



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 04:02 am BST

PDB ID : 1GH0  
Title : CRYSTAL STRUCTURE OF C-PHYCOCYANIN FROM SPIRULINA PLATENSIS  
Authors : Liang, D.-C.; Chang, W.-R.; Wang, X.-Q.  
Deposited on : 2000-10-29  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

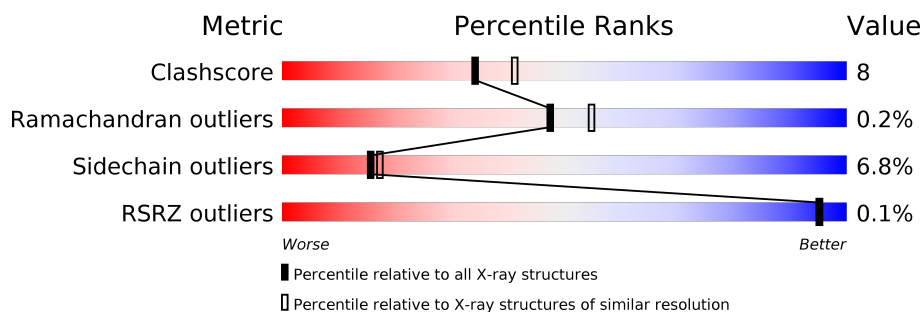
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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




















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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	162	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	162	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	E	162	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	G	162	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	I	162	<div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	K	162	<div> <div>86%</div> <div>14%</div> <div>.</div> </div>
1	M	162	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	162	 82% 16% .
1	Q	162	 75% 21% .
1	S	162	 79% 18% ..
1	U	162	 83% 17% .
1	W	162	 85% 13% .
2	B	172	 82% 17% .
2	D	172	 81% 17% .
2	F	172	 84% 14% .
2	H	172	 78% 20% .
2	J	172	 81% 17% .
2	L	172	 82% 17% .
2	N	172	 85% 14% .
2	P	172	 74% 22% .
2	R	172	 79% 17% .
2	T	172	 77% 20% .
2	V	172	 85% 14% .
2	X	172	 81% 18% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32493 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 C-PHYCOCYANIN ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	8	0	0
			1237	781	208	242	6			
1	C	162	Total	C	N	O	S	12	0	0
			1237	781	208	242	6			
1	E	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	G	162	Total	C	N	O	S	8	0	0
			1237	781	208	242	6			
1	I	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	K	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	M	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	O	162	Total	C	N	O	S	12	0	0
			1237	781	208	242	6			
1	Q	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	S	162	Total	C	N	O	S	8	0	0
			1237	781	208	242	6			
1	U	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			
1	W	162	Total	C	N	O	S	4	0	0
			1237	781	208	242	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ILE	see remark 999	UNP P72509
A	51	LEU	ARG	see remark 999	UNP P72509
A	148	VAL	GLY	see remark 999	UNP P72509
C	11	VAL	ILE	see remark 999	UNP P72509
C	51	LEU	ARG	see remark 999	UNP P72509

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Chain	Residue	Modelled	Actual	Comment	Reference
C	148	VAL	GLY	see remark 999	UNP P72509
E	11	VAL	ILE	see remark 999	UNP P72509
E	51	LEU	ARG	see remark 999	UNP P72509
E	148	VAL	GLY	see remark 999	UNP P72509
G	11	VAL	ILE	see remark 999	UNP P72509
G	51	LEU	ARG	see remark 999	UNP P72509
G	148	VAL	GLY	see remark 999	UNP P72509
I	11	VAL	ILE	see remark 999	UNP P72509
I	51	LEU	ARG	see remark 999	UNP P72509
I	148	VAL	GLY	see remark 999	UNP P72509
K	11	VAL	ILE	see remark 999	UNP P72509
K	51	LEU	ARG	see remark 999	UNP P72509
K	148	VAL	GLY	see remark 999	UNP P72509
M	11	VAL	ILE	see remark 999	UNP P72509
M	51	LEU	ARG	see remark 999	UNP P72509
M	148	VAL	GLY	see remark 999	UNP P72509
O	11	VAL	ILE	see remark 999	UNP P72509
O	51	LEU	ARG	see remark 999	UNP P72509
O	148	VAL	GLY	see remark 999	UNP P72509
Q	11	VAL	ILE	see remark 999	UNP P72509
Q	51	LEU	ARG	see remark 999	UNP P72509
Q	148	VAL	GLY	see remark 999	UNP P72509
S	11	VAL	ILE	see remark 999	UNP P72509
S	51	LEU	ARG	see remark 999	UNP P72509
S	148	VAL	GLY	see remark 999	UNP P72509
U	11	VAL	ILE	see remark 999	UNP P72509
U	51	LEU	ARG	see remark 999	UNP P72509
U	148	VAL	GLY	see remark 999	UNP P72509
W	11	VAL	ILE	see remark 999	UNP P72509
W	51	LEU	ARG	see remark 999	UNP P72509
W	148	VAL	GLY	see remark 999	UNP P72509

- Molecule 2 is a protein called C-PHYCOCYANIN BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1263	782	221	251	9			
2	D	172	Total	C	N	O	S	0	0	0
			1263	782	221	251	9			
2	F	172	Total	C	N	O	S	4	0	0
			1263	782	221	251	9			
2	H	172	Total	C	N	O	S	4	0	0
			1263	782	221	251	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	172	Total 1263	C 782	N 221	O 251	S 9	0	0	0
2	L	172	Total 1263	C 782	N 221	O 251	S 9	0	0	0
2	N	172	Total 1263	C 782	N 221	O 251	S 9	0	0	0
2	P	172	Total 1263	C 782	N 221	O 251	S 9	0	0	0
2	R	172	Total 1263	C 782	N 221	O 251	S 9	4	0	0
2	T	172	Total 1263	C 782	N 221	O 251	S 9	4	0	0
2	V	172	Total 1263	C 782	N 221	O 251	S 9	4	0	0
2	X	172	Total 1263	C 782	N 221	O 251	S 9	4	0	0

There are 60 discrepancies between the modelled and reference sequences:

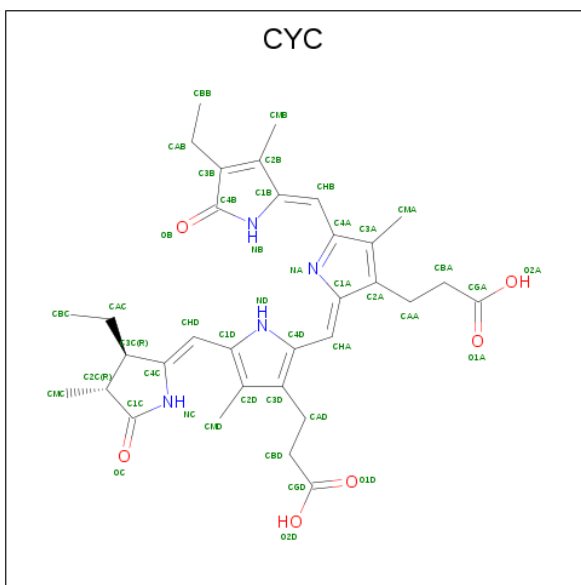
Chain	Residue	Modelled	Actual	Comment	Reference
B	40	VAL	ALA	see remark 999	UNP P72508
B	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
B	76	SER	ASN	see remark 999	UNP P72508
B	162	GLY	SER	see remark 999	UNP P72508
B	168	ALA	CYS	see remark 999	UNP P72508
D	40	VAL	ALA	see remark 999	UNP P72508
D	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
D	76	SER	ASN	see remark 999	UNP P72508
D	162	GLY	SER	see remark 999	UNP P72508
D	168	ALA	CYS	see remark 999	UNP P72508
F	40	VAL	ALA	see remark 999	UNP P72508
F	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
F	76	SER	ASN	see remark 999	UNP P72508
F	162	GLY	SER	see remark 999	UNP P72508
F	168	ALA	CYS	see remark 999	UNP P72508
H	40	VAL	ALA	see remark 999	UNP P72508
H	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
H	76	SER	ASN	see remark 999	UNP P72508
H	162	GLY	SER	see remark 999	UNP P72508
H	168	ALA	CYS	see remark 999	UNP P72508
J	40	VAL	ALA	see remark 999	UNP P72508
J	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
J	76	SER	ASN	see remark 999	UNP P72508

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Chain	Residue	Modelled	Actual	Comment	Reference
J	162	GLY	SER	see remark 999	UNP P72508
J	168	ALA	CYS	see remark 999	UNP P72508
L	40	VAL	ALA	see remark 999	UNP P72508
L	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
L	76	SER	ASN	see remark 999	UNP P72508
L	162	GLY	SER	see remark 999	UNP P72508
L	168	ALA	CYS	see remark 999	UNP P72508
N	40	VAL	ALA	see remark 999	UNP P72508
N	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
N	76	SER	ASN	see remark 999	UNP P72508
N	162	GLY	SER	see remark 999	UNP P72508
N	168	ALA	CYS	see remark 999	UNP P72508
P	40	VAL	ALA	see remark 999	UNP P72508
P	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
P	76	SER	ASN	see remark 999	UNP P72508
P	162	GLY	SER	see remark 999	UNP P72508
P	168	ALA	CYS	see remark 999	UNP P72508
R	40	VAL	ALA	see remark 999	UNP P72508
R	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
R	76	SER	ASN	see remark 999	UNP P72508
R	162	GLY	SER	see remark 999	UNP P72508
R	168	ALA	CYS	see remark 999	UNP P72508
T	40	VAL	ALA	see remark 999	UNP P72508
T	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
T	76	SER	ASN	see remark 999	UNP P72508
T	162	GLY	SER	see remark 999	UNP P72508
T	168	ALA	CYS	see remark 999	UNP P72508
V	40	VAL	ALA	see remark 999	UNP P72508
V	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
V	76	SER	ASN	see remark 999	UNP P72508
V	162	GLY	SER	see remark 999	UNP P72508
V	168	ALA	CYS	see remark 999	UNP P72508
X	40	VAL	ALA	see remark 999	UNP P72508
X	72	MEN	ASN	MODIFIED RESIDUE	UNP P72508
X	76	SER	ASN	see remark 999	UNP P72508
X	162	GLY	SER	see remark 999	UNP P72508
X	168	ALA	CYS	see remark 999	UNP P72508

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	C	1	Total 43	C 33	N 4	O 6	0	0
3	D	1	Total 43	C 33	N 4	O 6	0	0
3	D	1	Total 43	C 33	N 4	O 6	0	0
3	E	1	Total 43	C 33	N 4	O 6	0	0
3	F	1	Total 43	C 33	N 4	O 6	0	0
3	F	1	Total 43	C 33	N 4	O 6	0	0
3	G	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0
3	V	1	Total 43	C 33	N 4	O 6	0	0
3	V	1	Total 43	C 33	N 4	O 6	0	0
3	W	1	Total 43	C 33	N 4	O 6	0	0
3	X	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	36	Total	O			0	0
			36	36				
4	B	60	Total	O			0	0
			60	60				
4	C	39	Total	O			0	0
			39	39				
4	D	47	Total	O			0	0
			47	47				
4	E	53	Total	O			0	0
			53	53				
4	F	29	Total	O			0	0
			29	29				
4	G	40	Total	O			0	0
			40	40				
4	H	41	Total	O			0	0
			41	41				
4	I	39	Total	O			0	0
			39	39				
4	J	26	Total	O			0	0
			26	26				
4	K	57	Total	O			0	0
			57	57				
4	L	32	Total	O			0	0
			32	32				
4	M	31	Total	O			0	0
			31	31				
4	N	42	Total	O			0	0
			42	42				
4	O	35	Total	O			0	0
			35	35				
4	P	30	Total	O			0	0
			30	30				
4	Q	40	Total	O			0	0
			40	40				
4	R	39	Total	O			0	0
			39	39				

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	45	Total 45	O 45	0	0
4	T	29	Total 29	O 29	0	0
4	U	33	Total 33	O 33	0	0
4	V	48	Total 48	O 48	0	0
4	W	49	Total 49	O 49	0	0
4	X	25	Total 25	O 25	0	0

### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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: C-PHYCOCYANIN ALPHA SUBUNIT

Chain A: 




- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain C: 




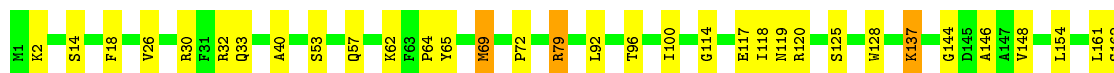
- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain E: 




- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain G: 




- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain I: 



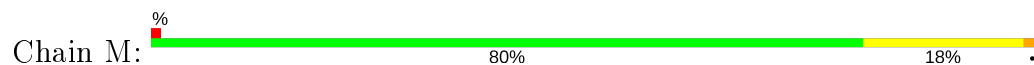
- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain K: 

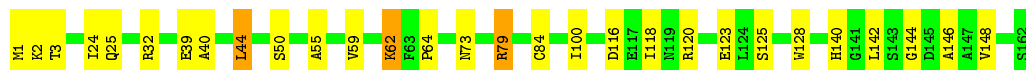
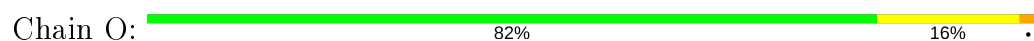




