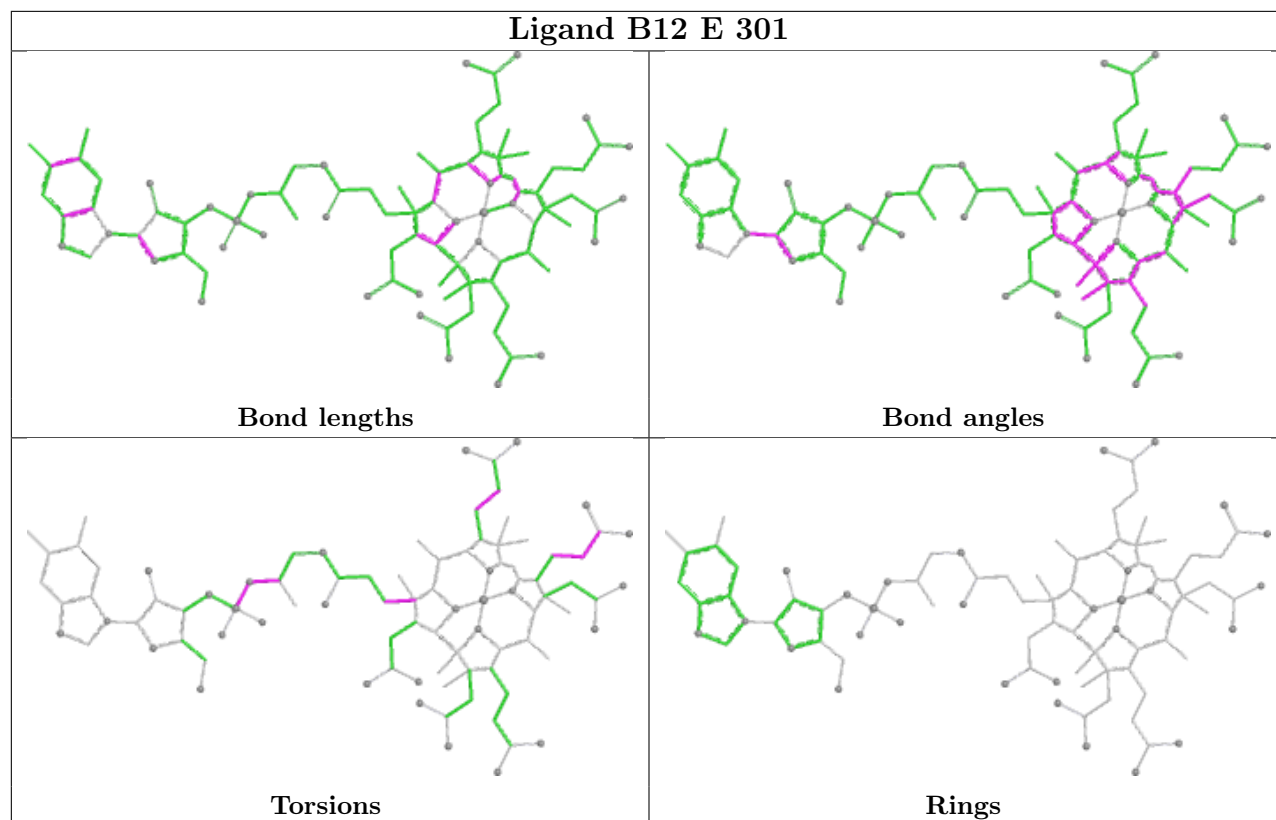
## Ligand 5AD F 401



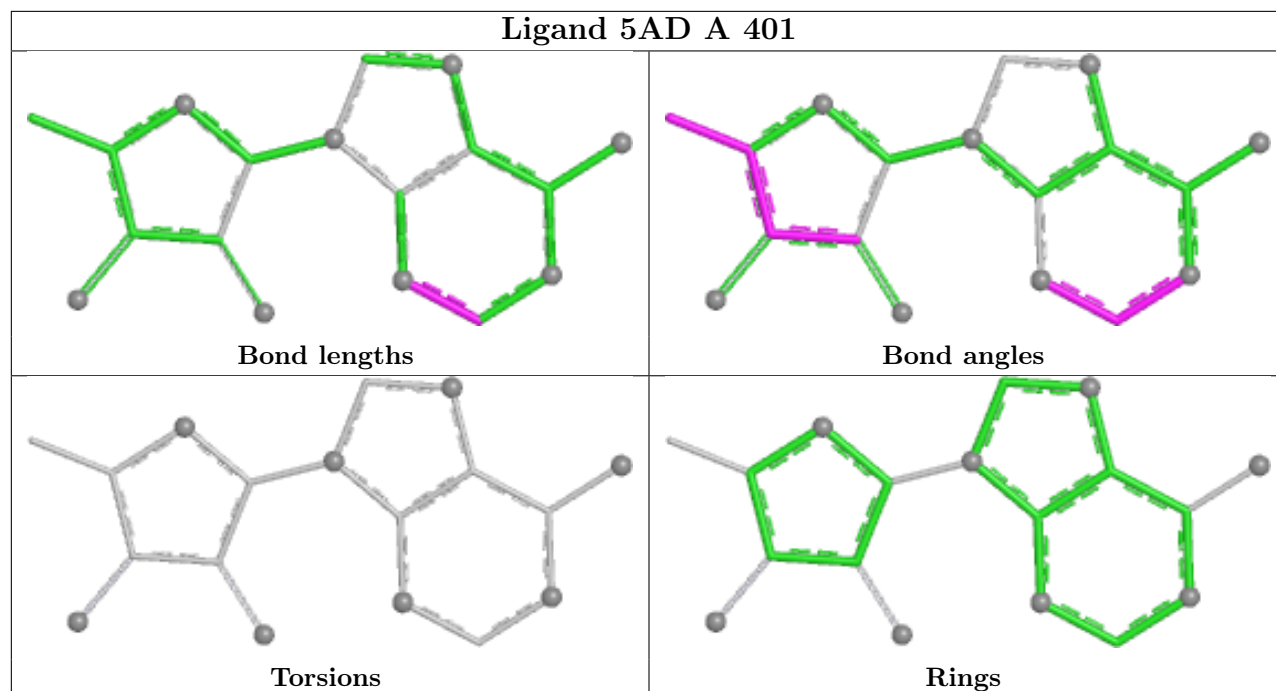
## Ligand 5AD G 401



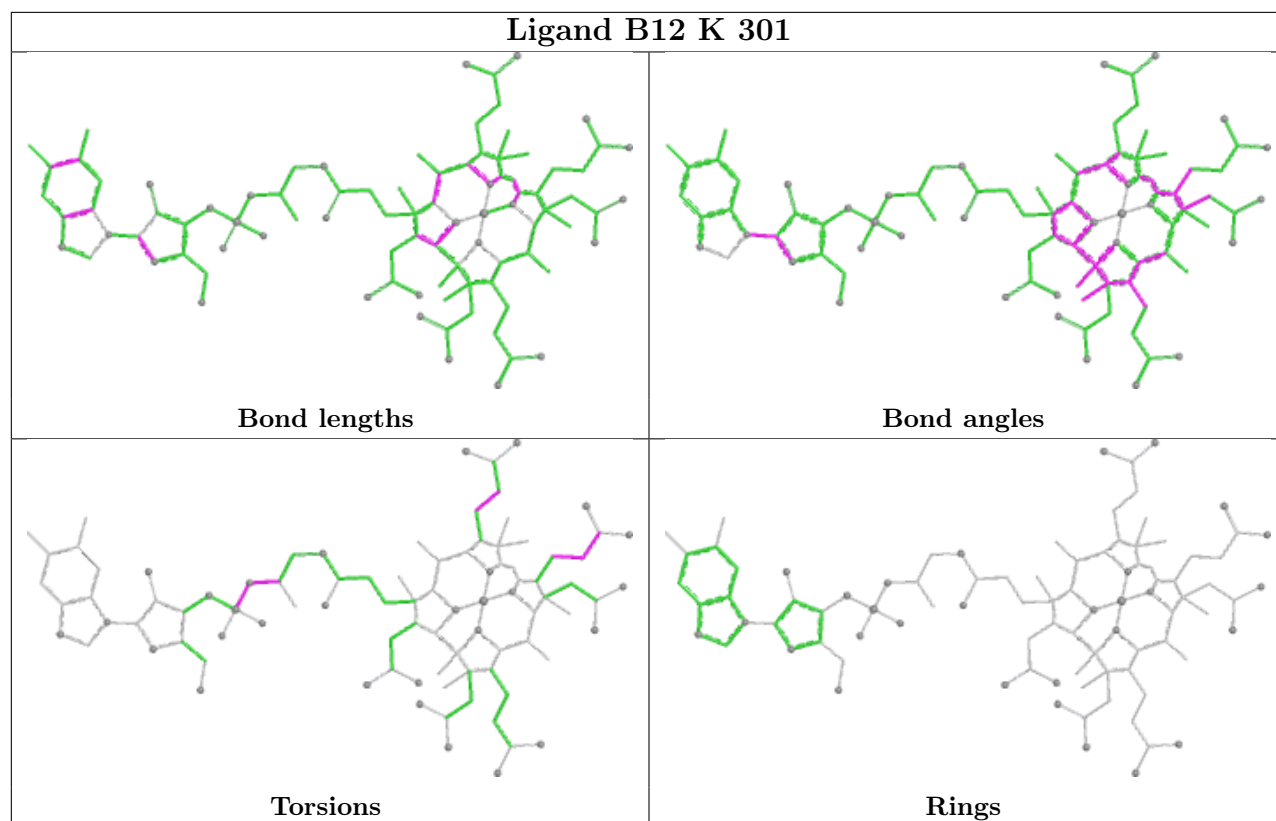




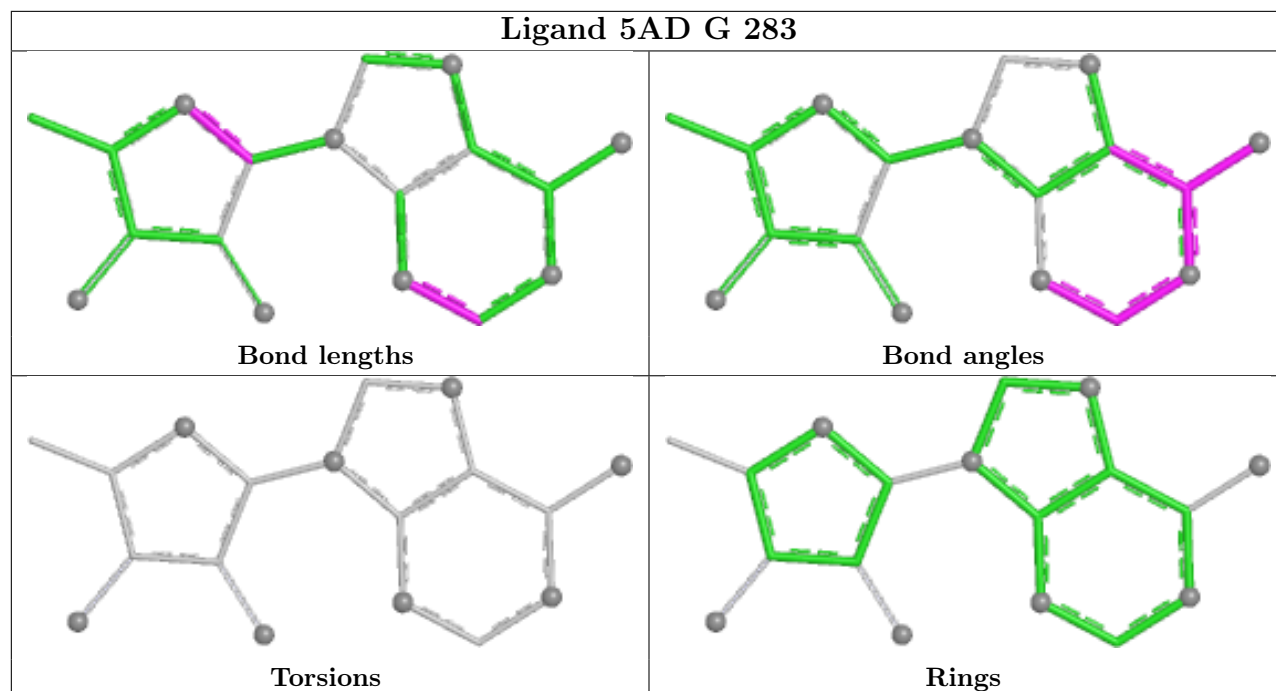