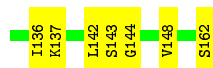
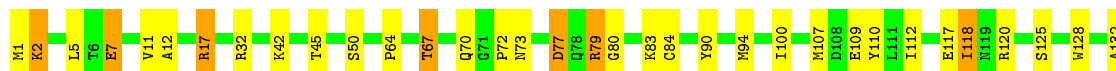
● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



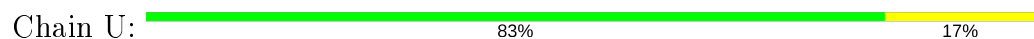
● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



● Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT





• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain B: 82% 17%



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain D: 81% 17%



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain F: 84% 14%



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain H: 78% 20%



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain J: 81% 17%




• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain L: 82% 17%




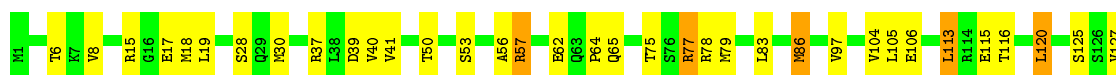
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain N:  85% 14%




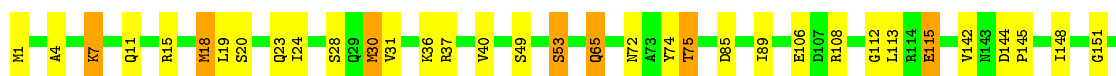
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain P:  74% 22%




• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain R:  79% 17%




• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain T:  77% 20%




• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain V:  85% 14%



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain X:  81% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.00Å 117.50Å 185.00Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.20) 90.9 (19.98-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.189 , 0.237 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MEN

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	0.35	0/1260	0.52	0/1703
1	C	0.34	0/1260	0.52	0/1703
1	E	0.36	0/1260	0.52	0/1703
1	G	0.38	0/1260	0.54	0/1703
1	I	0.36	0/1260	0.50	0/1703
1	K	0.43	0/1260	0.68	3/1703 (0.2%)
1	M	0.35	0/1260	0.52	0/1703
1	O	0.33	0/1260	0.51	0/1703
1	Q	0.36	0/1260	0.56	0/1703
1	S	0.35	0/1260	0.54	0/1703
1	U	0.34	0/1260	0.52	0/1703
1	W	0.35	0/1260	0.52	0/1703
2	B	0.36	0/1267	0.58	1/1714 (0.1%)
2	D	0.35	0/1267	0.54	0/1714
2	F	0.34	0/1267	0.56	0/1714
2	H	0.36	0/1267	0.63	2/1714 (0.1%)
2	J	0.34	0/1267	0.56	0/1714
2	L	0.35	0/1267	0.56	0/1714
2	N	0.34	0/1267	0.57	0/1714
2	P	0.34	0/1267	0.54	0/1714
2	R	0.33	0/1267	0.55	0/1714
2	T	0.34	0/1267	0.55	0/1714
2	V	0.34	0/1267	0.56	0/1714
2	X	0.35	0/1267	0.54	0/1714
All	All	0.35	0/30324	0.55	6/41004 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	79	ARG	NE-CZ-NH1	-14.14	113.23	120.30
2	H	25	ASP	CB-CG-OD2	9.61	126.94	118.30
1	K	79	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	K	79	ARG	CD-NE-CZ	-6.66	114.27	123.60
2	H	25	ASP	CB-CG-OD1	-5.79	113.09	118.30

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	1237	0	1216	18	0
1	C	1237	0	1216	30	0
1	E	1237	0	1216	12	0
1	G	1237	0	1216	17	0
1	I	1237	0	1216	25	0
1	K	1237	0	1216	19	0
1	M	1237	0	1216	19	0
1	O	1237	0	1216	19	0
1	Q	1237	0	1216	33	0
1	S	1237	0	1216	23	0
1	U	1237	0	1216	13	0
1	W	1237	0	1216	20	0
2	B	1263	0	1265	20	0
2	D	1263	0	1265	28	0
2	F	1263	0	1265	21	0
2	H	1263	0	1265	24	0
2	J	1263	0	1265	23	0
2	L	1263	0	1265	24	0
2	N	1263	0	1265	16	0
2	P	1263	0	1265	30	0
2	R	1263	0	1265	28	0
2	T	1263	0	1265	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	1263	0	1265	18	0
2	X	1263	0	1265	15	0
3	A	43	0	37	2	0
3	B	86	0	74	3	0
3	C	43	0	37	2	0
3	D	86	0	73	6	0
3	E	43	0	37	2	0
3	F	86	0	74	8	0
3	G	43	0	37	1	0
3	H	86	0	74	6	0
3	I	43	0	37	1	0
3	J	86	0	74	3	0
3	K	43	0	37	2	0
3	L	86	0	74	5	0
3	M	43	0	37	3	0
3	N	86	0	74	5	0
3	O	43	0	37	3	0
3	P	86	0	74	5	0
3	Q	43	0	37	4	0
3	R	86	0	74	6	0
3	S	43	0	37	2	0
3	T	86	0	73	10	0
3	U	43	0	37	1	0
3	V	86	0	73	5	0
3	W	43	0	37	3	0
3	X	86	0	74	5	0
4	A	36	0	0	1	0
4	B	60	0	0	2	0
4	C	39	0	0	4	0
4	D	47	0	0	0	0
4	E	53	0	0	1	0
4	F	29	0	0	3	0
4	G	40	0	0	0	0
4	H	41	0	0	0	0
4	I	39	0	0	1	0
4	J	26	0	0	0	0
4	K	57	0	0	2	0
4	L	32	0	0	0	0
4	M	31	0	0	1	0
4	N	42	0	0	0	0
4	O	35	0	0	0	0
4	P	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	40	0	0	1	0
4	R	39	0	0	1	0
4	S	45	0	0	0	0
4	T	29	0	0	3	0
4	U	33	0	0	0	0
4	V	48	0	0	1	0
4	W	49	0	0	1	0
4	X	25	0	0	3	0
All	All	32493	0	31101	525	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 8.

The worst 5 of 525 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:K:73:ASN:H	1:K:73:ASN:HD22	1.04	1.00
2:L:20:SER:H	2:L:23:GLN:HE21	1.10	0.99
2:T:20:SER:H	2:T:23:GLN:HE21	1.09	0.98
1:Q:100:ILE:HD13	2:R:19:LEU:HD22	1.43	0.97
1:S:73:ASN:H	1:S:73:ASN:HD22	1.08	0.94

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	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	C	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	E	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	I	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	K	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	25	26
1	M	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	O	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	Q	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	S	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25	26
1	U	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	W	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
2	B	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	D	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	F	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	H	169/172 (98%)	166 (98%)	2 (1%)	1 (1%)	25	26
2	J	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	L	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	N	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	P	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	26
2	R	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	T	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	V	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	3948/4008 (98%)	3856 (98%)	83 (2%)	9 (0%)	47	55

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	2	LYS
2	L	75	THR
2	R	75	THR
1	S	2	LYS
1	E	2	LYS

### 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	125/125 (100%)	119 (95%)	6 (5%)	25	32
1	C	125/125 (100%)	115 (92%)	10 (8%)	12	12
1	E	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	G	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	I	125/125 (100%)	119 (95%)	6 (5%)	25	32
1	K	125/125 (100%)	120 (96%)	5 (4%)	31	40
1	M	125/125 (100%)	115 (92%)	10 (8%)	12	12
1	O	125/125 (100%)	114 (91%)	11 (9%)	10	10
1	Q	125/125 (100%)	110 (88%)	15 (12%)	5	4
1	S	125/125 (100%)	113 (90%)	12 (10%)	8	8
1	U	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	W	125/125 (100%)	118 (94%)	7 (6%)	21	25
2	B	130/130 (100%)	124 (95%)	6 (5%)	27	34
2	D	130/130 (100%)	125 (96%)	5 (4%)	33	42
2	F	130/130 (100%)	122 (94%)	8 (6%)	18	21
2	H	130/130 (100%)	125 (96%)	5 (4%)	33	42
2	J	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	L	130/130 (100%)	121 (93%)	9 (7%)	15	16
2	N	130/130 (100%)	124 (95%)	6 (5%)	27	34
2	P	130/130 (100%)	116 (89%)	14 (11%)	6	6
2	R	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	T	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	V	130/130 (100%)	123 (95%)	7 (5%)	22	26
2	X	130/130 (100%)	118 (91%)	12 (9%)	9	9
All	All	3060/3060 (100%)	2852 (93%)	208 (7%)	16	17

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	118	ILE
2	P	50	THR
1	W	53	SER
2	N	18	MET
1	O	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	35	ASN
2	N	35	ASN
2	X	35	ASN
2	L	47	ASN
2	L	54	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	MEN	R	72	2	7,8,9	0.77	0	6,9,11	0.56	0
2	MEN	X	72	2	7,8,9	0.87	0	6,9,11	0.48	0
2	MEN	T	72	2	7,8,9	0.93	1 (14%)	6,9,11	0.54	0
2	MEN	J	72	2	7,8,9	0.86	0	6,9,11	0.60	0
2	MEN	P	72	2	7,8,9	0.90	1 (14%)	6,9,11	0.45	0
2	MEN	V	72	2	7,8,9	0.88	0	6,9,11	0.60	0
2	MEN	L	72	2	7,8,9	0.86	0	6,9,11	0.53	0
2	MEN	B	72	2	7,8,9	0.74	0	6,9,11	0.52	0
2	MEN	H	72	2	7,8,9	0.89	1 (14%)	6,9,11	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MEN	N	72	2	7,8,9	0.82	0	6,9,11	0.55	0
2	MEN	D	72	2	7,8,9	0.79	0	6,9,11	0.57	0
2	MEN	F	72	2	7,8,9	0.84	0	6,9,11	0.53	0

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
2	MEN	R	72	2	-	3/7/8/10	-
2	MEN	X	72	2	-	4/7/8/10	-
2	MEN	T	72	2	-	2/7/8/10	-
2	MEN	J	72	2	-	2/7/8/10	-
2	MEN	P	72	2	-	2/7/8/10	-
2	MEN	V	72	2	-	3/7/8/10	-
2	MEN	L	72	2	-	3/7/8/10	-
2	MEN	B	72	2	-	3/7/8/10	-
2	MEN	H	72	2	-	2/7/8/10	-
2	MEN	N	72	2	-	3/7/8/10	-
2	MEN	D	72	2	-	3/7/8/10	-
2	MEN	F	72	2	-	3/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	72	MEN	CE2-ND2	-2.16	1.41	1.45
2	P	72	MEN	CE2-ND2	-2.08	1.41	1.45
2	H	72	MEN	CE2-ND2	-2.07	1.41	1.45

There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	72	MEN	N-CA-CB-CG
2	F	72	MEN	CA-CB-CG-OD1
2	P	72	MEN	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	L	72	MEN	CA-CB-CG-OD1
2	N	72	MEN	CA-CB-CG-OD1

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	72	MEN	1	0
2	T	72	MEN	3	0
2	J	72	MEN	1	0
2	L	72	MEN	1	0
2	B	72	MEN	1	0
2	N	72	MEN	1	0
2	F	72	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

36 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	CYC	R	1153	2	36,46,46	1.90	7 (19%)	44,67,67	1.94	14 (31%)
3	CYC	N	1082	2	36,46,46	2.04	8 (22%)	44,67,67	1.79	10 (22%)
3	CYC	J	1153	2	36,46,46	1.75	7 (19%)	44,67,67	1.92	11 (25%)
3	CYC	H	1153	2	36,46,46	1.59	7 (19%)	44,67,67	1.97	11 (25%)
3	CYC	C	1084	1	36,46,46	2.15	8 (22%)	44,67,67	1.74	8 (18%)
3	CYC	T	1082	2	36,46,46	2.13	7 (19%)	44,67,67	1.86	9 (20%)
3	CYC	V	1082	2	36,46,46	2.09	7 (19%)	44,67,67	1.80	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CYC	G	1084	1	36,46,46	1.97	7 (19%)	44,67,67	1.76	9 (20%)
3	CYC	O	1084	1	36,46,46	2.04	8 (22%)	44,67,67	1.72	8 (18%)
3	CYC	X	1153	2	36,46,46	1.92	7 (19%)	44,67,67	1.98	11 (25%)
3	CYC	S	1084	1	36,46,46	2.05	8 (22%)	44,67,67	1.75	8 (18%)
3	CYC	Q	1084	1	36,46,46	2.03	8 (22%)	44,67,67	1.72	9 (20%)
3	CYC	W	1084	1	36,46,46	2.05	10 (27%)	44,67,67	1.75	9 (20%)
3	CYC	P	1153	2	36,46,46	1.67	8 (22%)	44,67,67	1.94	11 (25%)
3	CYC	N	1153	2	36,46,46	1.74	8 (22%)	44,67,67	1.91	12 (27%)
3	CYC	L	1082	2	36,46,46	2.11	9 (25%)	44,67,67	1.76	9 (20%)
3	CYC	F	1153	2	36,46,46	1.75	9 (25%)	44,67,67	1.89	11 (25%)
3	CYC	E	1084	1	36,46,46	2.06	9 (25%)	44,67,67	1.77	7 (15%)
3	CYC	K	1084	1	36,46,46	2.20	9 (25%)	44,67,67	1.74	8 (18%)
3	CYC	V	1153	2	36,46,46	1.92	9 (25%)	44,67,67	2.18	13 (29%)
3	CYC	D	1082	2	36,46,46	1.96	8 (22%)	44,67,67	1.78	11 (25%)
3	CYC	T	1153	2	36,46,46	1.77	7 (19%)	44,67,67	2.01	12 (27%)
3	CYC	F	1082	2	36,46,46	1.97	7 (19%)	44,67,67	1.82	10 (22%)
3	CYC	U	1084	1	36,46,46	2.13	9 (25%)	44,67,67	1.80	7 (15%)
3	CYC	B	1082	2	36,46,46	2.12	7 (19%)	44,67,67	1.81	10 (22%)
3	CYC	L	1153	2	36,46,46	1.79	8 (22%)	44,67,67	2.04	13 (29%)
3	CYC	H	1082	2	36,46,46	2.05	8 (22%)	44,67,67	1.83	10 (22%)
3	CYC	A	1084	1	36,46,46	1.99	8 (22%)	44,67,67	1.76	8 (18%)
3	CYC	R	1082	2	36,46,46	2.52	13 (36%)	44,67,67	2.05	12 (27%)
3	CYC	I	1084	1	36,46,46	2.12	8 (22%)	44,67,67	1.78	9 (20%)
3	CYC	X	1082	2	36,46,46	2.11	10 (27%)	44,67,67	1.82	10 (22%)
3	CYC	M	1084	1	36,46,46	2.06	8 (22%)	44,67,67	1.77	8 (18%)
3	CYC	J	1082	2	36,46,46	1.98	8 (22%)	44,67,67	1.80	10 (22%)
3	CYC	D	1153	2	36,46,46	1.75	7 (19%)	44,67,67	1.99	12 (27%)
3	CYC	B	1153	2	36,46,46	2.03	8 (22%)	44,67,67	2.00	13 (29%)
3	CYC	P	1082	2	36,46,46	1.96	8 (22%)	44,67,67	1.99	12 (27%)

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	CYC	R	1153	2	-	6/21/74/74	0/4/4/4
3	CYC	N	1082	2	-	7/21/74/74	0/4/4/4
3	CYC	J	1153	2	-	6/21/74/74	0/4/4/4
3	CYC	H	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	C	1084	1	-	6/21/74/74	0/4/4/4
3	CYC	T	1082	2	-	7/21/74/74	0/4/4/4
3	CYC	V	1082	2	-	6/21/74/74	0/4/4/4
3	CYC	G	1084	1	-	5/21/74/74	0/4/4/4
3	CYC	O	1084	1	-	6/21/74/74	0/4/4/4
3	CYC	X	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	S	1084	1	-	4/21/74/74	0/4/4/4
3	CYC	Q	1084	1	-	5/21/74/74	0/4/4/4
3	CYC	W	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	P	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	N	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	L	1082	2	-	6/21/74/74	0/4/4/4
3	CYC	F	1153	2	-	5/21/74/74	0/4/4/4
3	CYC	E	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	K	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	V	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	D	1082	2	-	8/21/74/74	0/4/4/4
3	CYC	T	1153	2	-	4/21/74/74	0/4/4/4
3	CYC	F	1082	2	-	4/21/74/74	0/4/4/4
3	CYC	U	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	B	1082	2	-	5/21/74/74	0/4/4/4
3	CYC	L	1153	2	-	5/21/74/74	0/4/4/4
3	CYC	H	1082	2	-	6/21/74/74	0/4/4/4
3	CYC	A	1084	1	-	6/21/74/74	0/4/4/4
3	CYC	R	1082	2	-	5/21/74/74	0/4/4/4
3	CYC	I	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	X	1082	2	-	5/21/74/74	0/4/4/4
3	CYC	M	1084	1	-	7/21/74/74	0/4/4/4
3	CYC	J	1082	2	-	6/21/74/74	0/4/4/4
3	CYC	D	1153	2	-	6/21/74/74	0/4/4/4
3	CYC	B	1153	2	-	5/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	P	1082	2	-	5/21/74/74	0/4/4/4

The worst 5 of 292 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1082	CYC	CHA-C1A	9.73	1.43	1.35
3	K	1084	CYC	CHA-C1A	8.93	1.42	1.35
3	T	1082	CYC	CHA-C1A	8.85	1.42	1.35
3	B	1082	CYC	CHA-C1A	8.50	1.42	1.35
3	V	1082	CYC	CHA-C1A	8.42	1.42	1.35

The worst 5 of 365 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1153	CYC	C2C-C1C-NC	5.93	113.39	108.27
3	R	1082	CYC	C2C-C1C-NC	5.74	113.22	108.27
3	X	1153	CYC	C2C-C1C-NC	5.66	113.15	108.27
3	B	1153	CYC	C2C-C1C-NC	5.66	113.15	108.27
3	T	1153	CYC	C2C-C1C-NC	5.65	113.14	108.27

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1153	CYC	NA-C4A-CHB-C1B
3	R	1153	CYC	C3A-C4A-CHB-C1B
3	R	1153	CYC	C4B-C3B-CAB-CBB
3	R	1153	CYC	C2C-C3C-CAC-CBC
3	R	1153	CYC	C4C-C3C-CAC-CBC

There are no ring outliers.

33 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1153	CYC	4	0
3	N	1082	CYC	4	0
3	H	1153	CYC	3	0
3	C	1084	CYC	2	0
3	T	1082	CYC	4	0
3	V	1082	CYC	1	0
3	G	1084	CYC	1	0

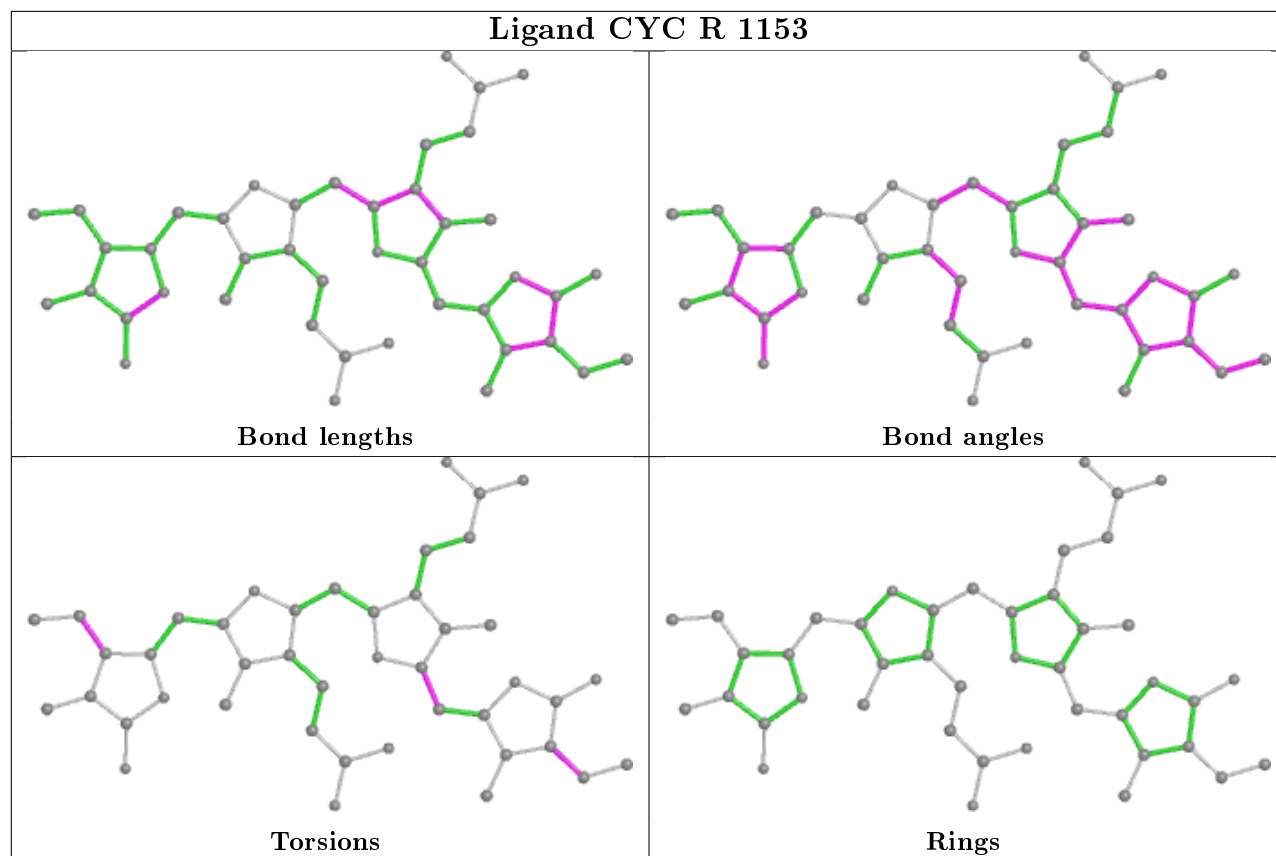
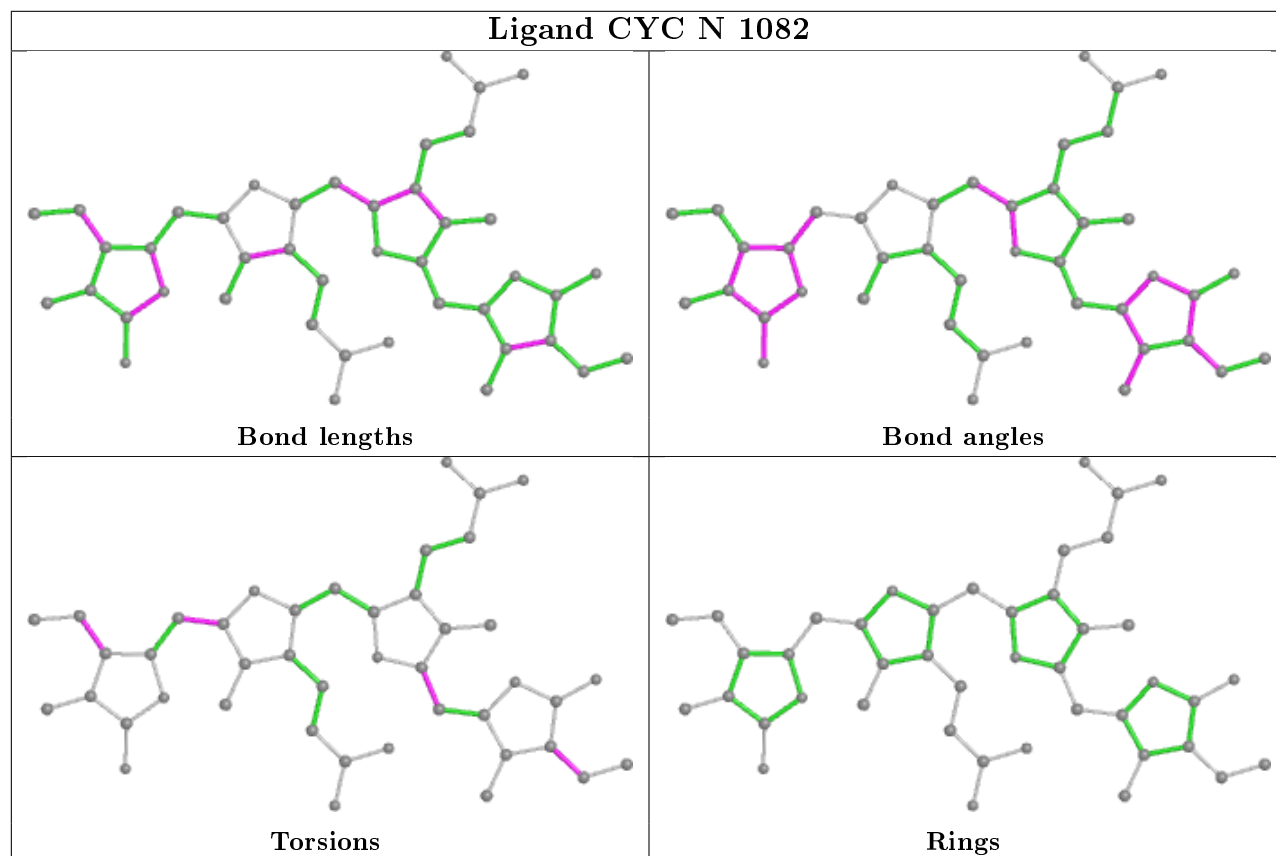
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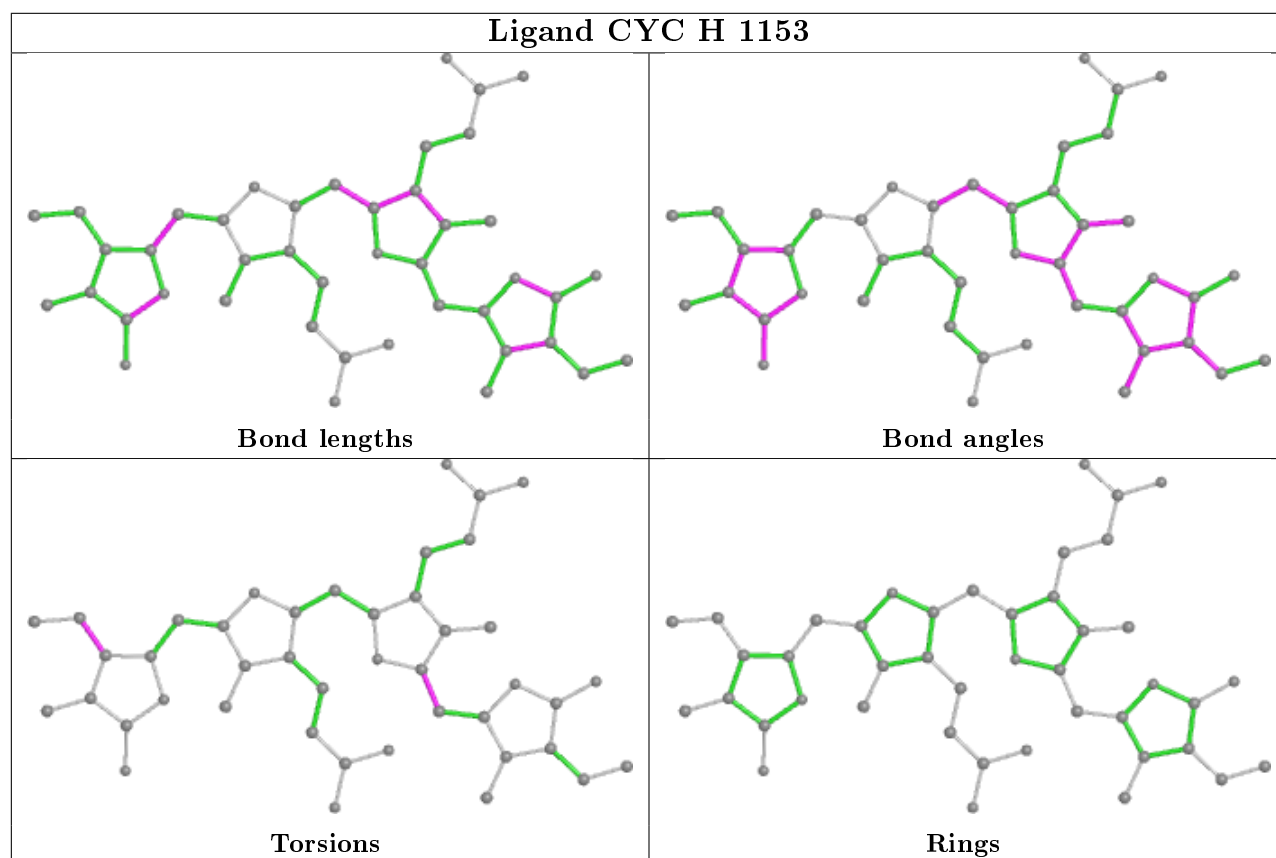
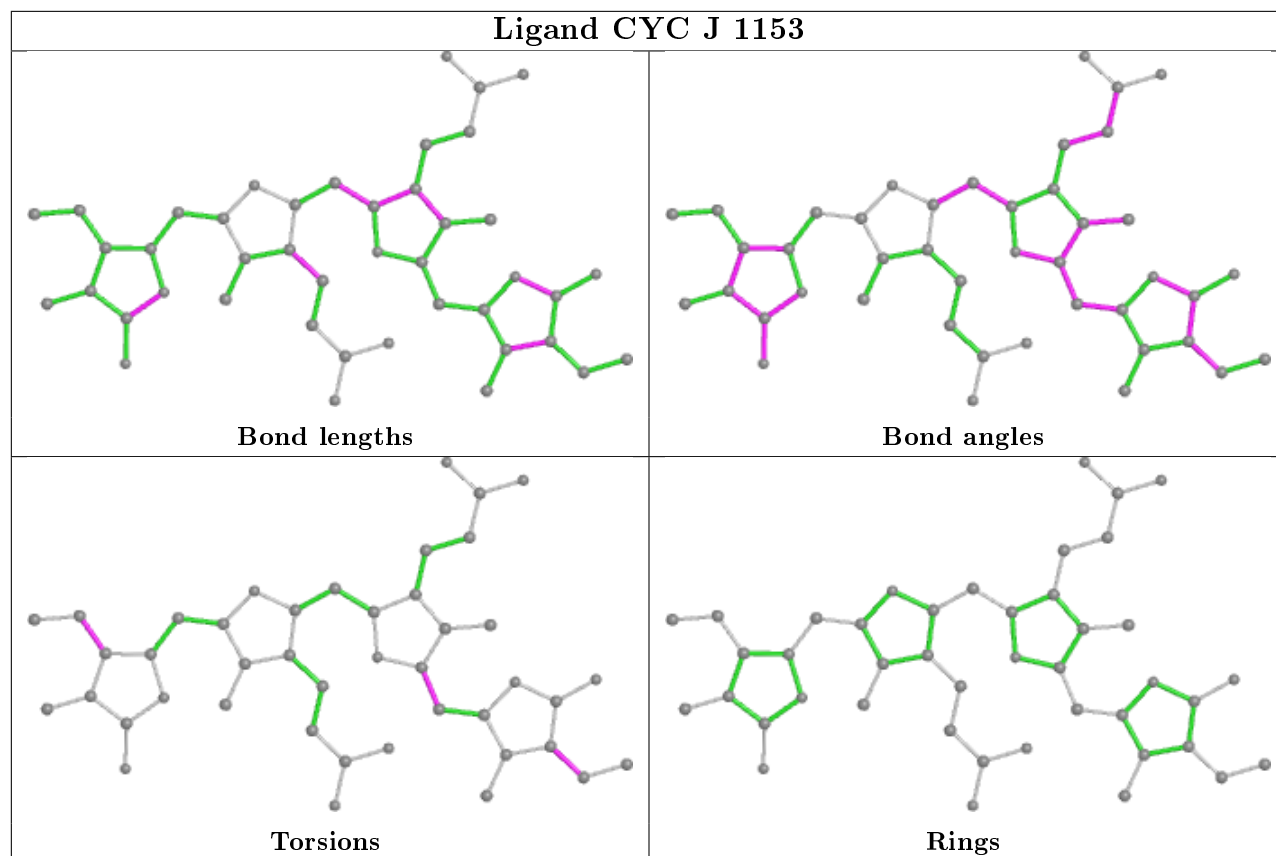