## Ligand 5AD A 401



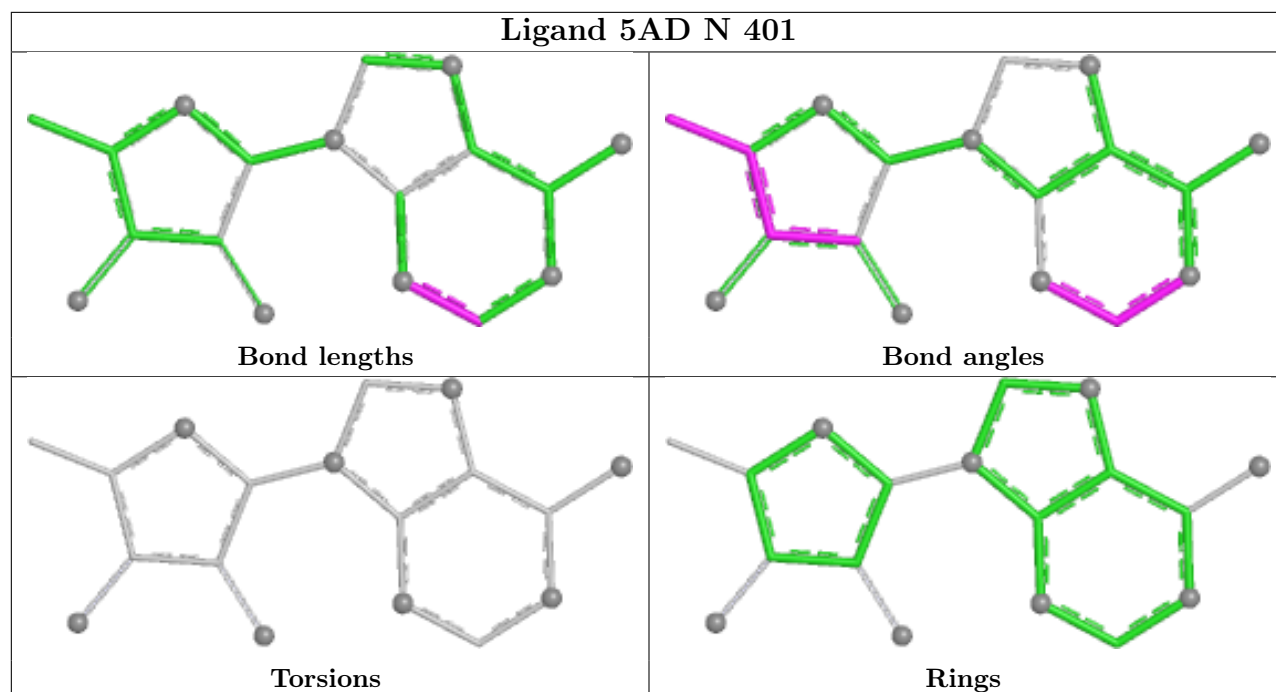
## Ligand B12 K 301

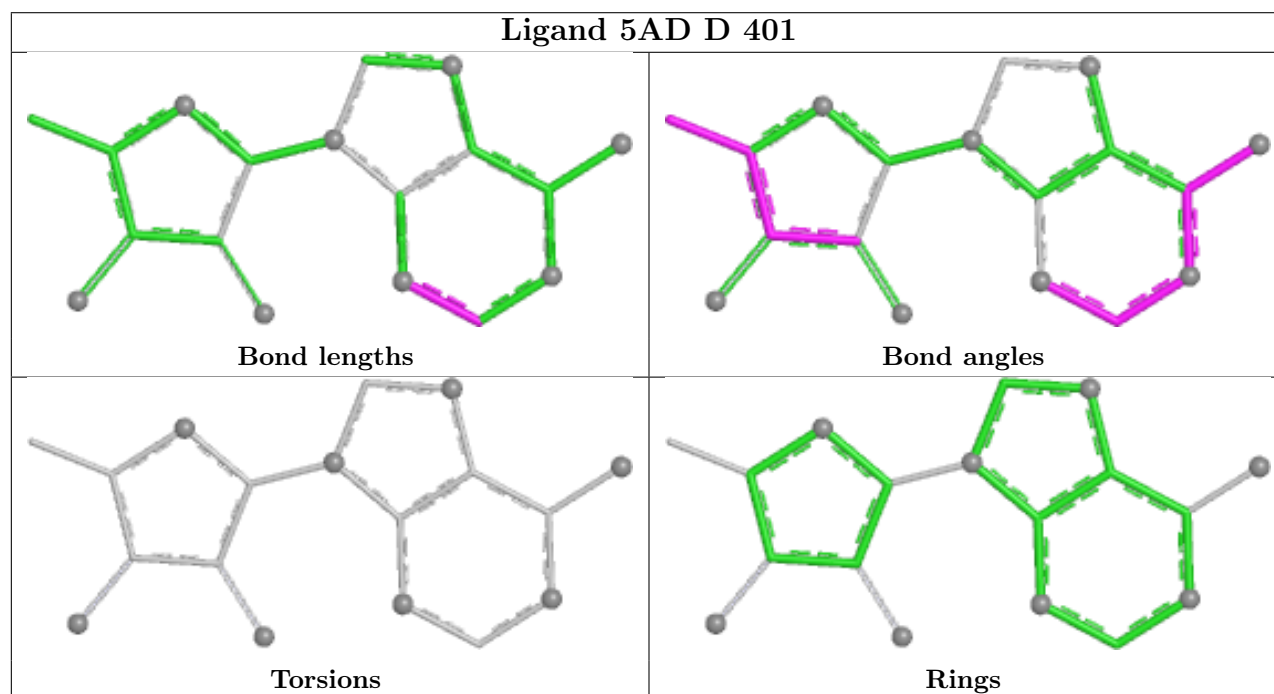
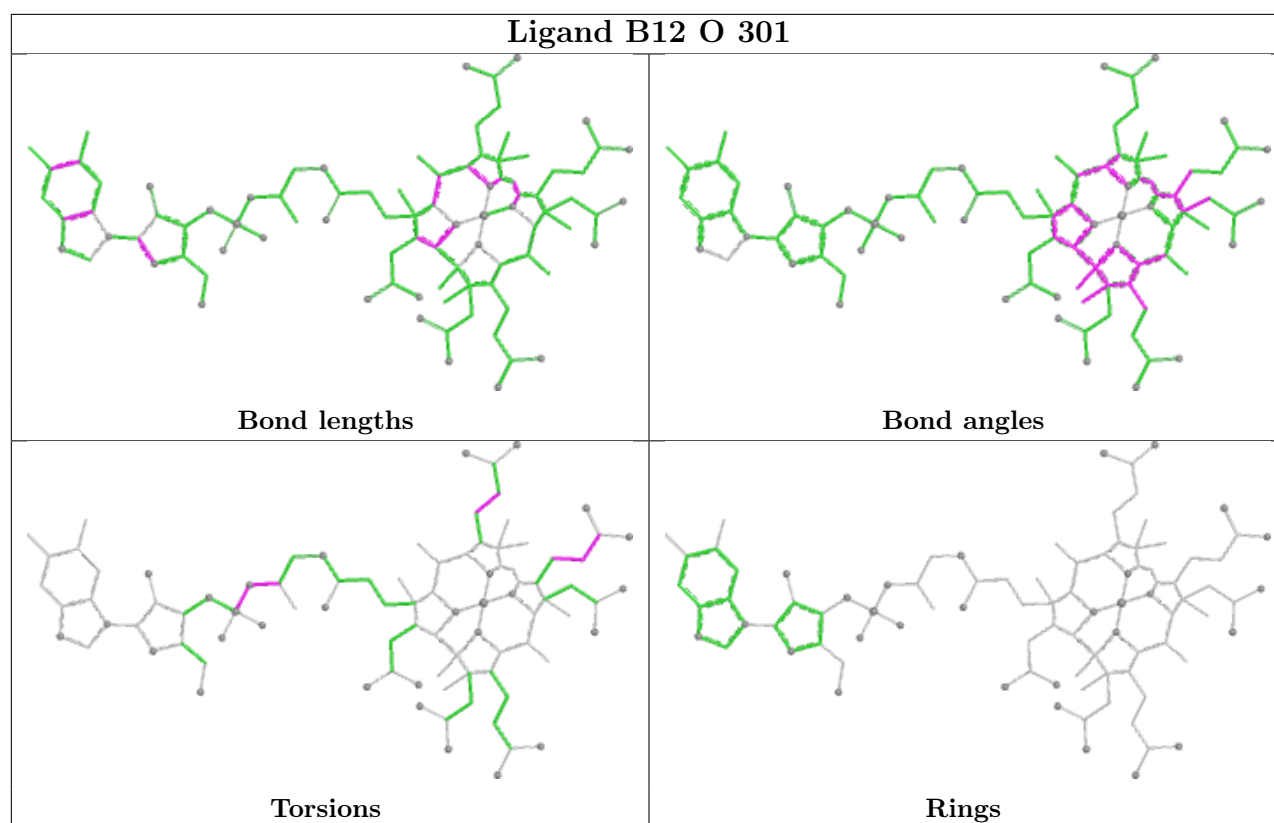


## Ligand 5AD G 283

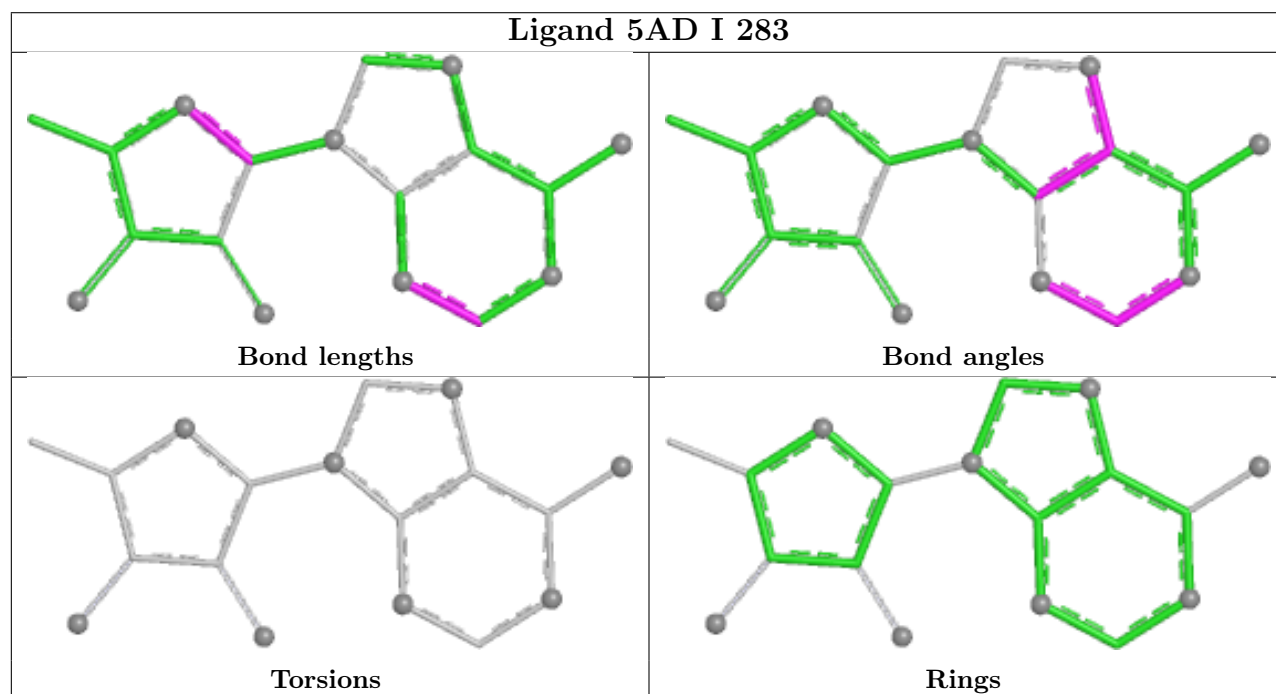
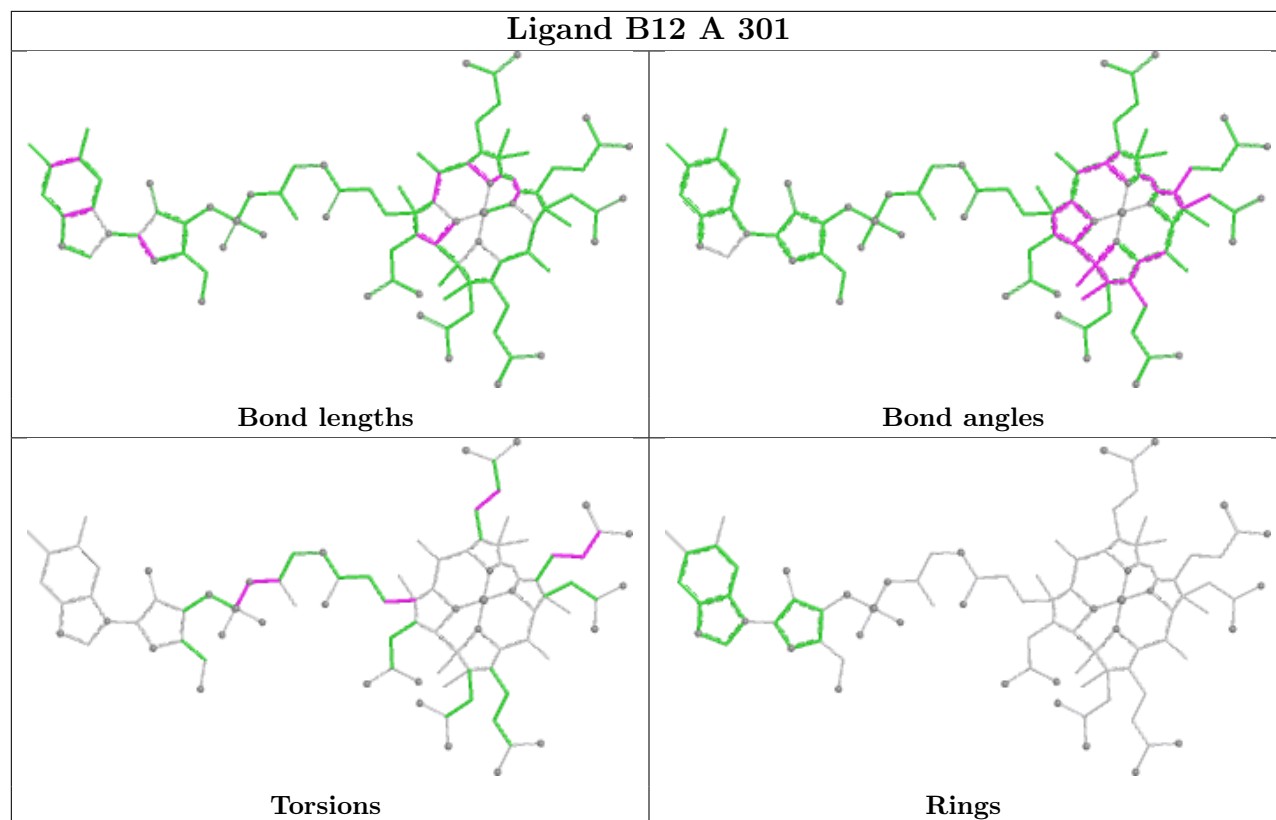