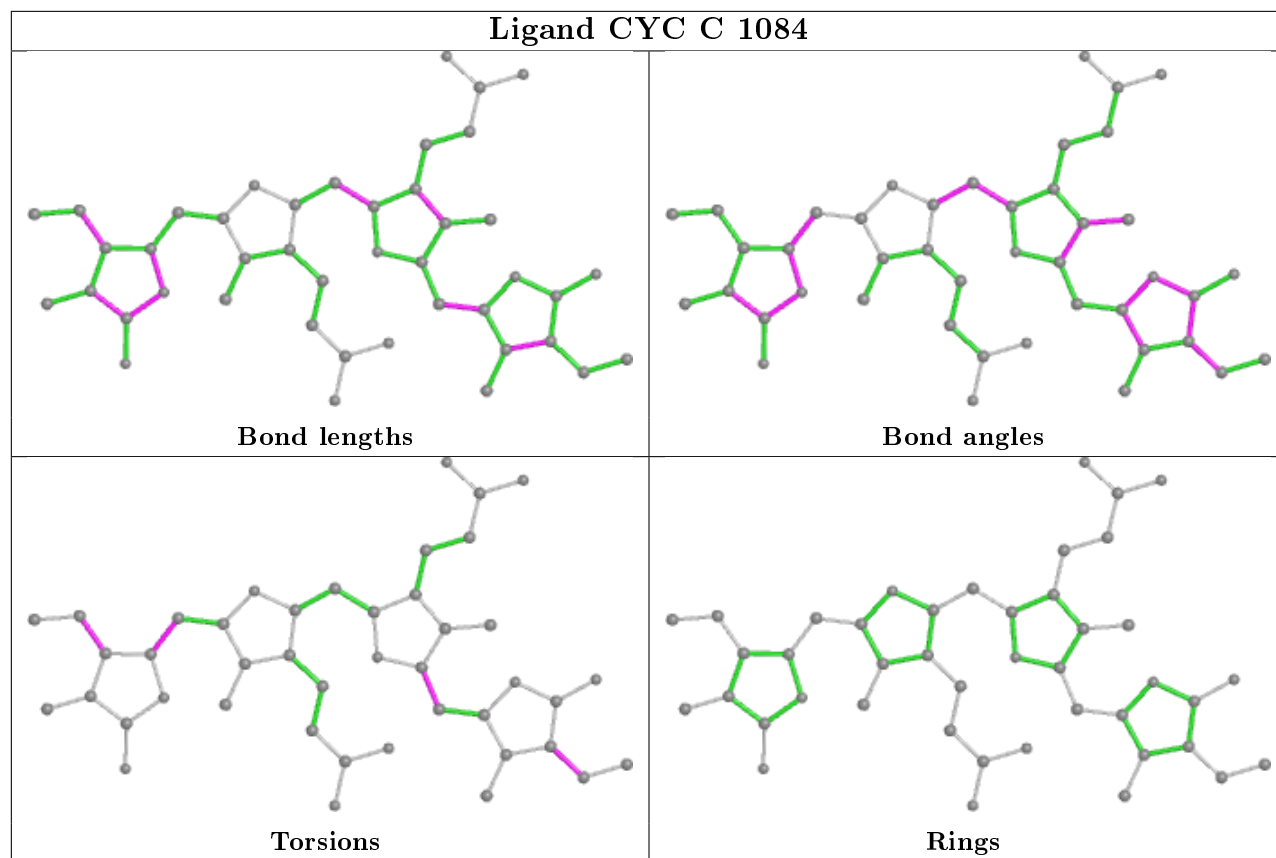
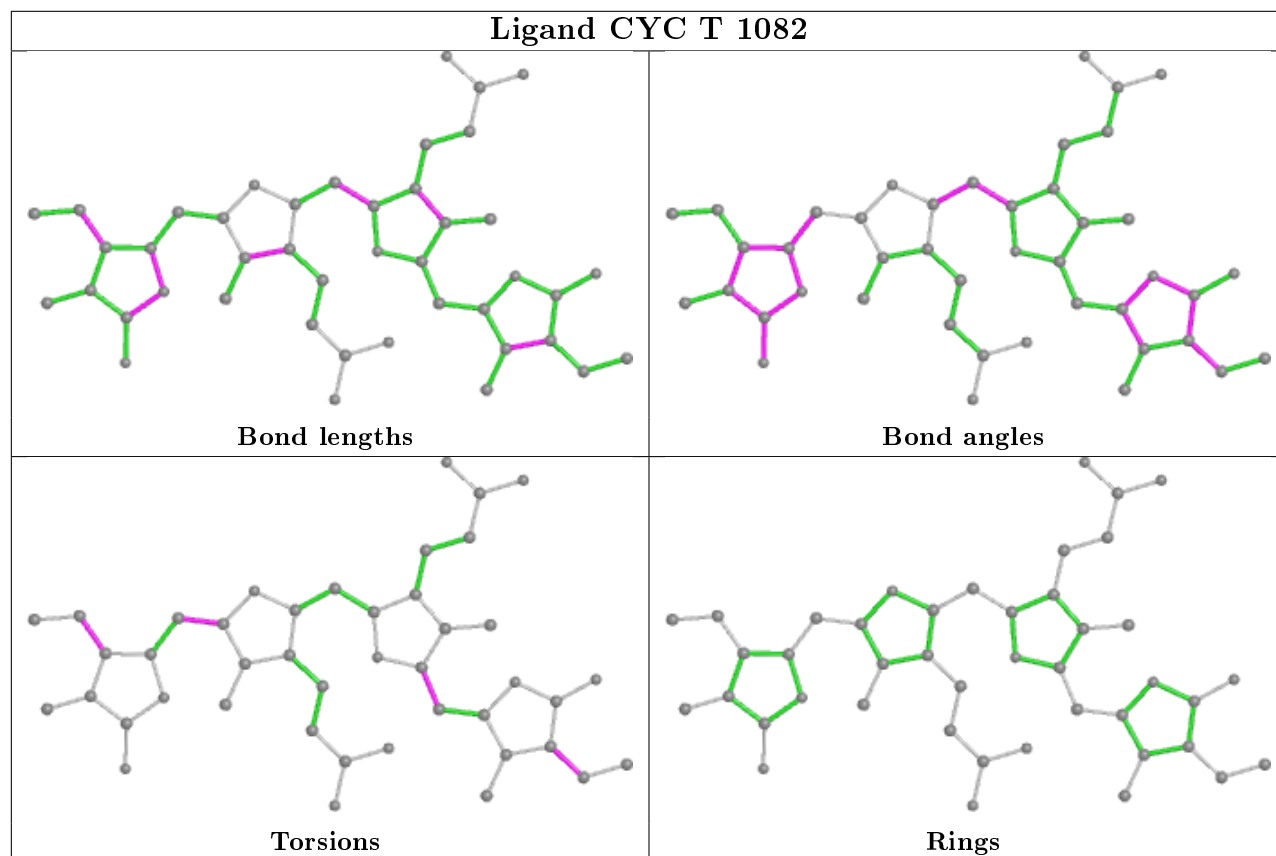
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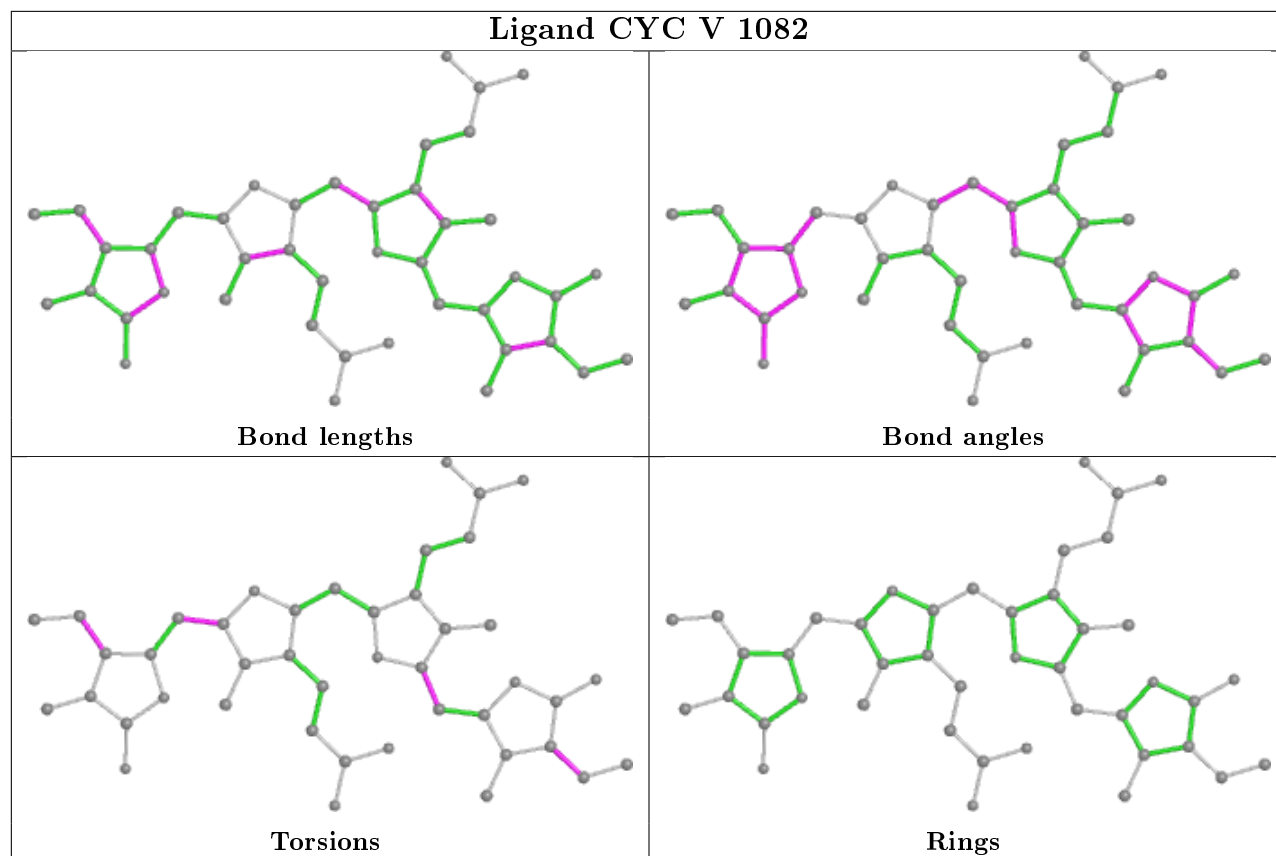
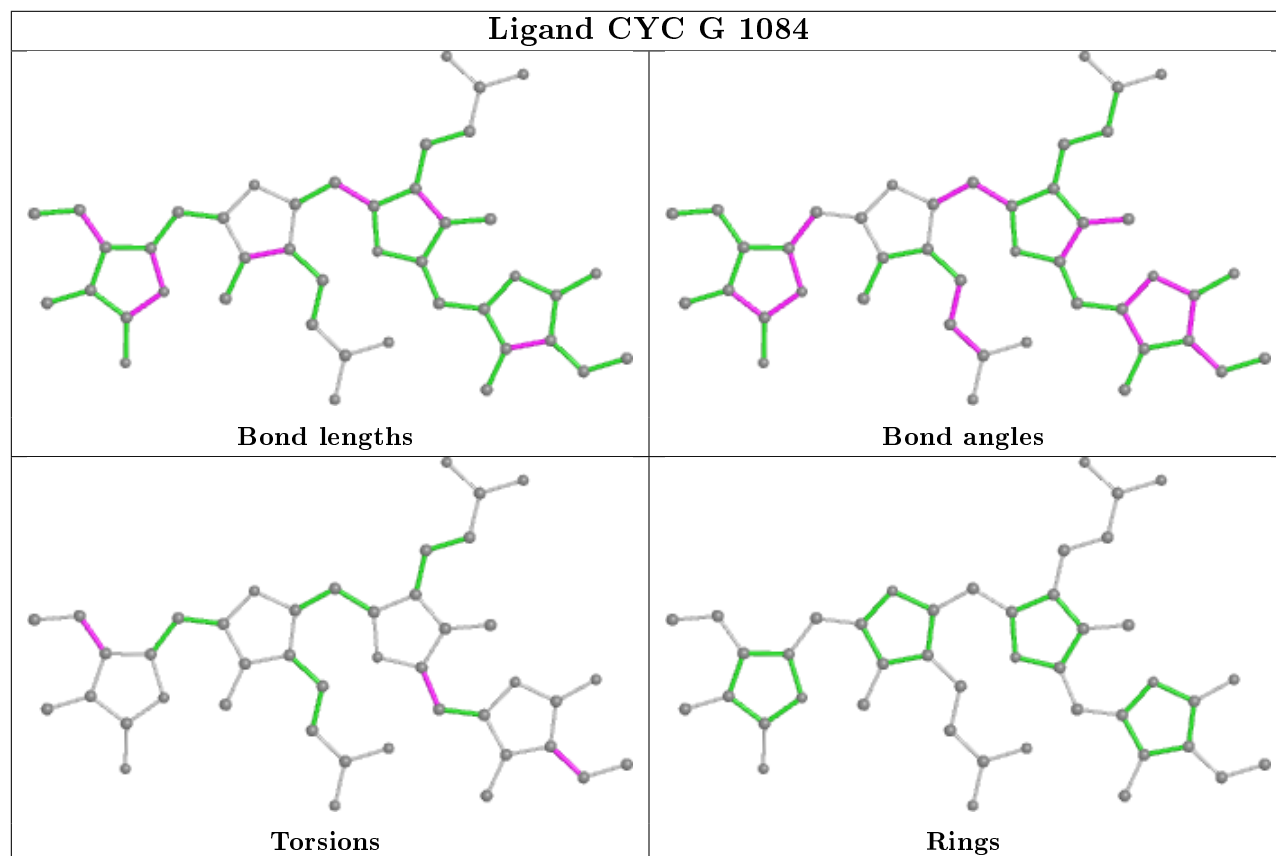
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1084	CYC	3	0
3	X	1153	CYC	4	0
3	S	1084	CYC	2	0
3	Q	1084	CYC	4	0
3	W	1084	CYC	3	0
3	P	1153	CYC	5	0
3	N	1153	CYC	1	0
3	L	1082	CYC	2	0
3	F	1153	CYC	3	0
3	E	1084	CYC	2	0
3	K	1084	CYC	2	0
3	V	1153	CYC	4	0
3	D	1082	CYC	2	0
3	T	1153	CYC	6	0
3	F	1082	CYC	5	0
3	U	1084	CYC	1	0
3	B	1082	CYC	3	0
3	L	1153	CYC	3	0
3	H	1082	CYC	3	0
3	A	1084	CYC	2	0
3	R	1082	CYC	2	0
3	I	1084	CYC	1	0
3	X	1082	CYC	1	0
3	M	1084	CYC	3	0
3	J	1082	CYC	3	0
3	D	1153	CYC	4	0

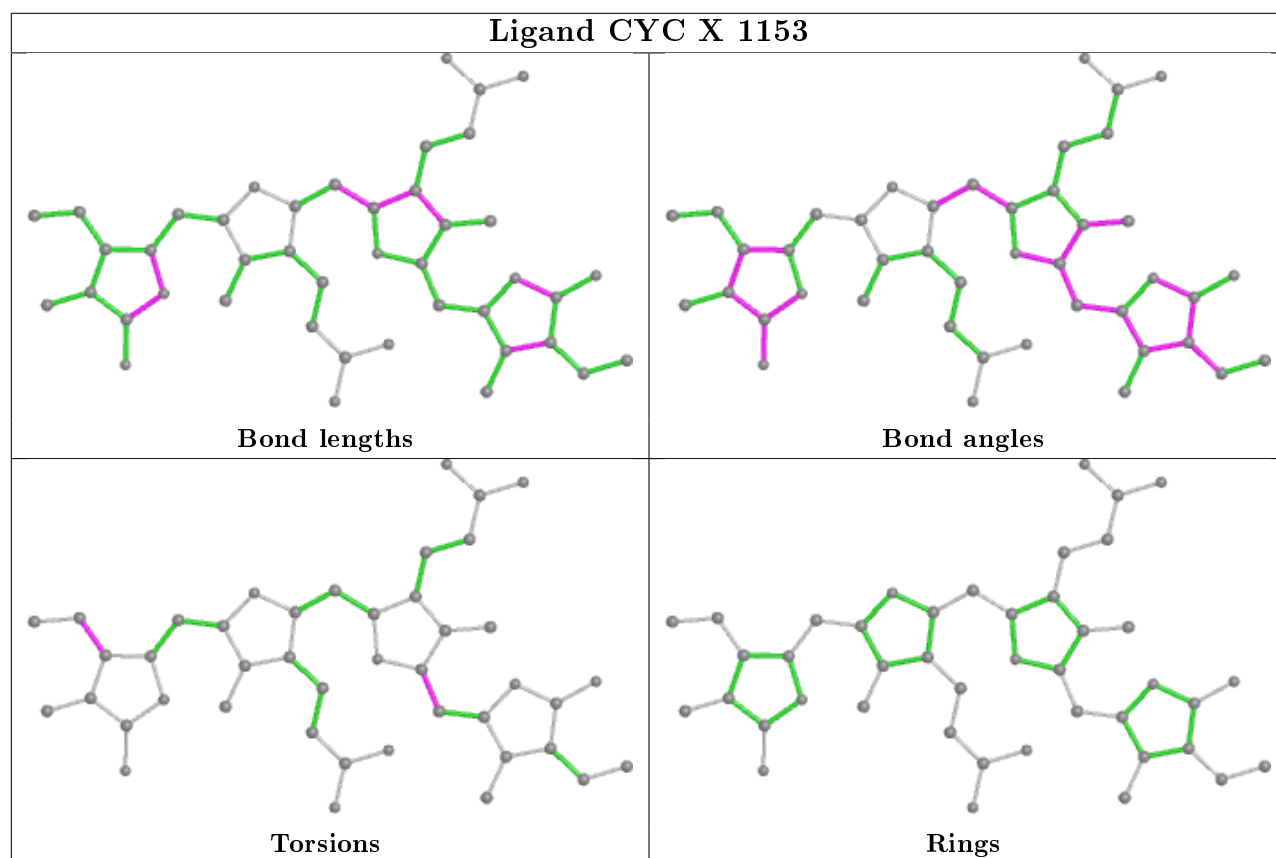
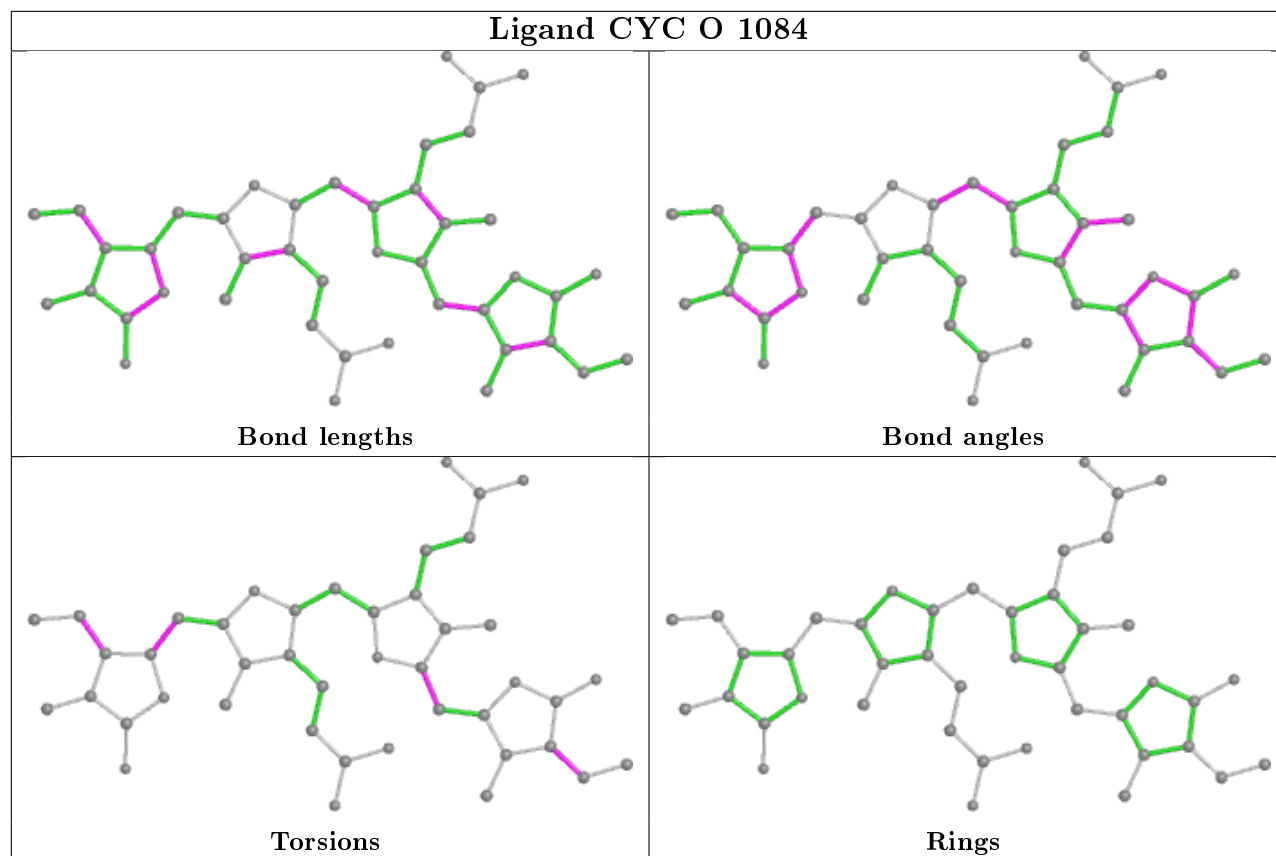
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