## Ligand 5AD N 401

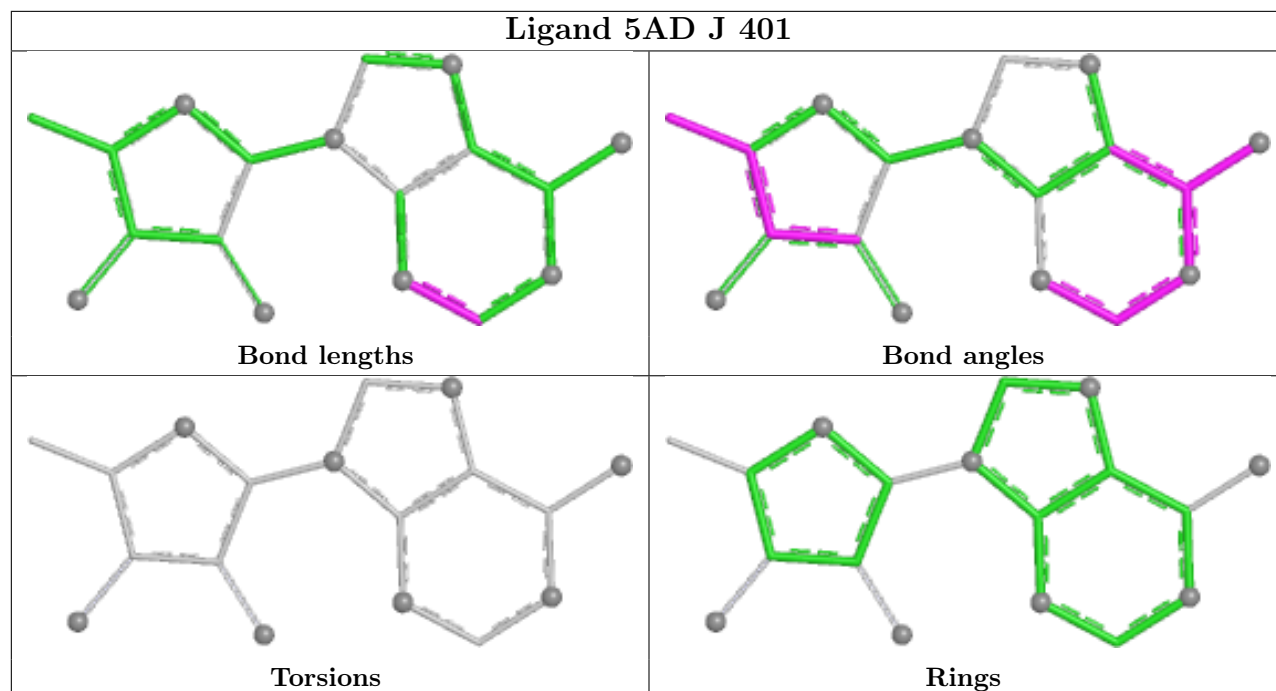




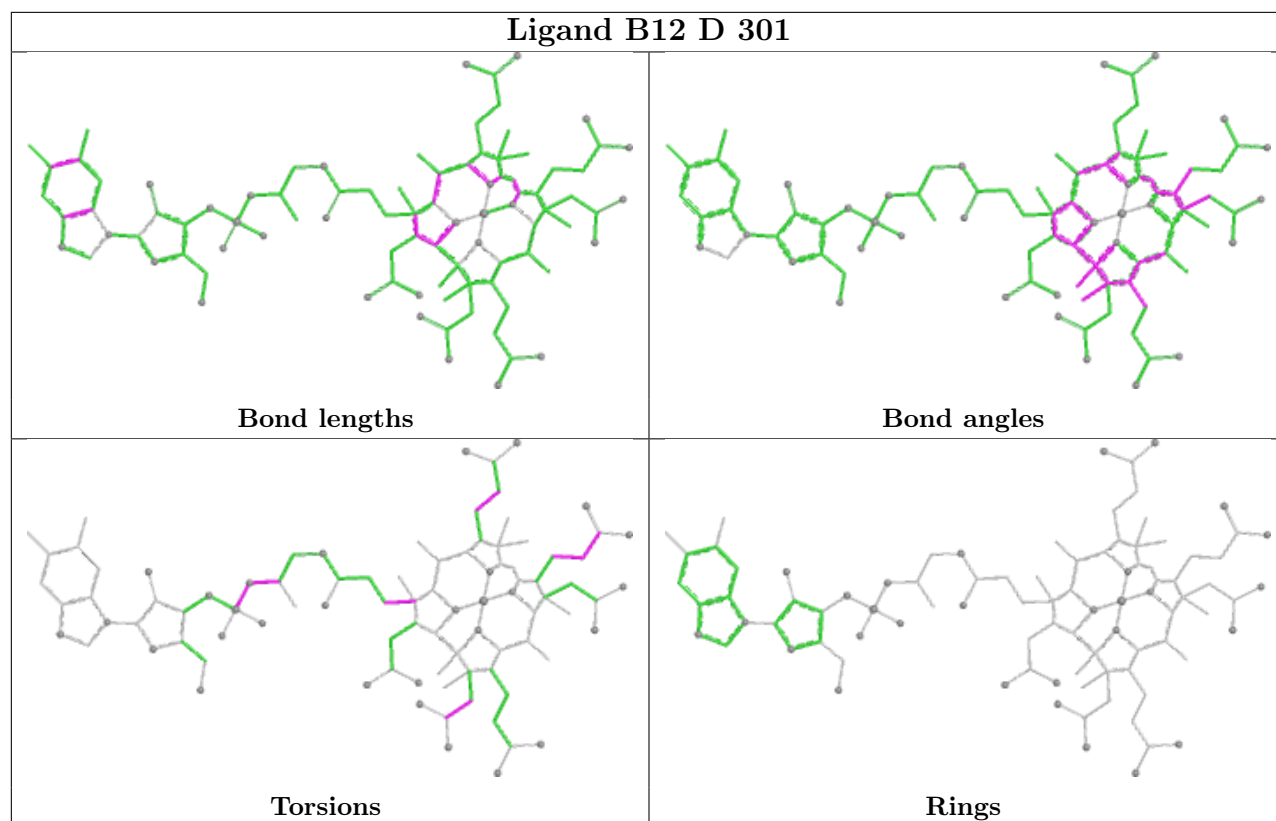




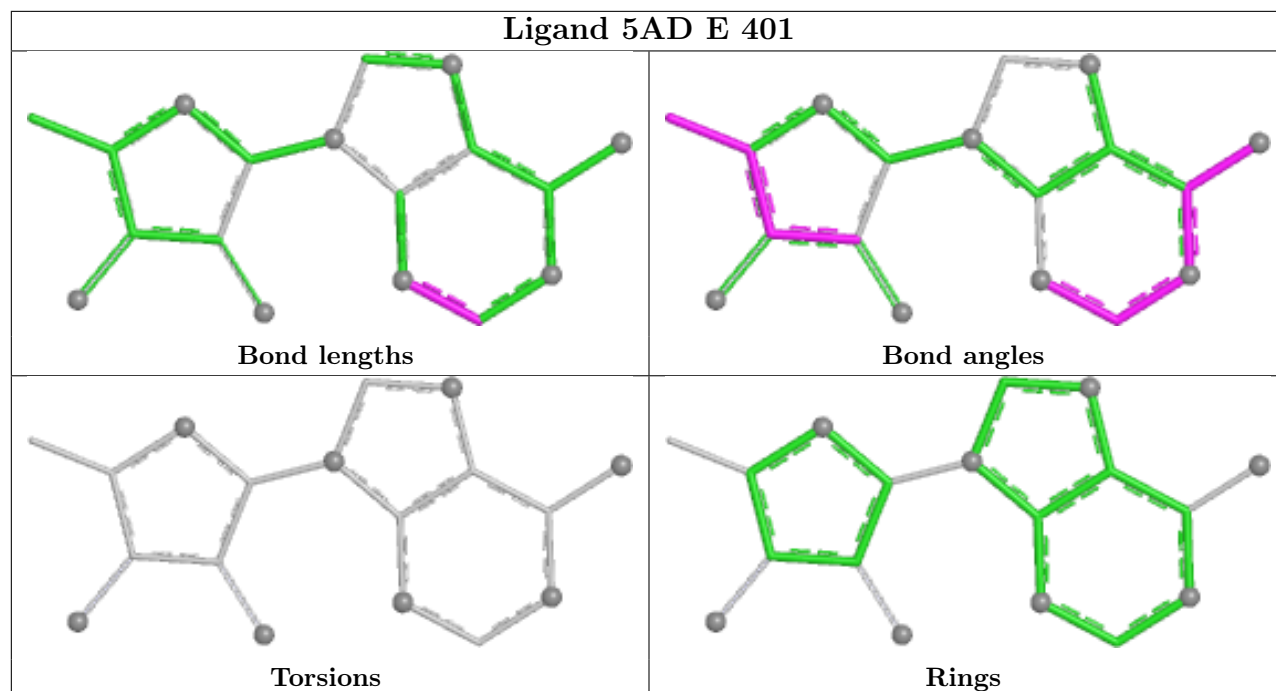
## Ligand 5AD J 401



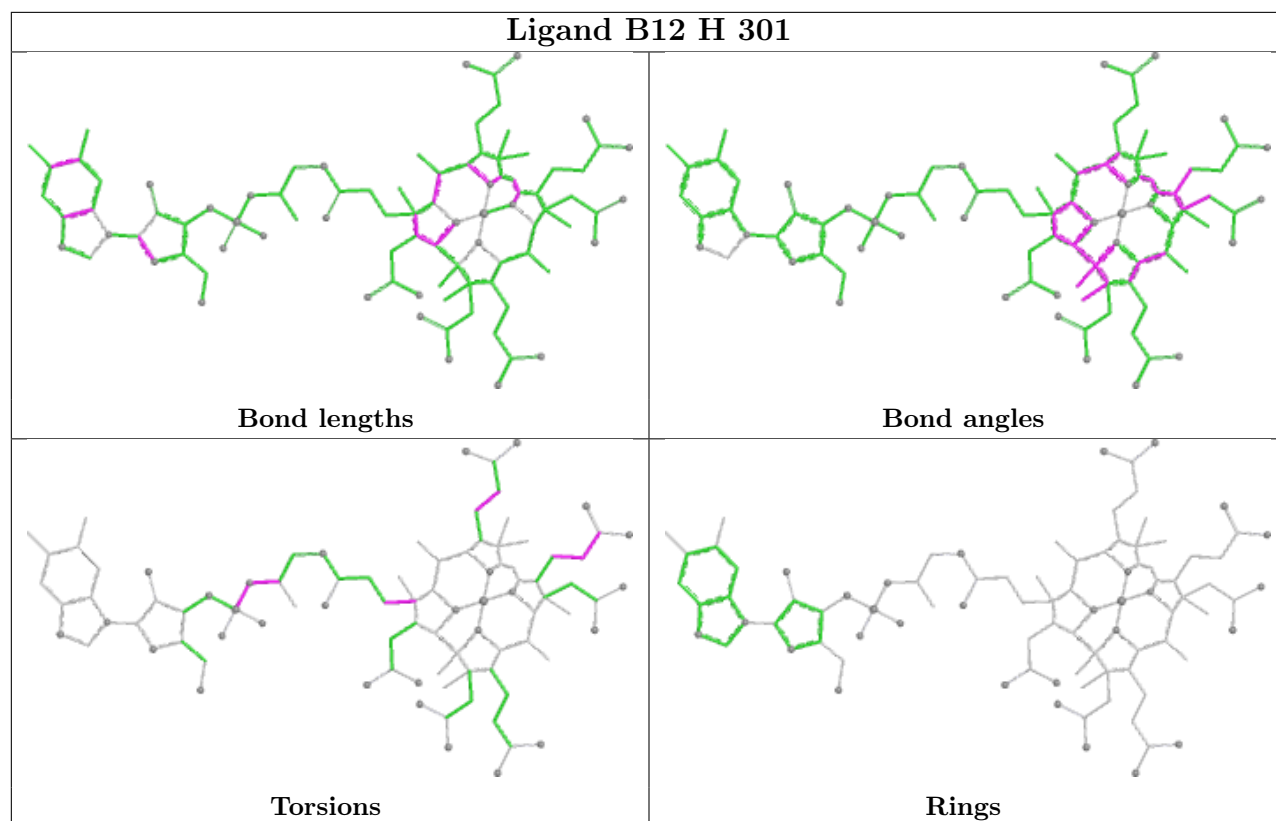
## Ligand B12 D 301

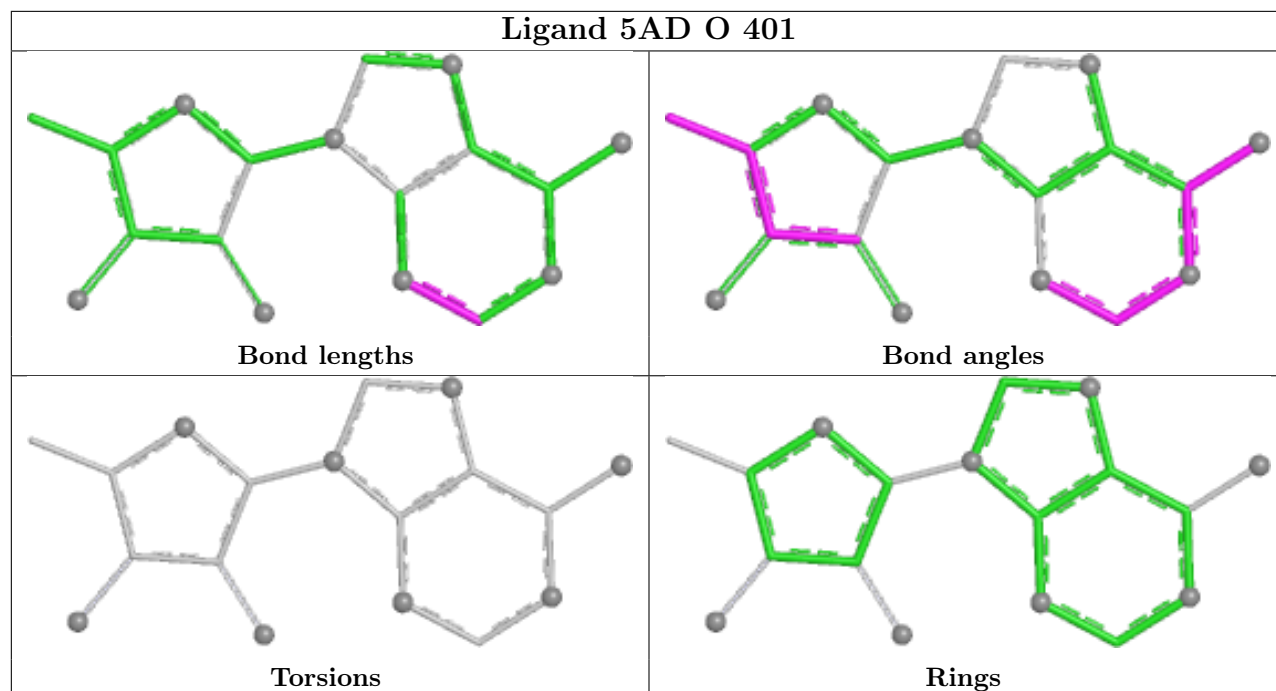


## Ligand 5AD E 401



## Ligand B12 H 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	225/286 (78%)	-0.15	1 (0%) 89 87	24, 40, 57, 70	0
1	B	226/286 (79%)	-0.07	3 (1%) 74 71	26, 40, 59, 70	0
1	C	226/286 (79%)	0.12	2 (0%) 81 78	29, 42, 60, 76	2 (0%)
1	D	227/286 (79%)	-0.32	2 (0%) 81 78	23, 35, 52, 73	1 (0%)
1	E	228/286 (79%)	-0.48	1 (0%) 89 87	18, 31, 51, 72	1 (0%)
1	F	226/286 (79%)	-0.58	1 (0%) 89 87	16, 28, 47, 63	3 (1%)
1	G	226/286 (79%)	-0.58	5 (2%) 62 59	16, 27, 48, 68	0
1	H	225/286 (78%)	-0.57	3 (1%) 74 71	17, 27, 47, 66	0
1	I	226/286 (79%)	-0.51	2 (0%) 81 78	19, 30, 51, 71	1 (0%)
1	J	225/286 (78%)	-0.58	1 (0%) 89 87	19, 28, 50, 71	1 (0%)
1	K	225/286 (78%)	-0.43	0 100 100	19, 32, 51, 67	1 (0%)
1	L	229/286 (80%)	-0.57	3 (1%) 74 71	16, 28, 45, 71	2 (0%)
1	M	229/286 (80%)	-0.62	2 (0%) 81 78	16, 28, 45, 63	1 (0%)
1	N	230/286 (80%)	-0.37	1 (0%) 89 87	20, 33, 51, 76	0
1	O	226/286 (79%)	-0.55	1 (0%) 89 87	18, 30, 47, 68	1 (0%)
1	P	228/286 (79%)	-0.50	2 (0%) 81 78	18, 31, 51, 68	0
All	All	3627/4576 (79%)	-0.42	30 (0%) 82 80	16, 32, 54, 76	14 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	4.7
1	P	231	LEU	4.6
1	F	3	PRO	4.3
1	C	231	LEU	4.1
1	O	231	LEU	4.1