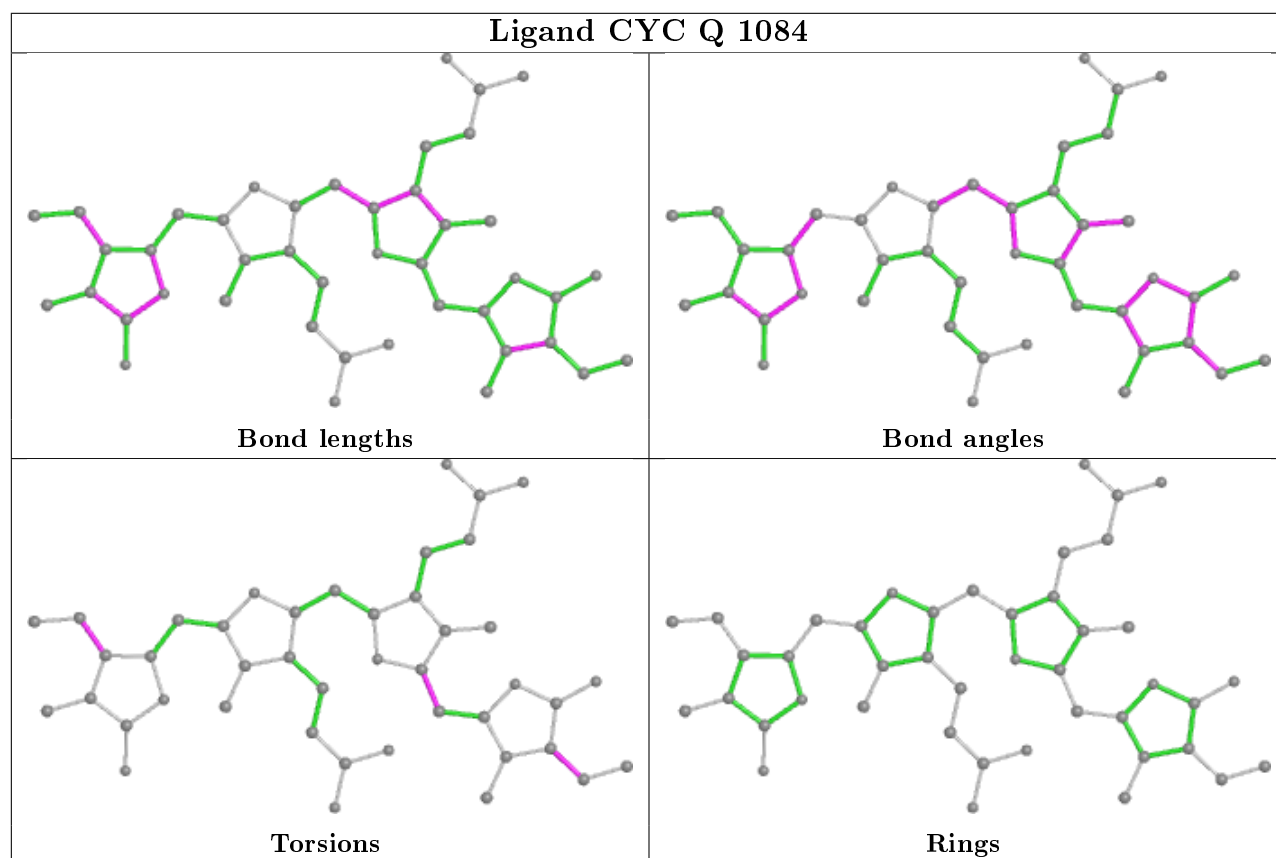
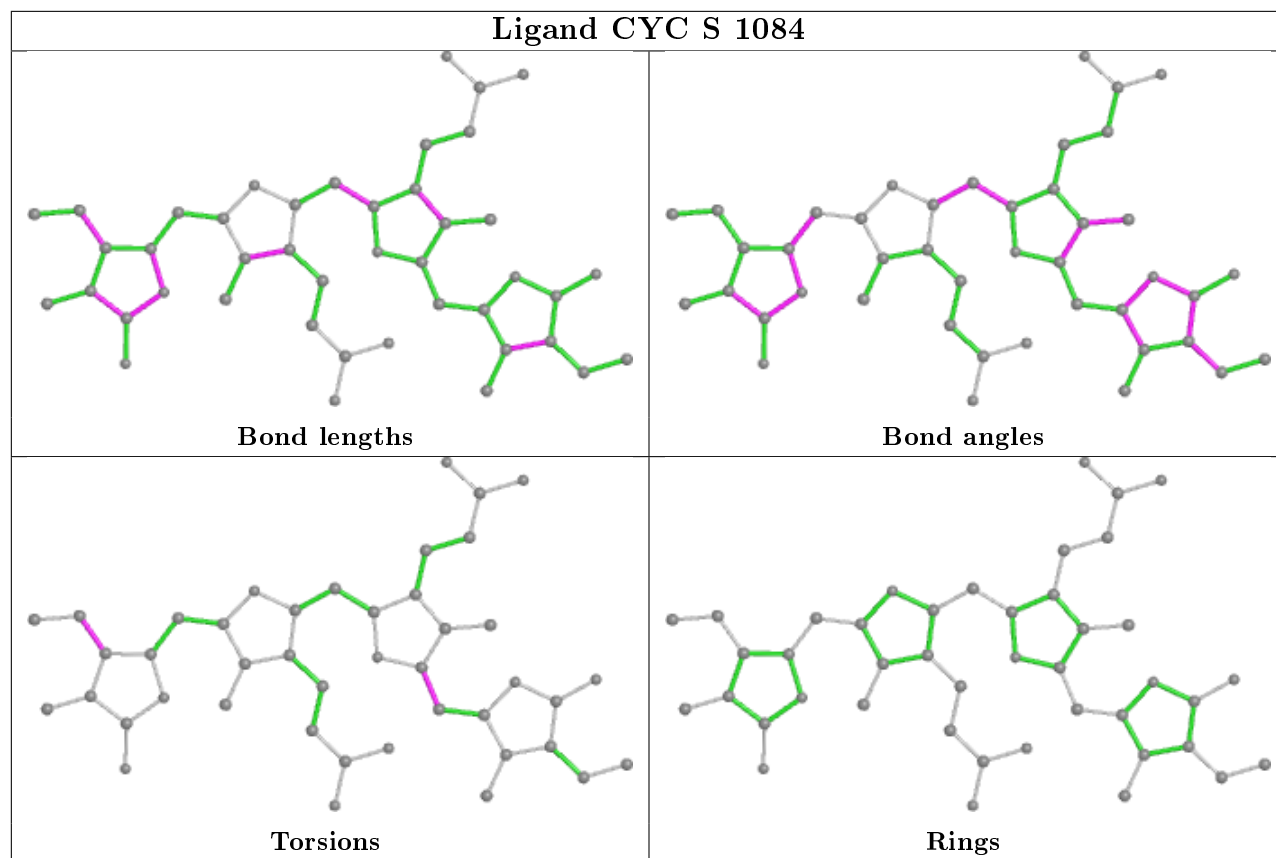
**Ligand CYC R 1153****Ligand CYC N 1082**

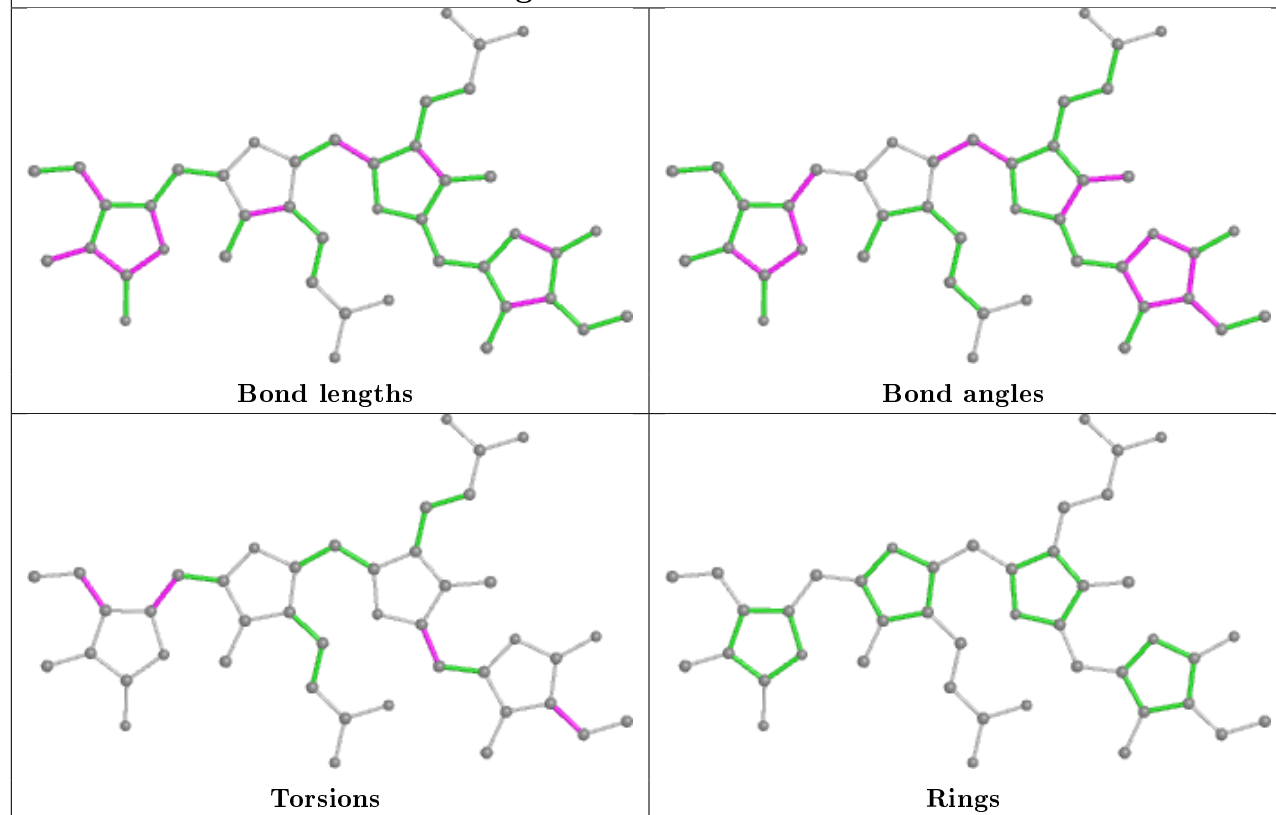
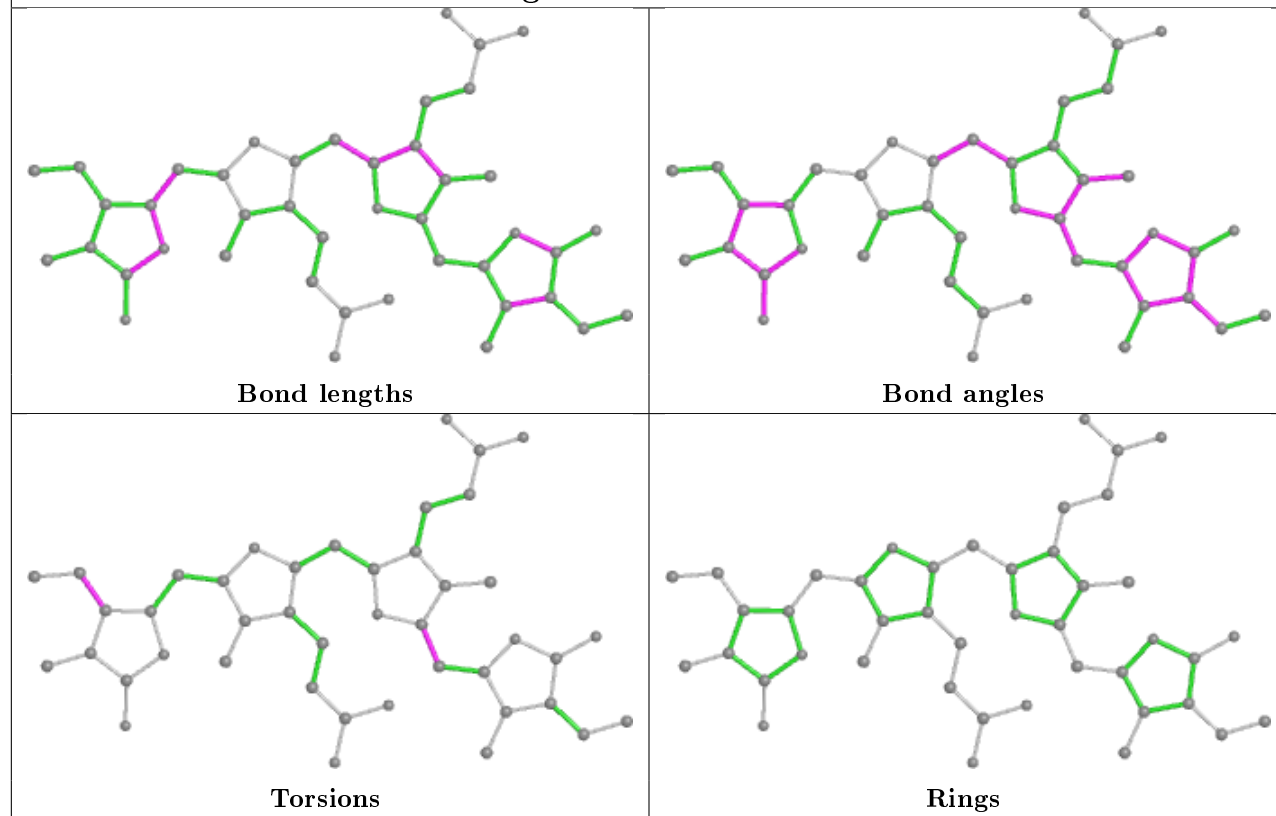


**Ligand CYC C 1084****Ligand CYC T 1082**

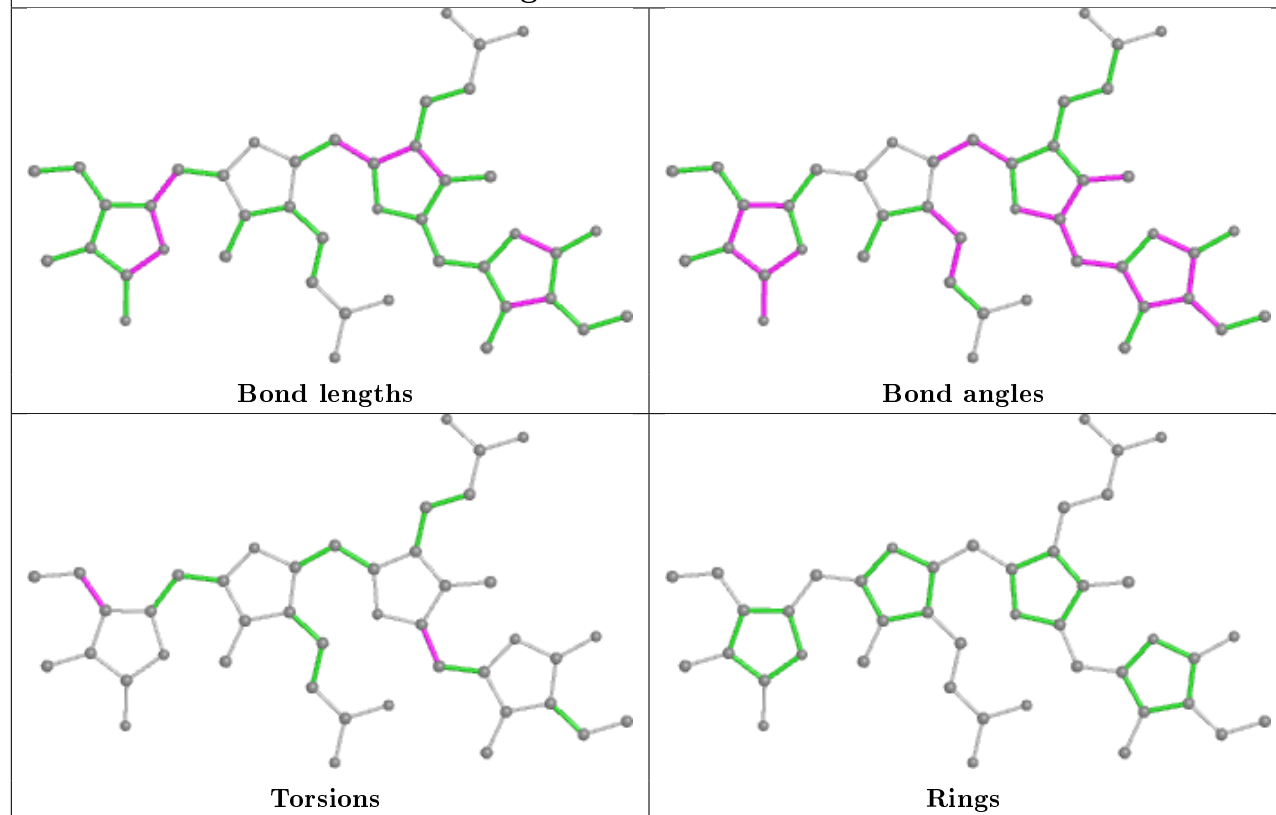
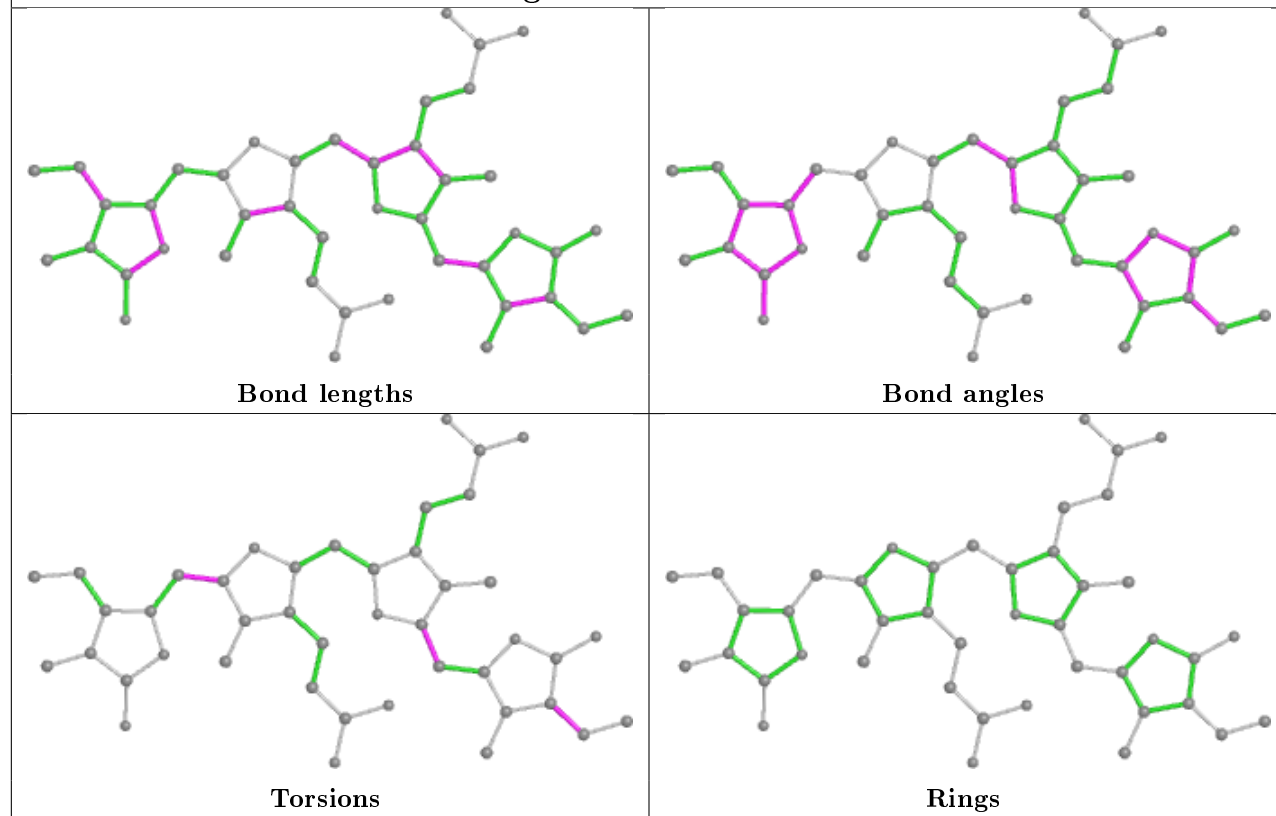
**Ligand CYC V 1082****Ligand CYC G 1084**

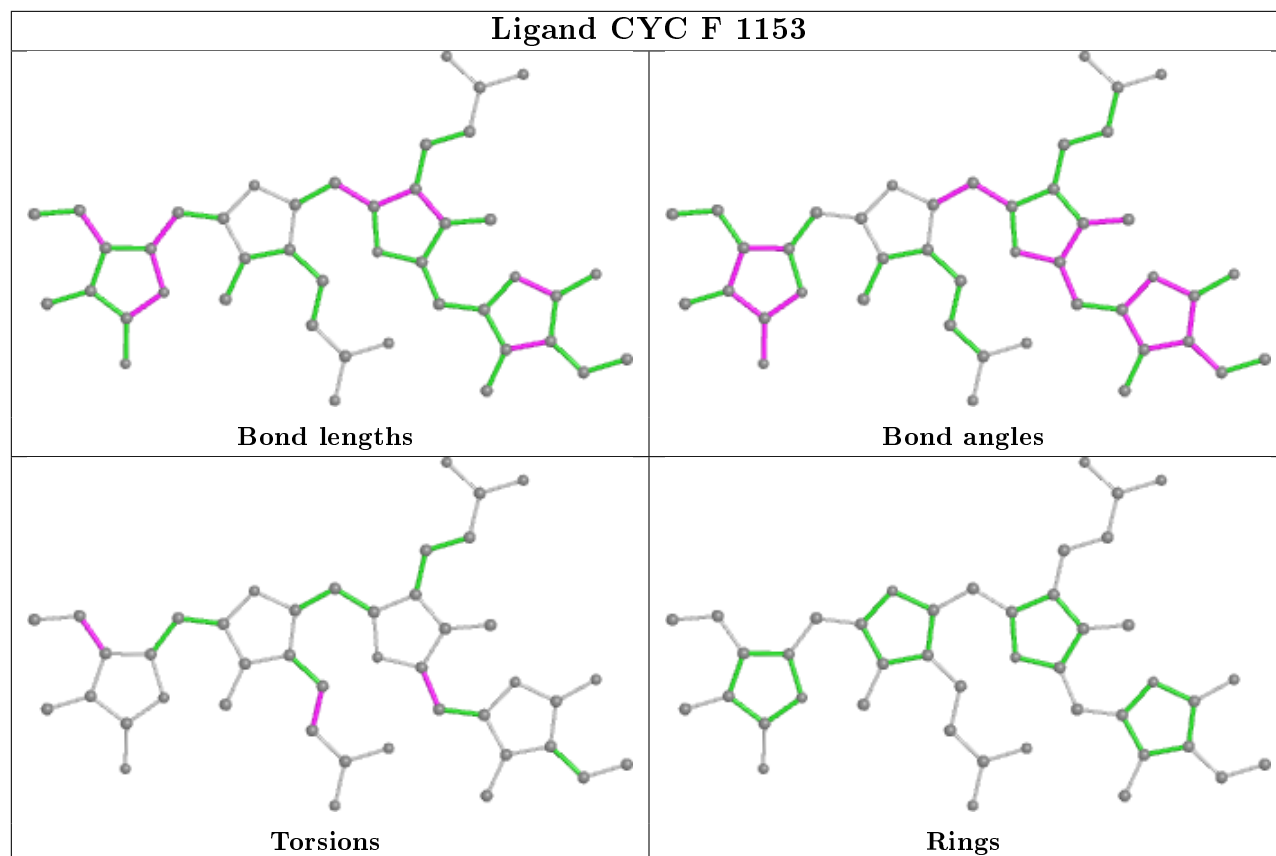
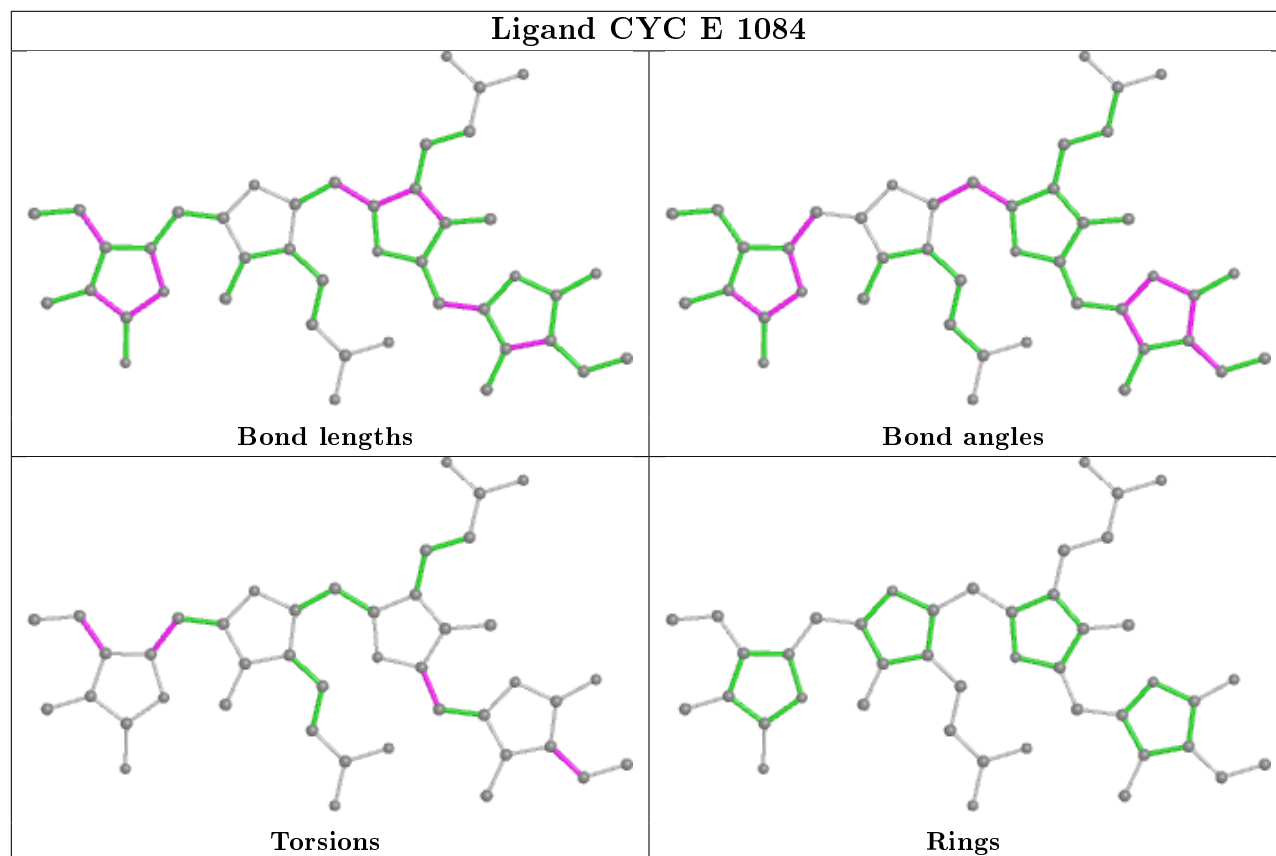