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	DHL	G	601	4/4	0.67	0.27	57,59,61,64	0
4	DHL	A	601	4/4	0.68	0.26	79,79,79,80	0
4	DHL	O	601	4/4	0.70	0.34	29,30,32,35	4
5	5AD	G	283	18/18	0.72	0.19	55,68,72,72	0
5	5AD	I	283	18/18	0.75	0.18	59,64,71,73	0
4	DHL	I	601	4/4	0.76	0.34	41,42,42,42	4
4	DHL	D	601	4/4	0.77	0.25	62,62,63,64	0
4	DHL	M	601	4/4	0.81	0.21	54,55,56,56	0
6	EDO	E	283	4/4	0.83	0.20	55,55,55,59	0
4	DHL	C	601	4/4	0.85	0.28	22,23,25,30	4
4	DHL	L	601	4/4	0.88	0.15	51,51,51,51	0
4	DHL	F	601	4/4	0.88	0.16	52,52,53,54	0
5	5AD	C	401	18/18	0.89	0.12	31,39,46,46	0
4	DHL	N	601	4/4	0.89	0.17	51,55,58,61	0
3	FLC	D	501	13/13	0.90	0.10	43,44,45,45	0
4	DHL	K	601	4/4	0.90	0.15	50,51,51,53	0
3	FLC	C	501	13/13	0.90	0.13	61,62,63,63	0
5	5AD	O	401	18/18	0.90	0.11	25,31,35,39	0
5	5AD	B	401	18/18	0.90	0.11	35,40,43,43	0
6	EDO	P	284	4/4	0.90	0.21	48,49,49,53	0
4	DHL	J	601	4/4	0.91	0.13	43,47,51,54	0
5	5AD	K	401	18/18	0.91	0.11	23,32,34,35	0
5	5AD	L	401	18/18	0.91	0.11	24,32,44,47	0
3	FLC	B	501	13/13	0.91	0.10	53,54,55,55	0
5	5AD	E	401	18/18	0.91	0.10	24,31,38,38	0
6	EDO	P	283	4/4	0.91	0.18	43,44,45,48	0
5	5AD	A	401	18/18	0.91	0.09	41,44,47,49	0

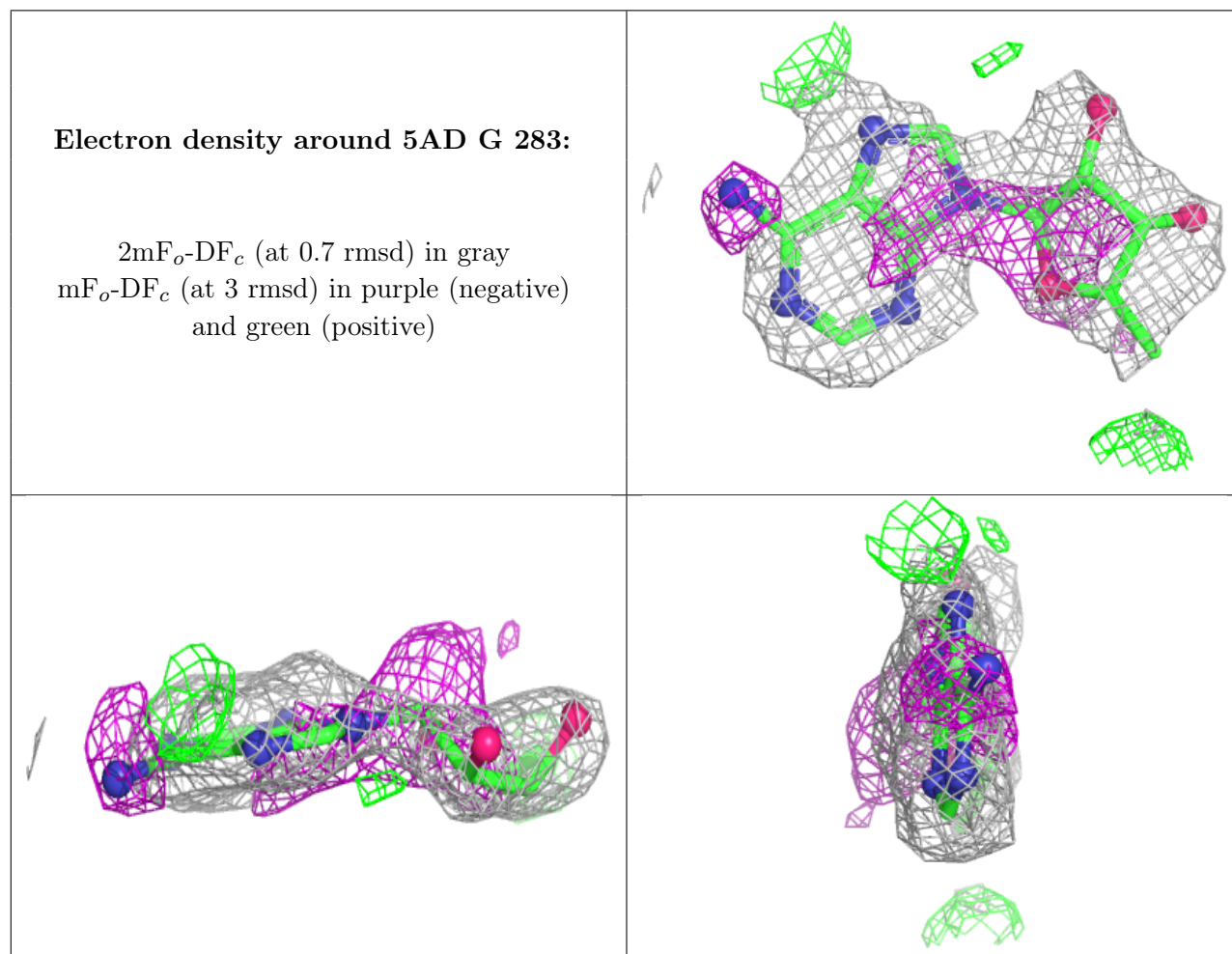
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FLC	P	501	13/13	0.92	0.10	39,40,41,42	0
5	5AD	F	401	18/18	0.92	0.10	24,31,35,38	0
5	5AD	M	401	18/18	0.92	0.10	26,34,40,43	0
5	5AD	N	401	18/18	0.92	0.10	22,31,39,40	0
3	FLC	K	501	13/13	0.92	0.10	37,38,39,39	0
5	5AD	H	401	18/18	0.92	0.10	23,29,38,38	0
5	5AD	I	401	18/18	0.92	0.10	28,34,38,39	0
5	5AD	D	401	18/18	0.92	0.09	31,35,47,48	0
3	FLC	N	501	13/13	0.93	0.09	38,39,40,41	0
3	FLC	G	501	13/13	0.93	0.09	33,34,35,36	0
5	5AD	G	401	18/18	0.93	0.09	28,32,38,39	0
5	5AD	J	401	18/18	0.94	0.09	22,28,37,38	0
3	FLC	F	501	13/13	0.94	0.08	31,32,33,33	0
3	FLC	L	501	13/13	0.94	0.09	35,35,36,37	0
3	FLC	M	501	13/13	0.94	0.08	35,36,37,37	0
3	FLC	E	501	13/13	0.94	0.09	36,37,38,38	0
4	DHL	P	601	4/4	0.94	0.12	38,38,38,40	0
5	5AD	P	401	18/18	0.94	0.09	26,32,36,37	0
3	FLC	O	501	13/13	0.94	0.08	36,37,38,38	0
3	FLC	H	501	13/13	0.94	0.08	37,38,39,39	0
3	FLC	J	501	13/13	0.94	0.07	35,36,37,38	0
4	DHL	H	601	4/4	0.95	0.11	39,40,41,42	0
3	FLC	A	501	13/13	0.95	0.07	43,44,45,46	0
3	FLC	I	501	13/13	0.95	0.08	34,34,35,36	0
2	B12	C	301	91/91	0.96	0.09	28,35,46,55	0
2	B12	B	301	91/91	0.96	0.08	29,35,42,49	0
2	B12	G	301	91/91	0.97	0.07	15,21,28,29	0
2	B12	H	301	91/91	0.97	0.07	16,22,26,29	0
2	B12	I	301	91/91	0.97	0.07	17,23,30,33	0
2	B12	J	301	91/91	0.97	0.07	18,23,30,32	0
2	B12	K	301	91/91	0.97	0.07	17,25,29,34	0
2	B12	M	301	91/91	0.97	0.07	10,21,28,31	0
2	B12	N	301	91/91	0.97	0.07	15,23,29,32	0
2	B12	O	301	91/91	0.97	0.07	15,22,29,32	0
2	B12	P	301	91/91	0.97	0.07	17,24,29,31	0
2	B12	A	301	91/91	0.97	0.07	27,33,41,44	0
2	B12	D	301	91/91	0.97	0.08	17,28,37,38	0
2	B12	F	301	91/91	0.97	0.07	12,21,28,30	0
2	B12	L	301	91/91	0.98	0.07	14,20,28,30	0
2	B12	E	301	91/91	0.98	0.07	17,23,30,32	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

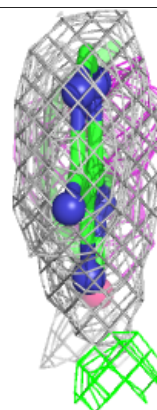
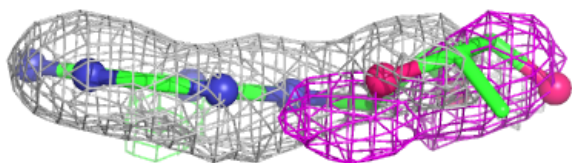
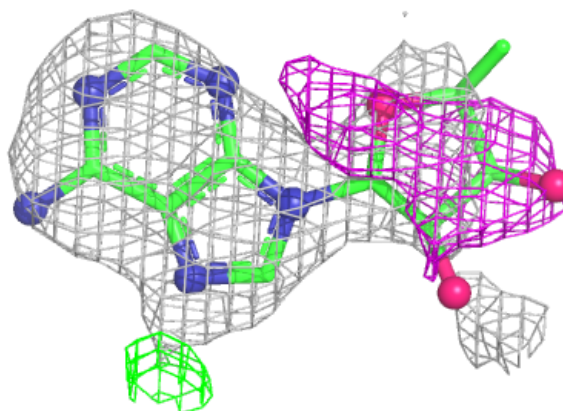
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



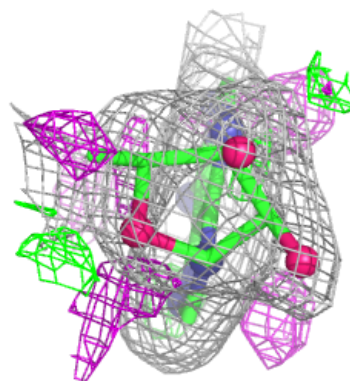
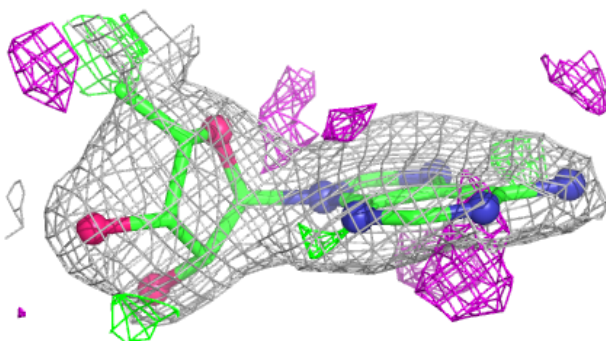
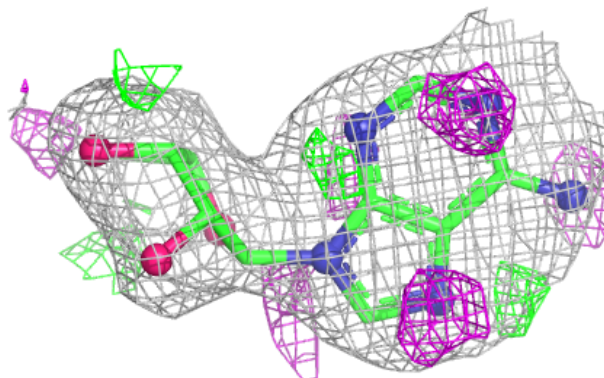


**Electron density around 5AD I 283:**

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

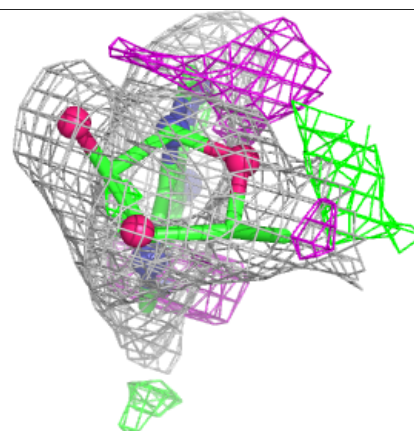
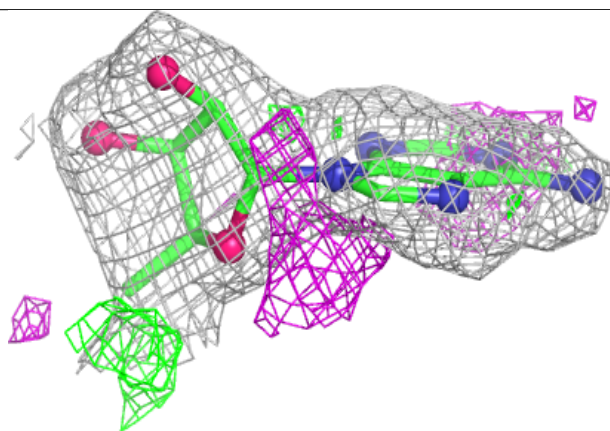
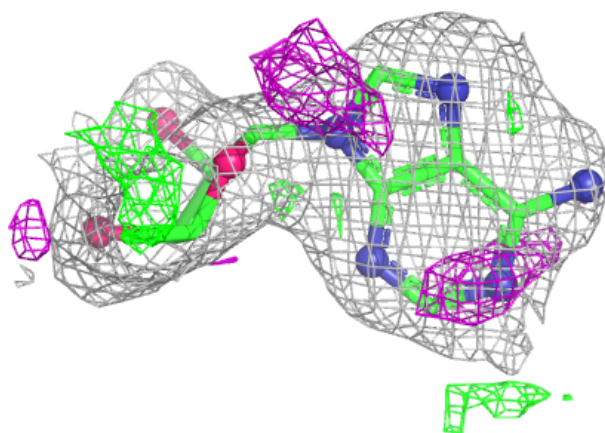
**Electron density around 5AD C 401:**

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

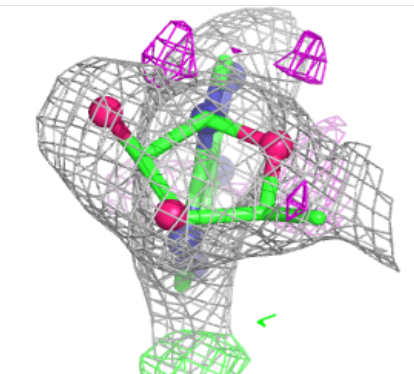
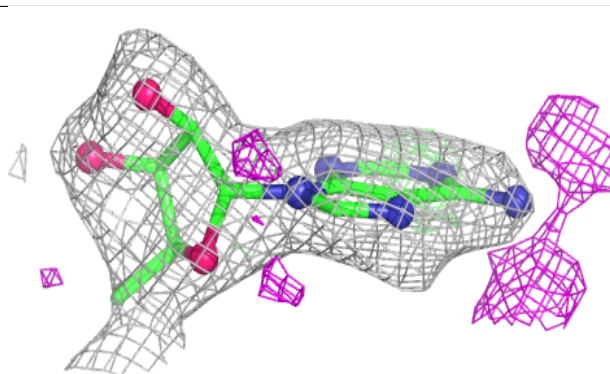
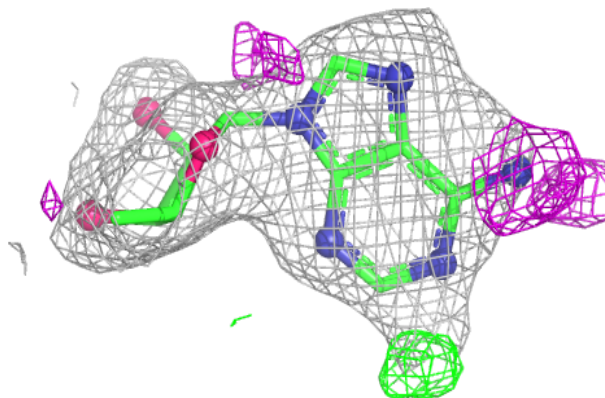


**Electron density around 5AD O 401:**

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

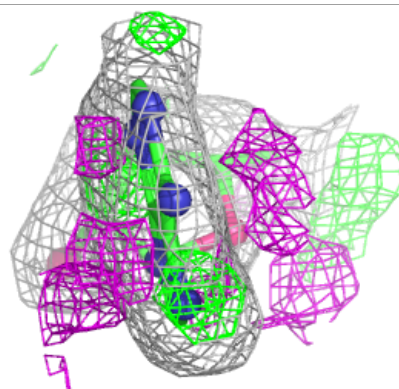
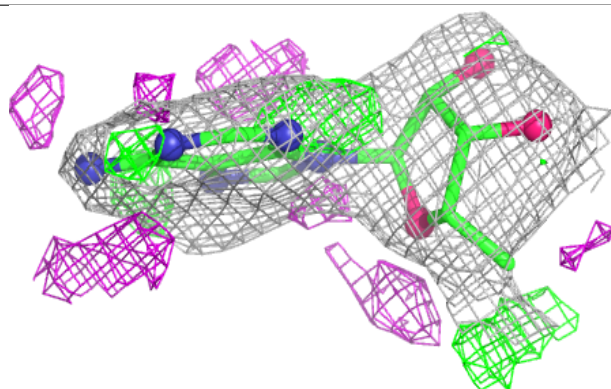
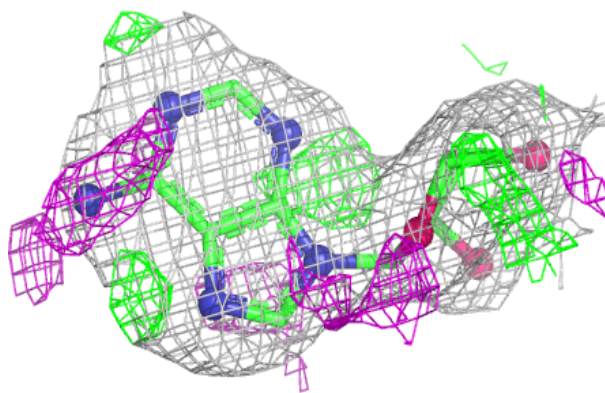
**Electron density around 5AD B 401:**

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

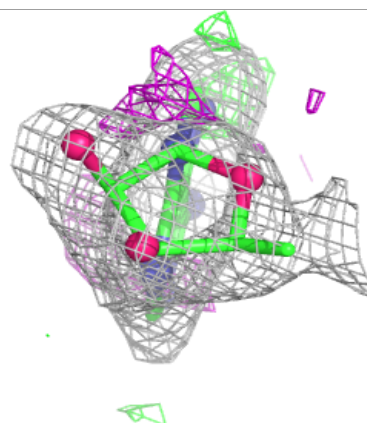
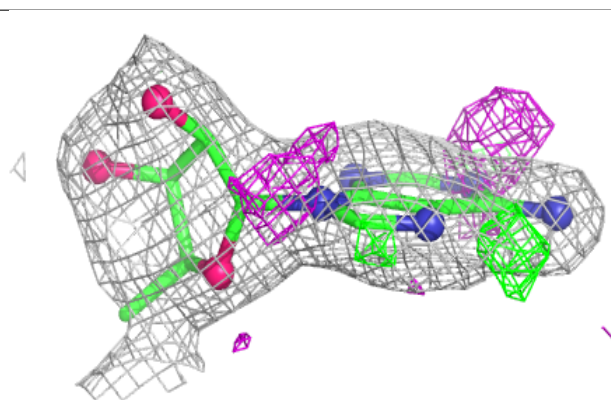
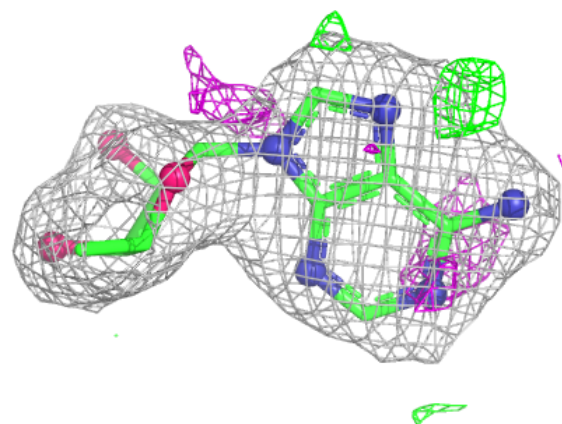


**Electron density around 5AD K 401:**

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

**Electron density around 5AD L 401:**

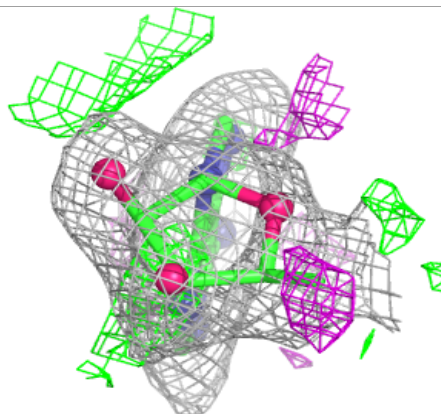
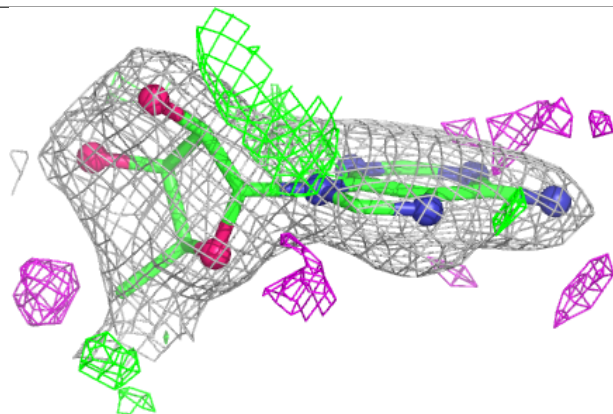
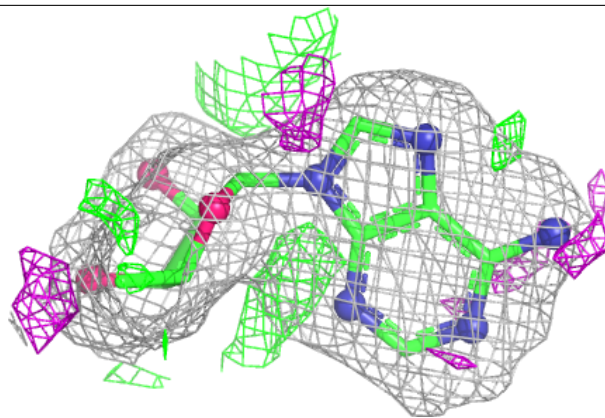
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





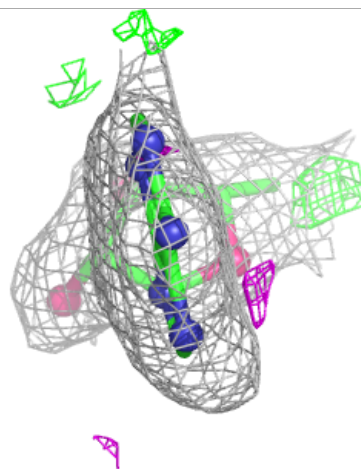
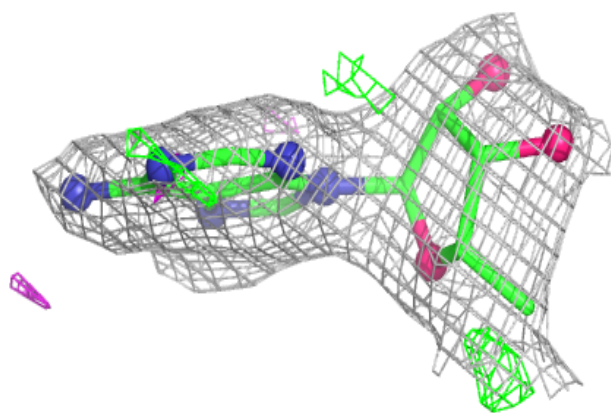
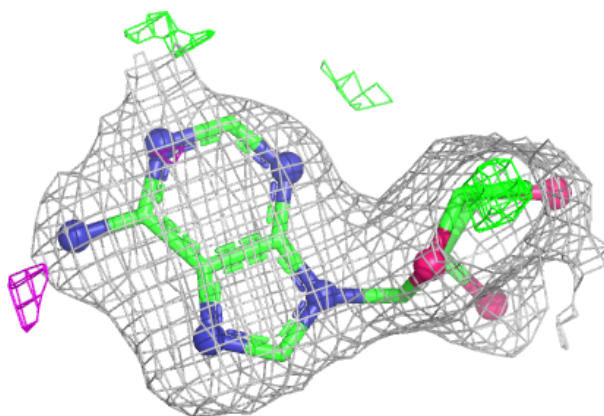
**Electron density around 5AD E 401:**

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



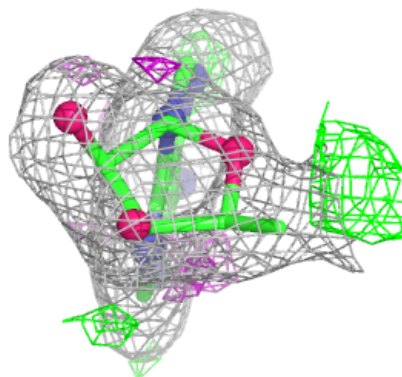
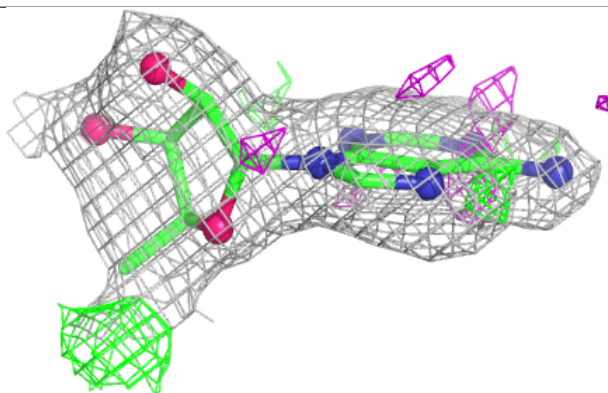
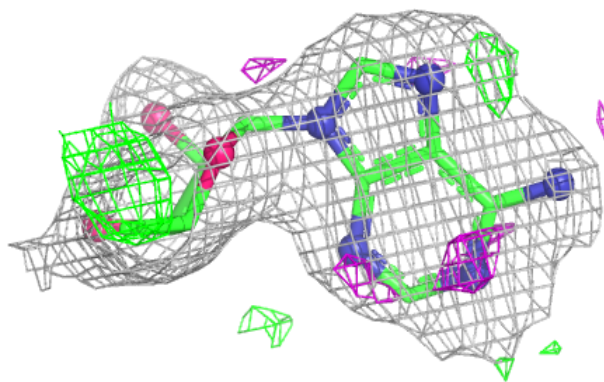
**Electron density around 5AD A 401:**

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



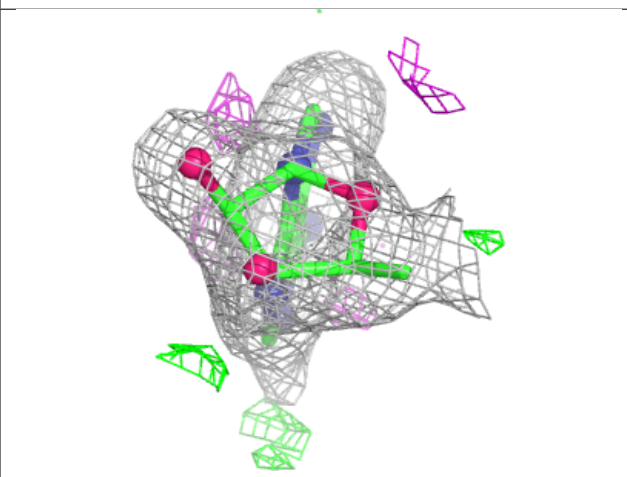
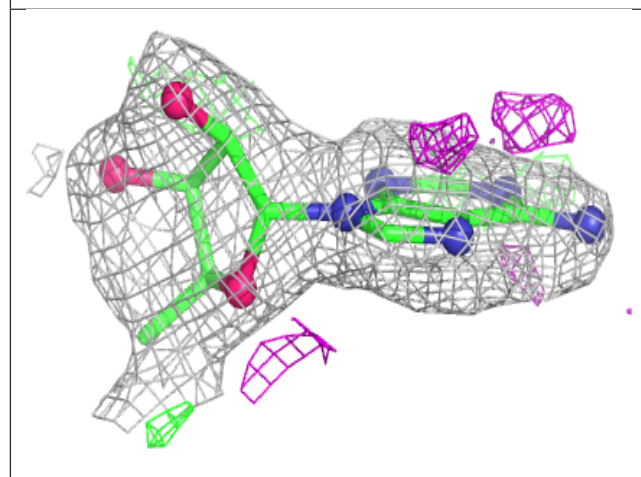
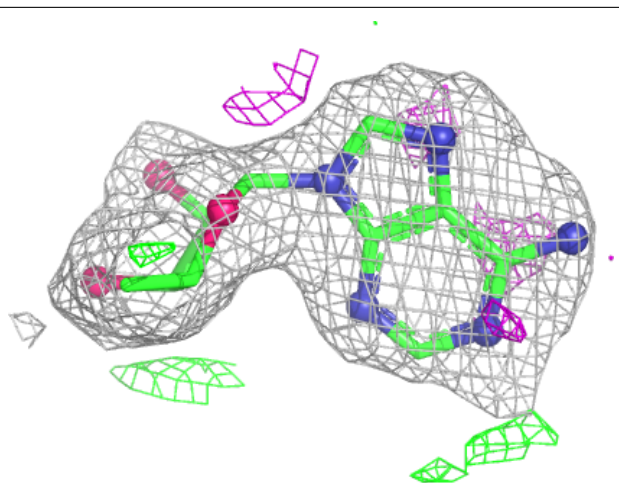
**Electron density around 5AD F 401:**

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



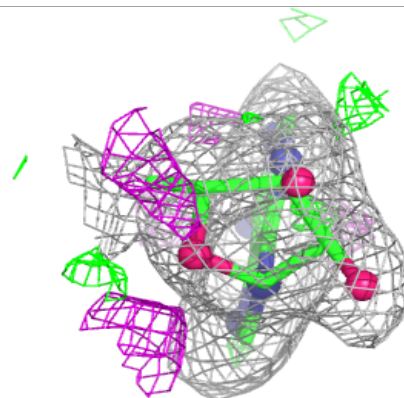
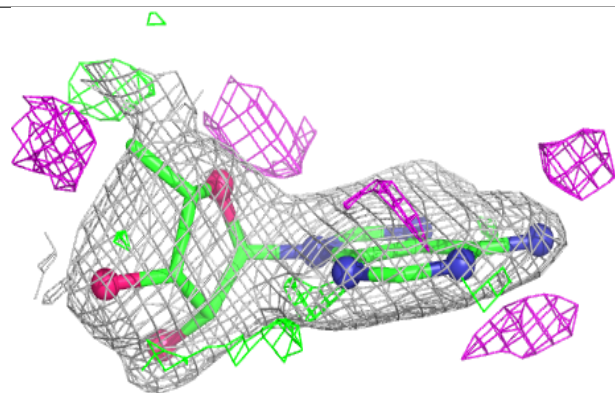
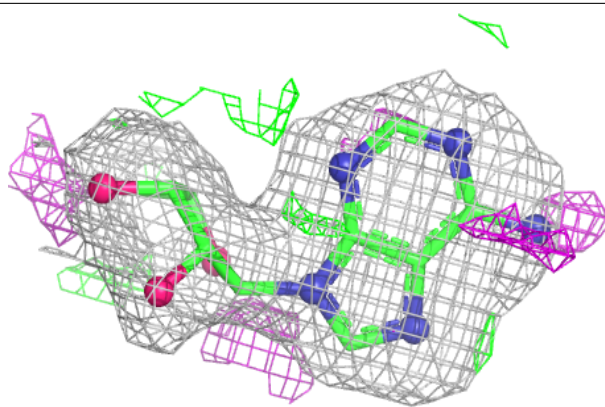
**Electron density around 5AD M 401:**

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



**Electron density around 5AD N 401:**

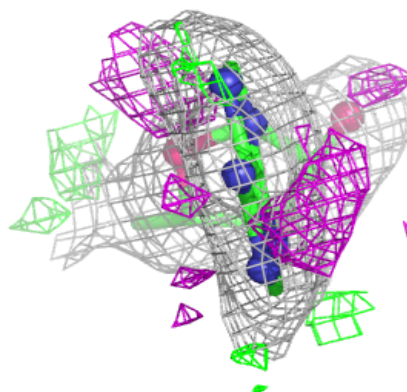
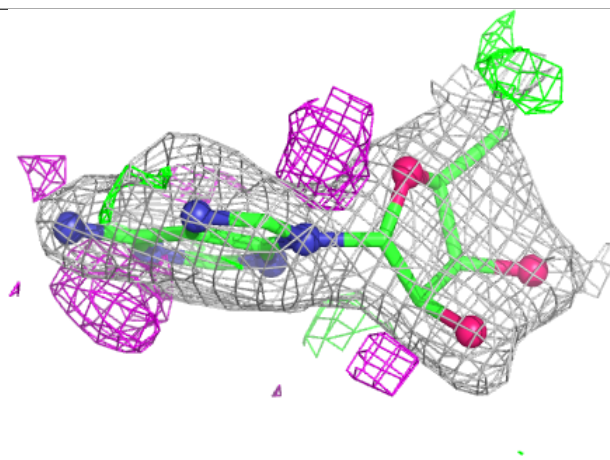
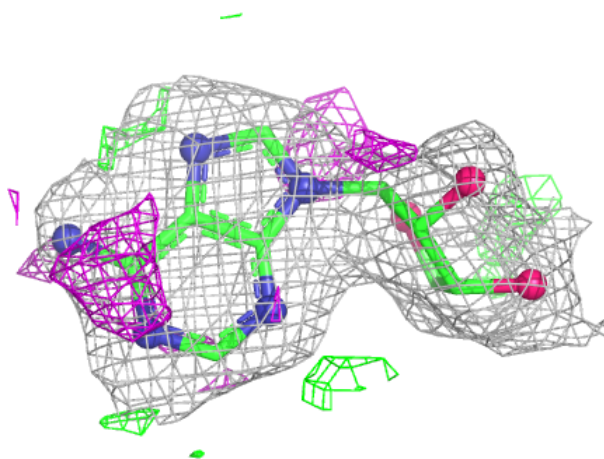
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)





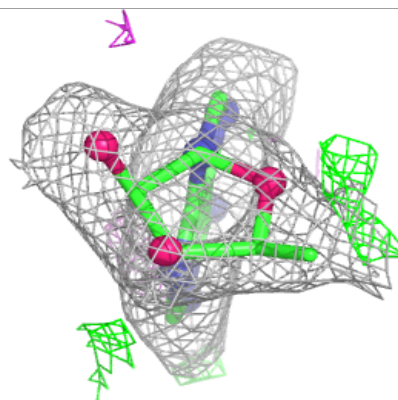
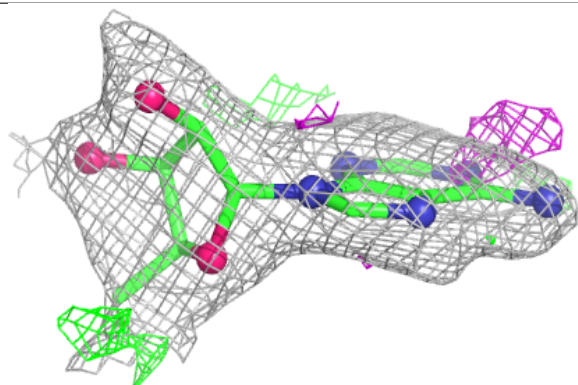
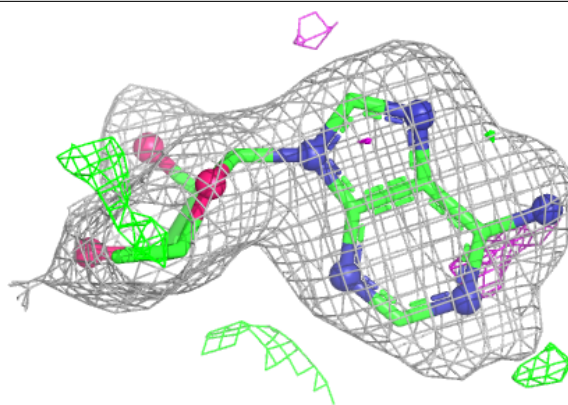
**Electron density around 5AD H 401:**

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

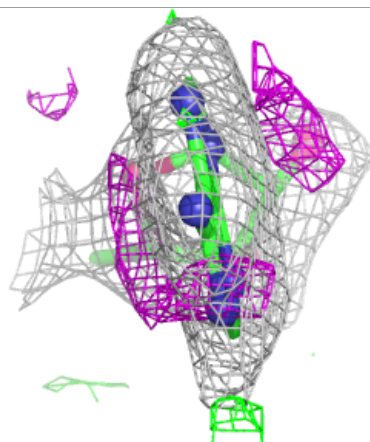
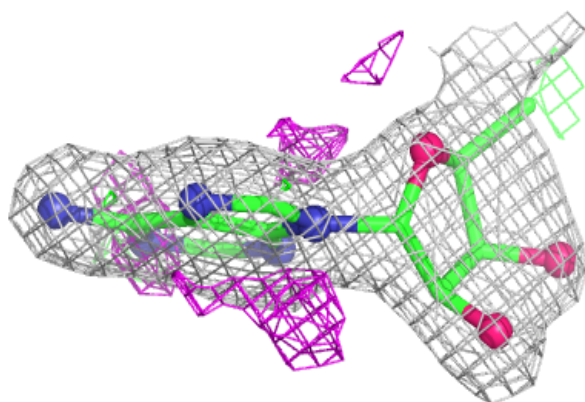
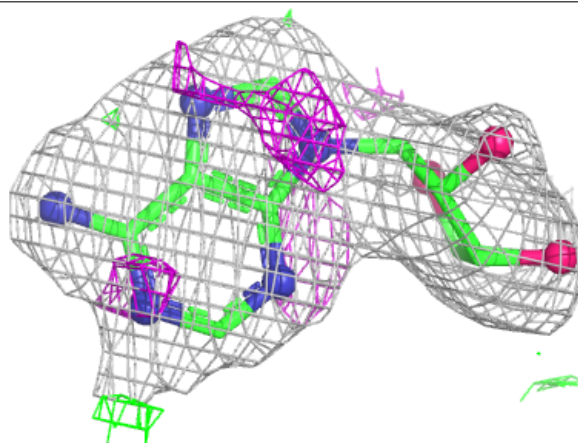


**Electron density around 5AD I 401:**

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

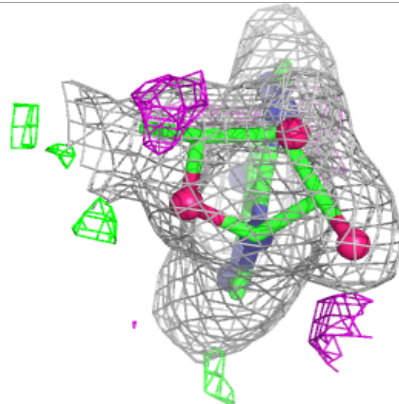
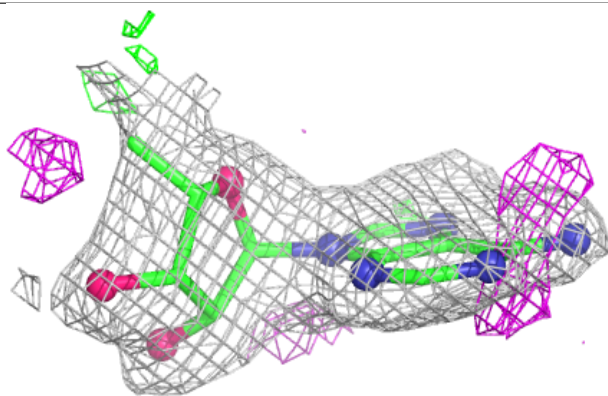
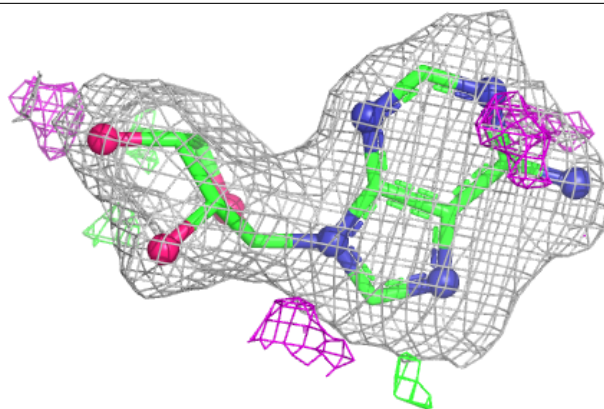
**Electron density around 5AD D 401:**

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

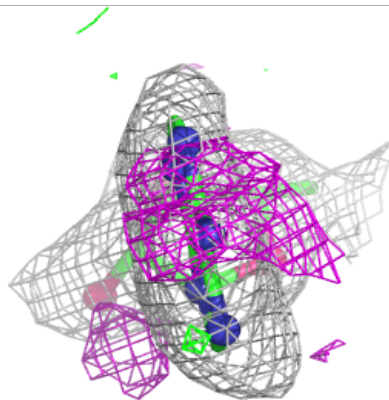
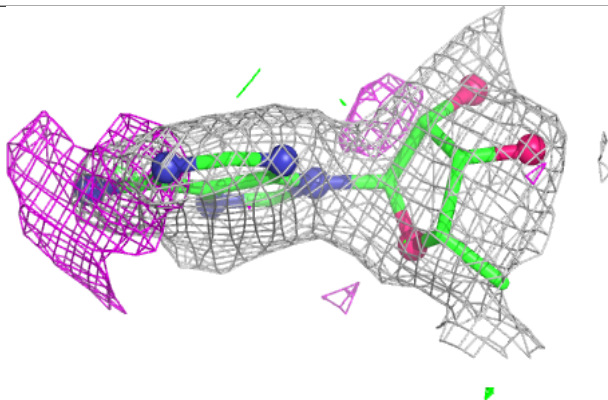
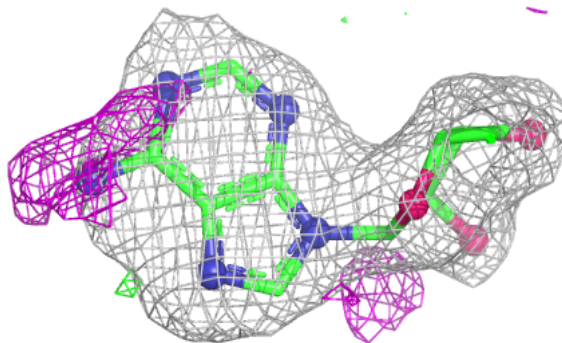


**Electron density around 5AD G 401:**

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

**Electron density around 5AD J 401:**

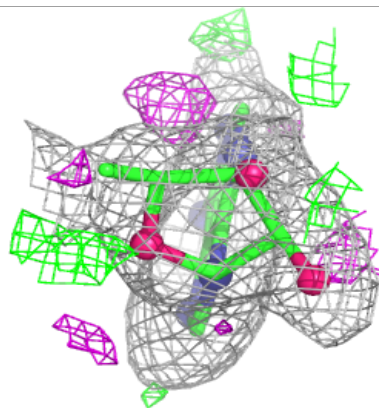
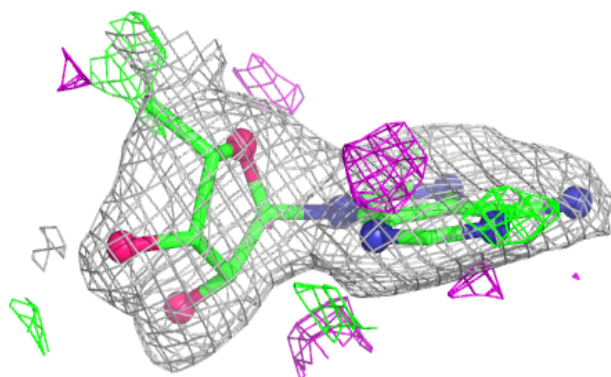
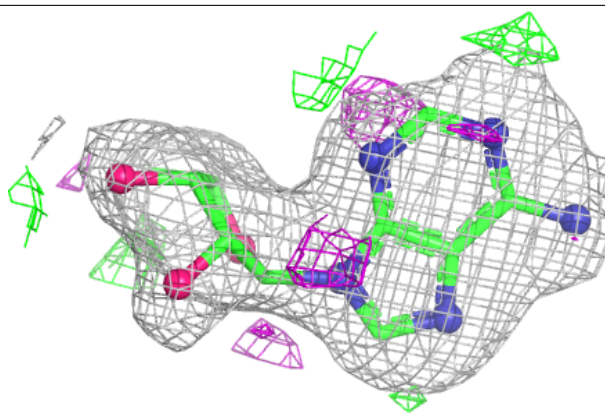
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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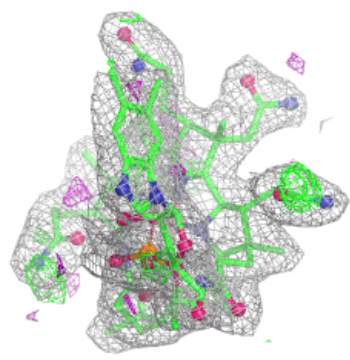
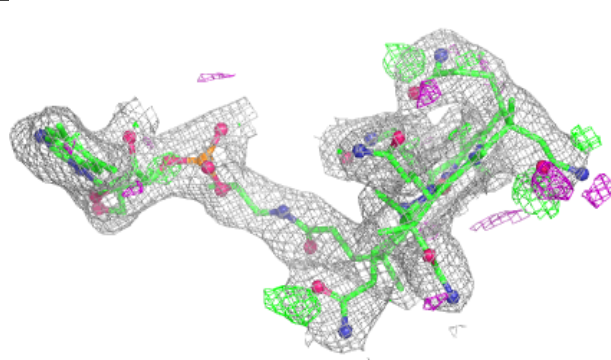
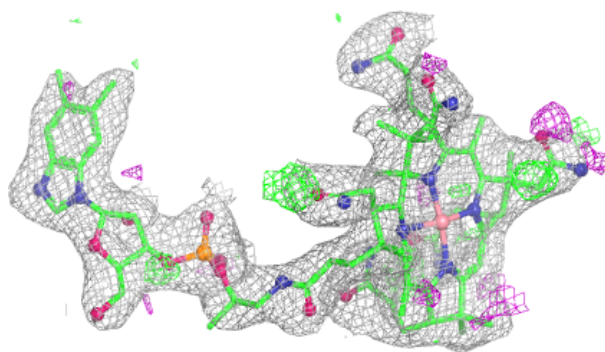


**Electron density around 5AD P 401:**

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

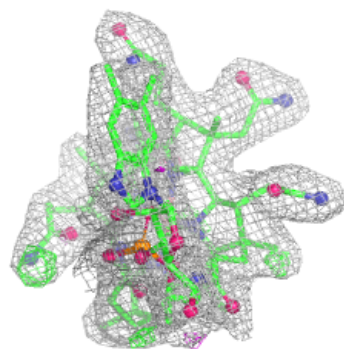
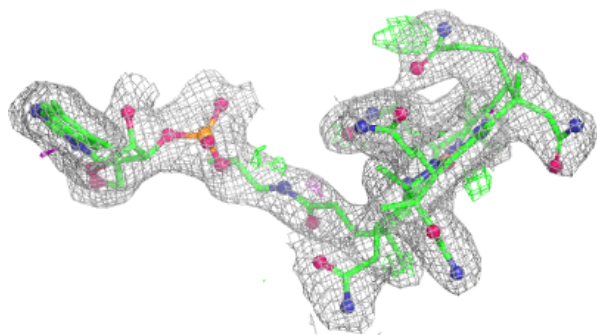
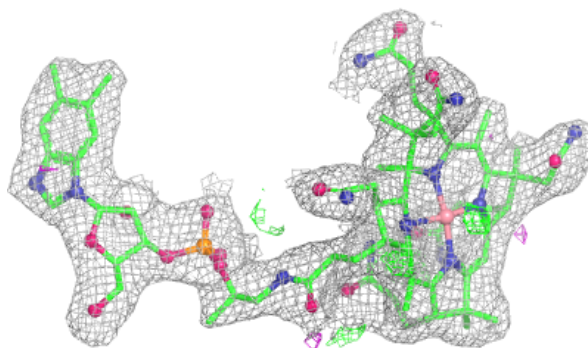
**Electron density around B12 C 301:**

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

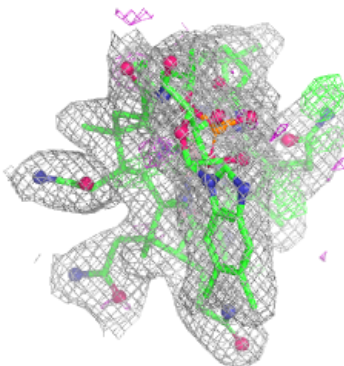
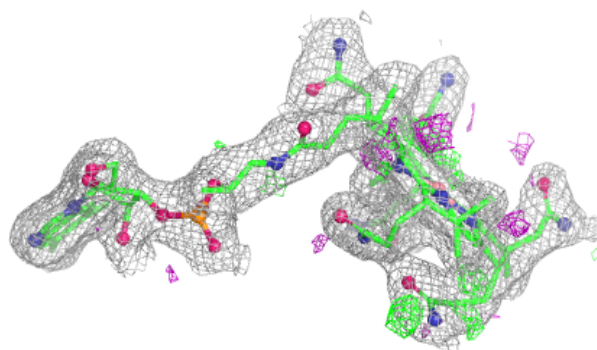
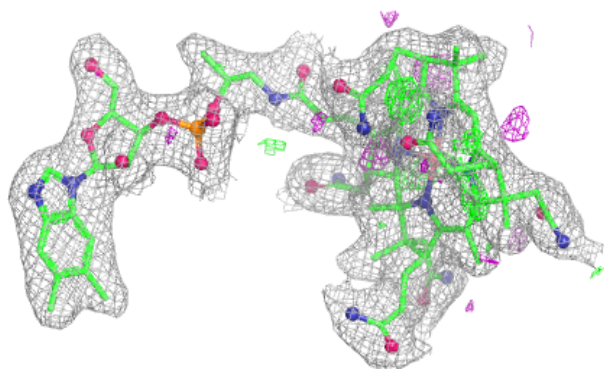


**Electron density around B12 B 301:**

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

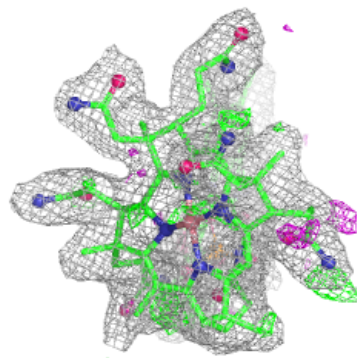
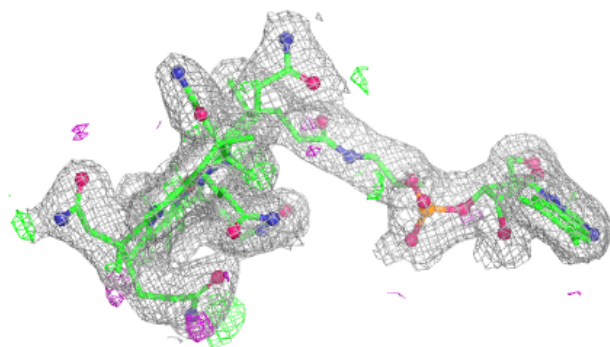
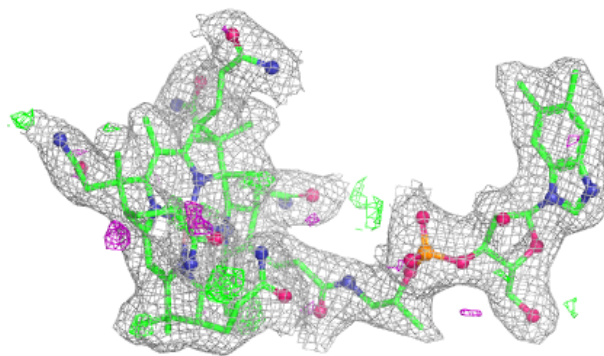
**Electron density around B12 G 301:**

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

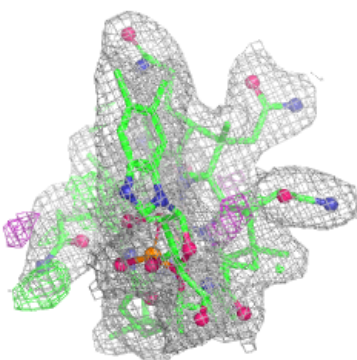
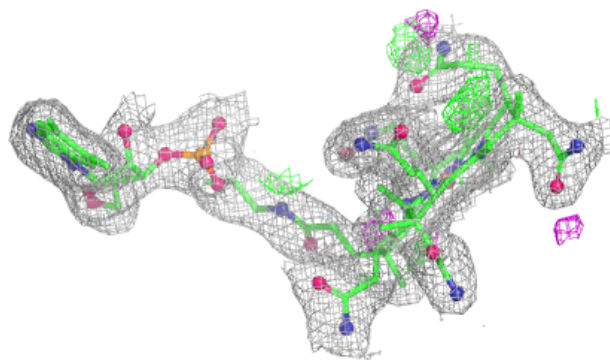
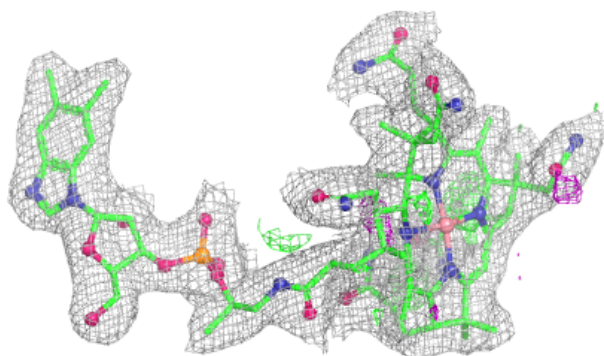


**Electron density around B12 H 301:**

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

**Electron density around B12 I 301:**

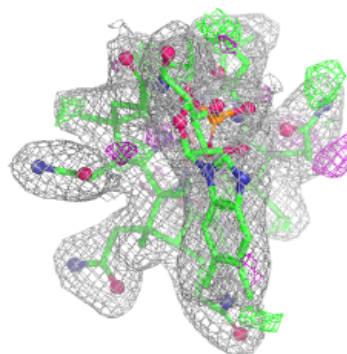
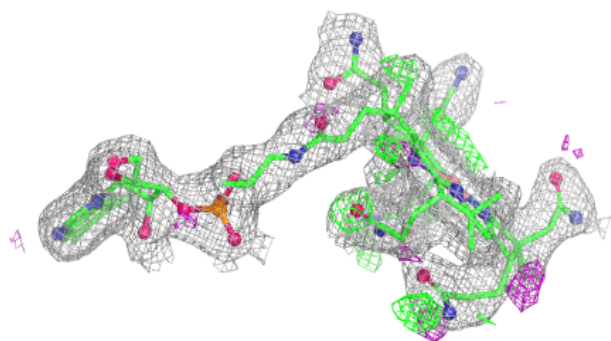
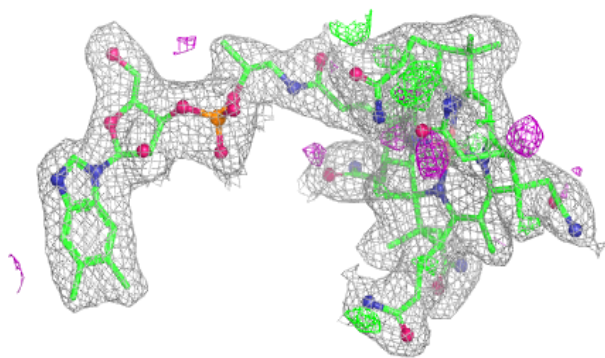
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



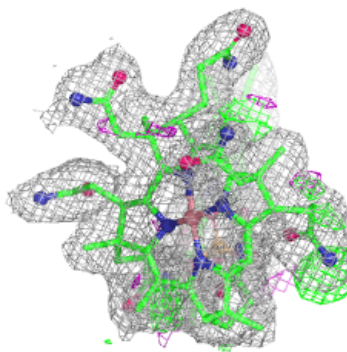
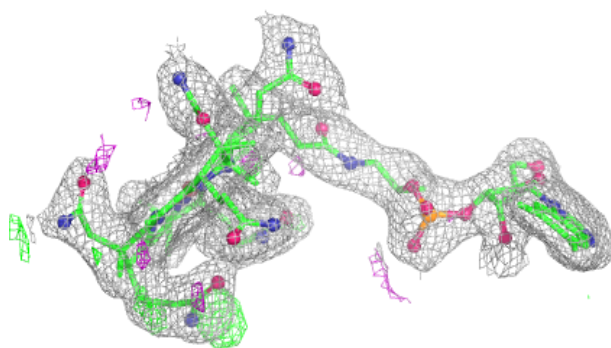
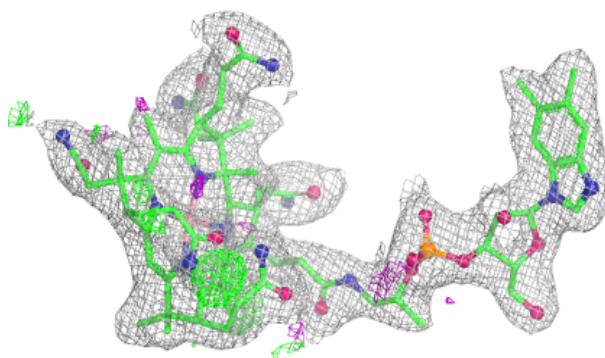


**Electron density around B12 J 301:**

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

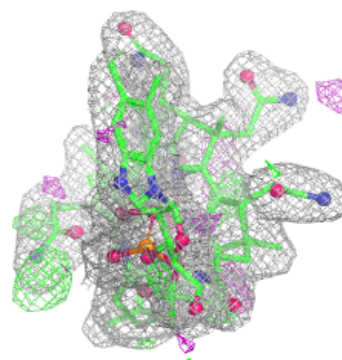
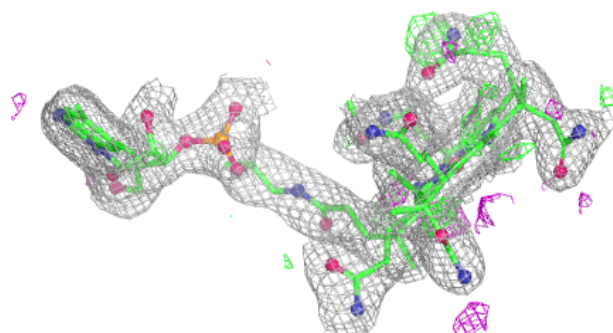
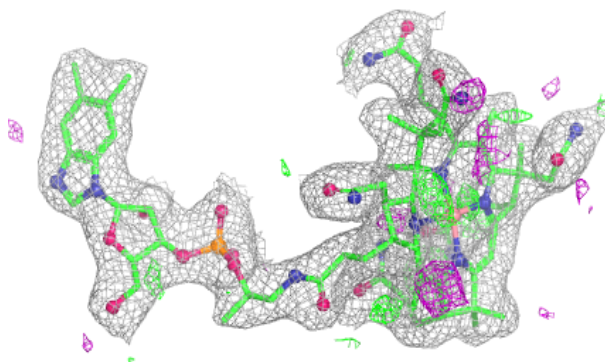
**Electron density around B12 K 301:**

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

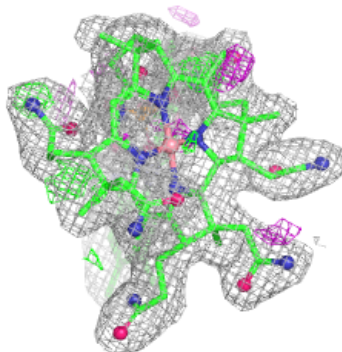
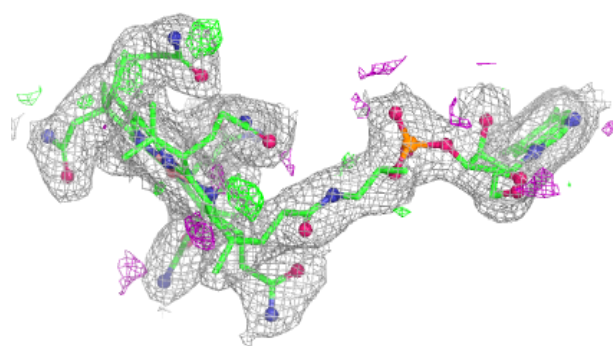
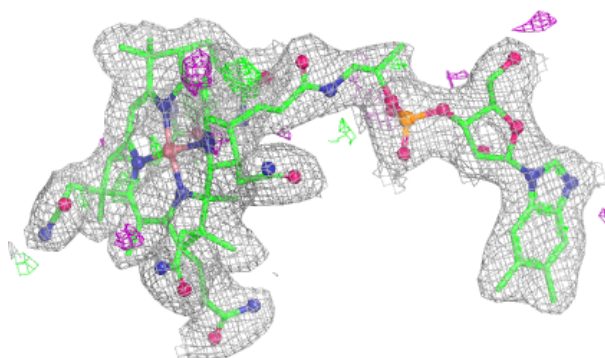


**Electron density around B12 M 301:**

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

**Electron density around B12 N 301:**

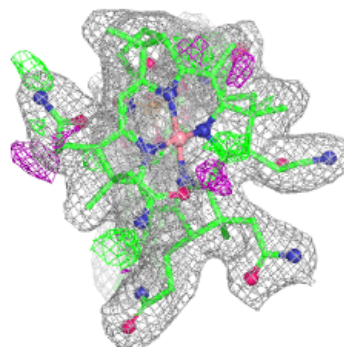
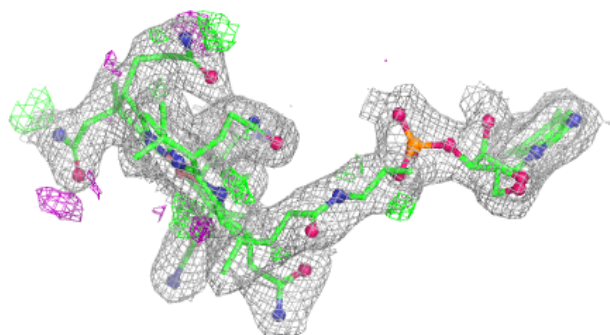
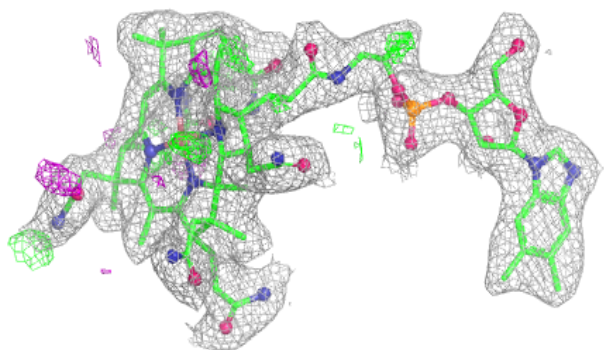
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



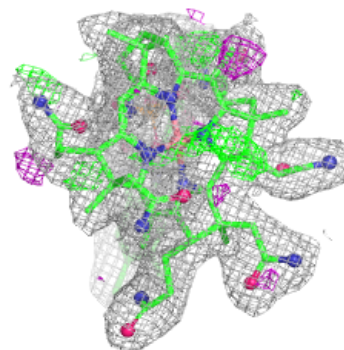
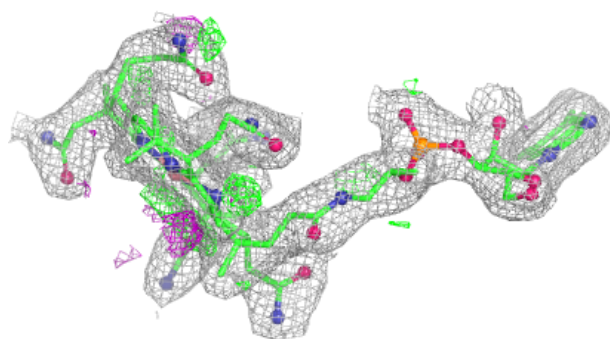
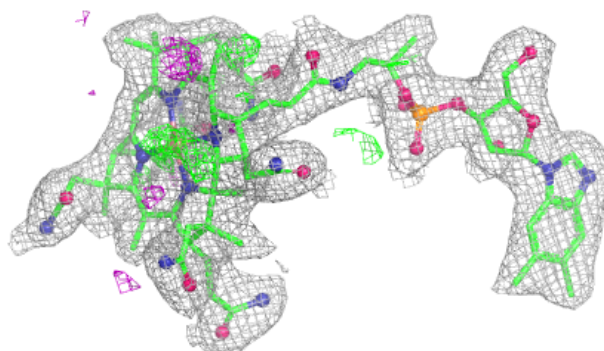


**Electron density around B12 O 301:**

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

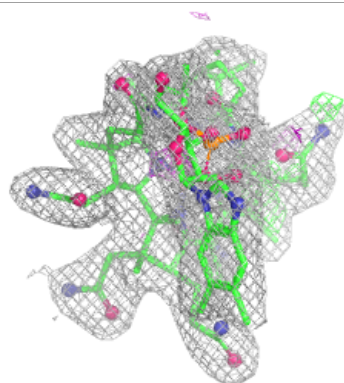
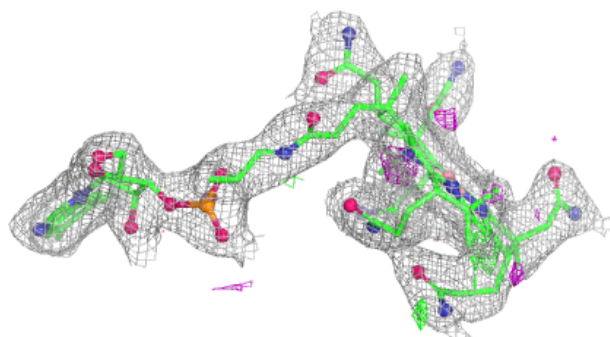
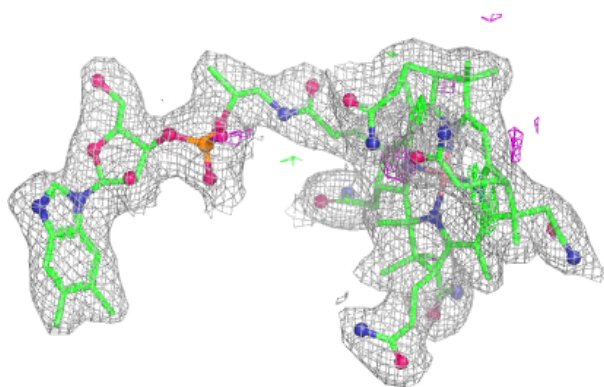
**Electron density around B12 P 301:**

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

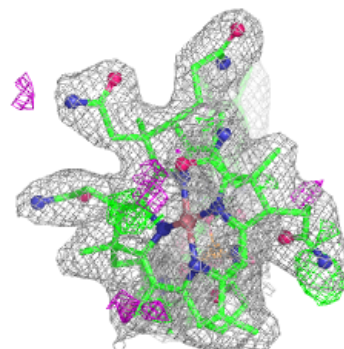
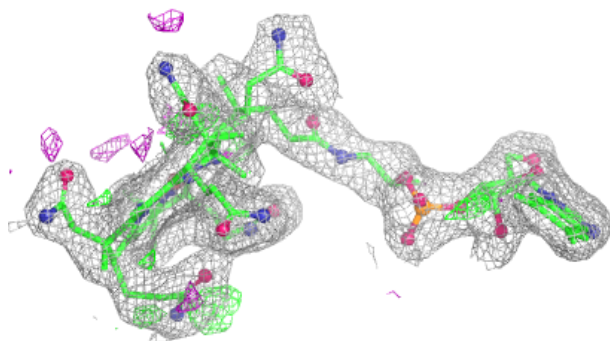
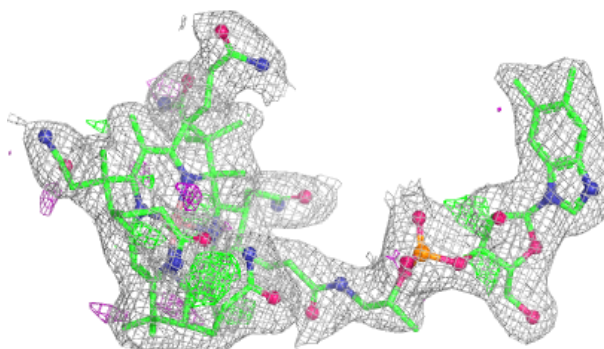


**Electron density around B12 A 301:**

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

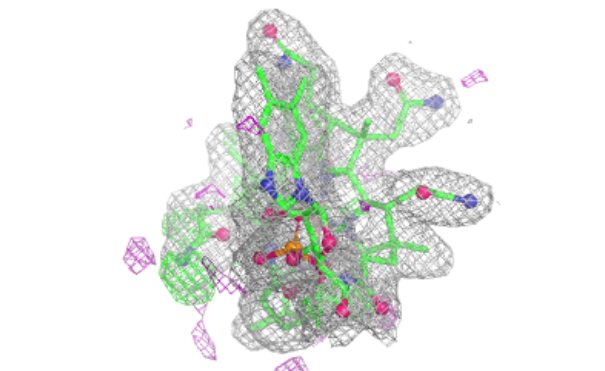
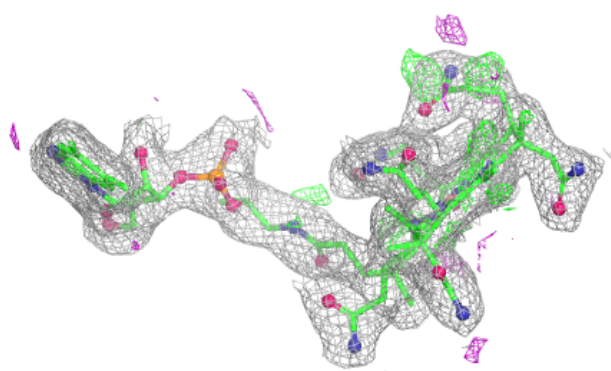
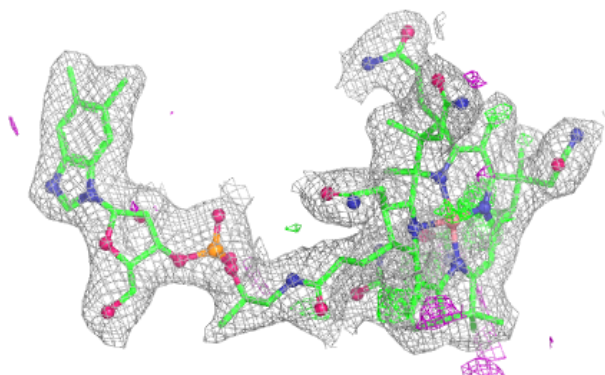
**Electron density around B12 D 301:**

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

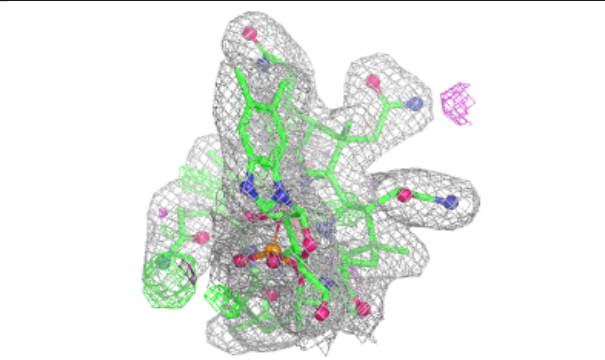
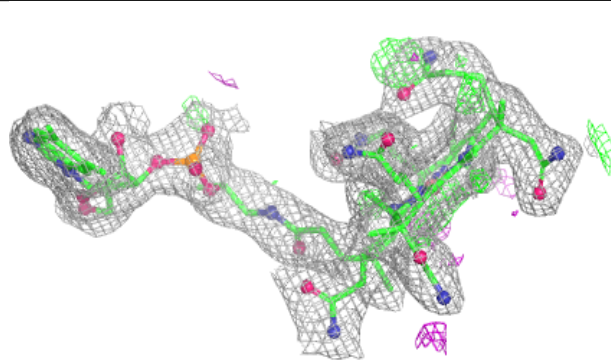
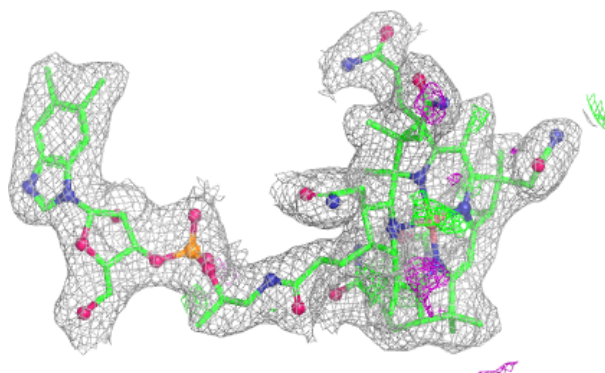


**Electron density around B12 F 301:**

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

**Electron density around B12 L 301:**

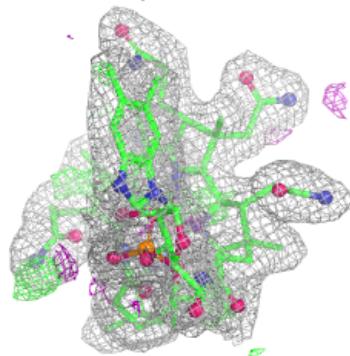
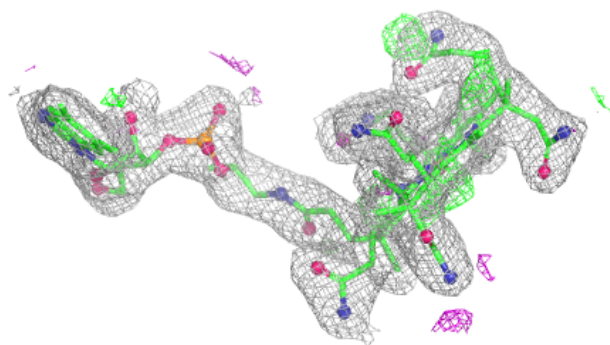
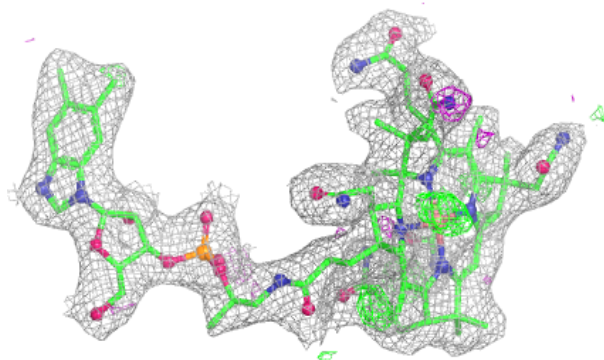
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around B12 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.