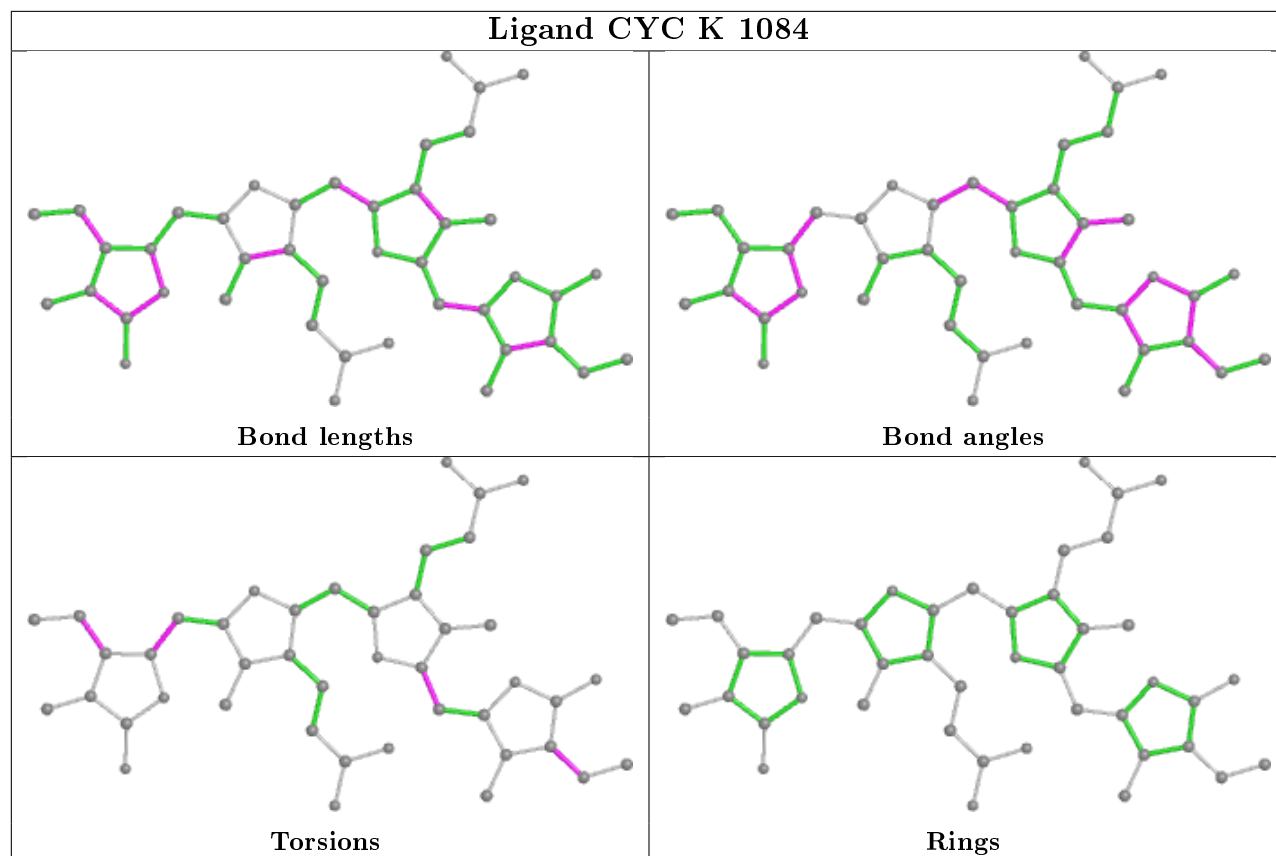
**Ligand CYC W 1084****Ligand CYC P 1153**



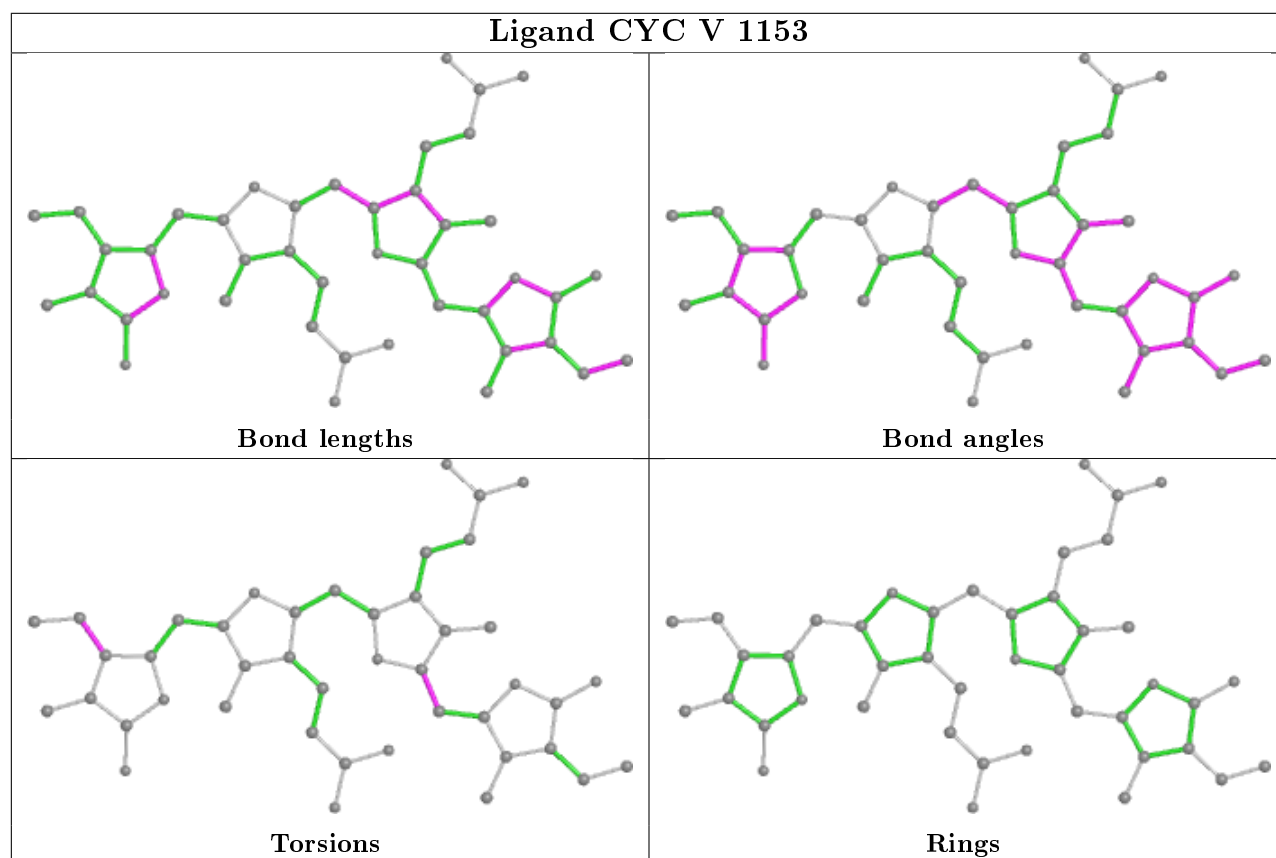
**Ligand CYC N 1153****Ligand CYC L 1082**

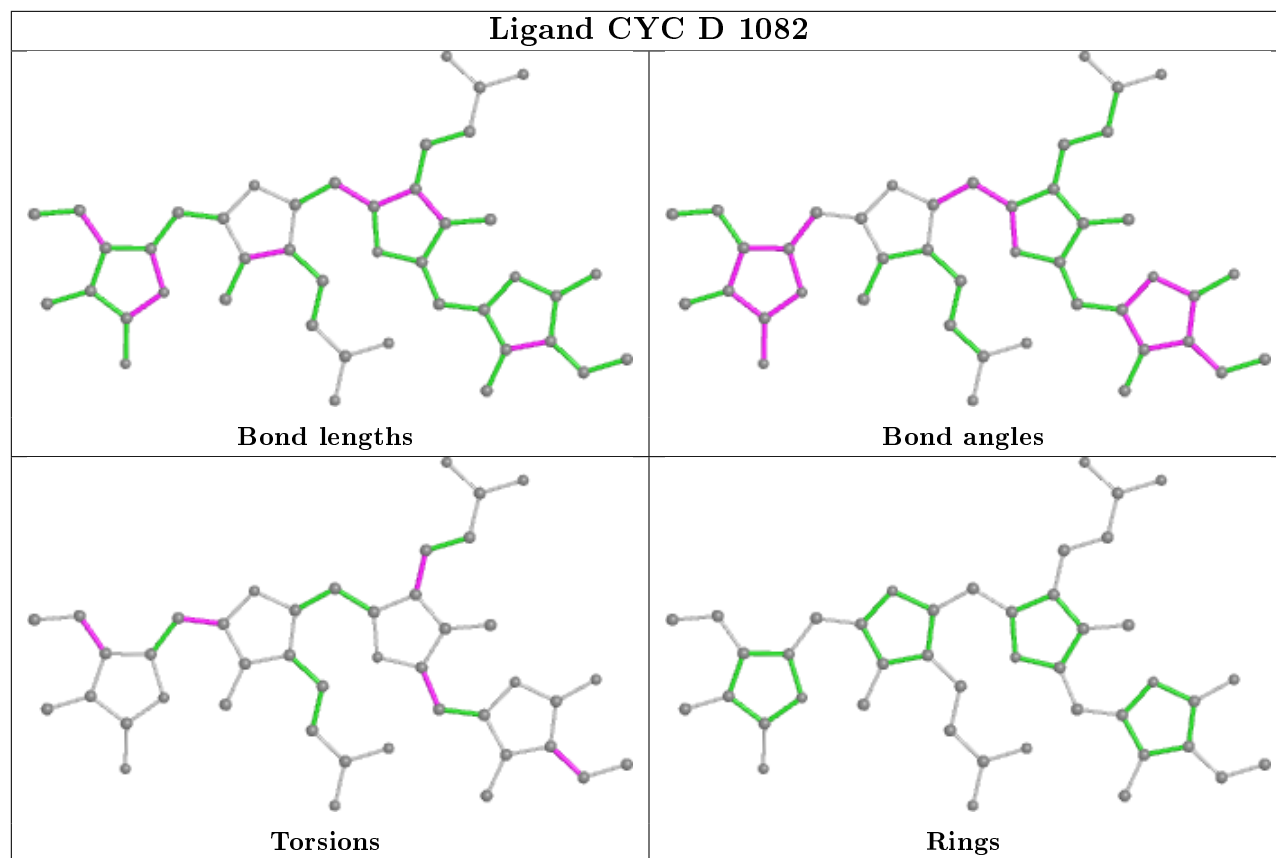
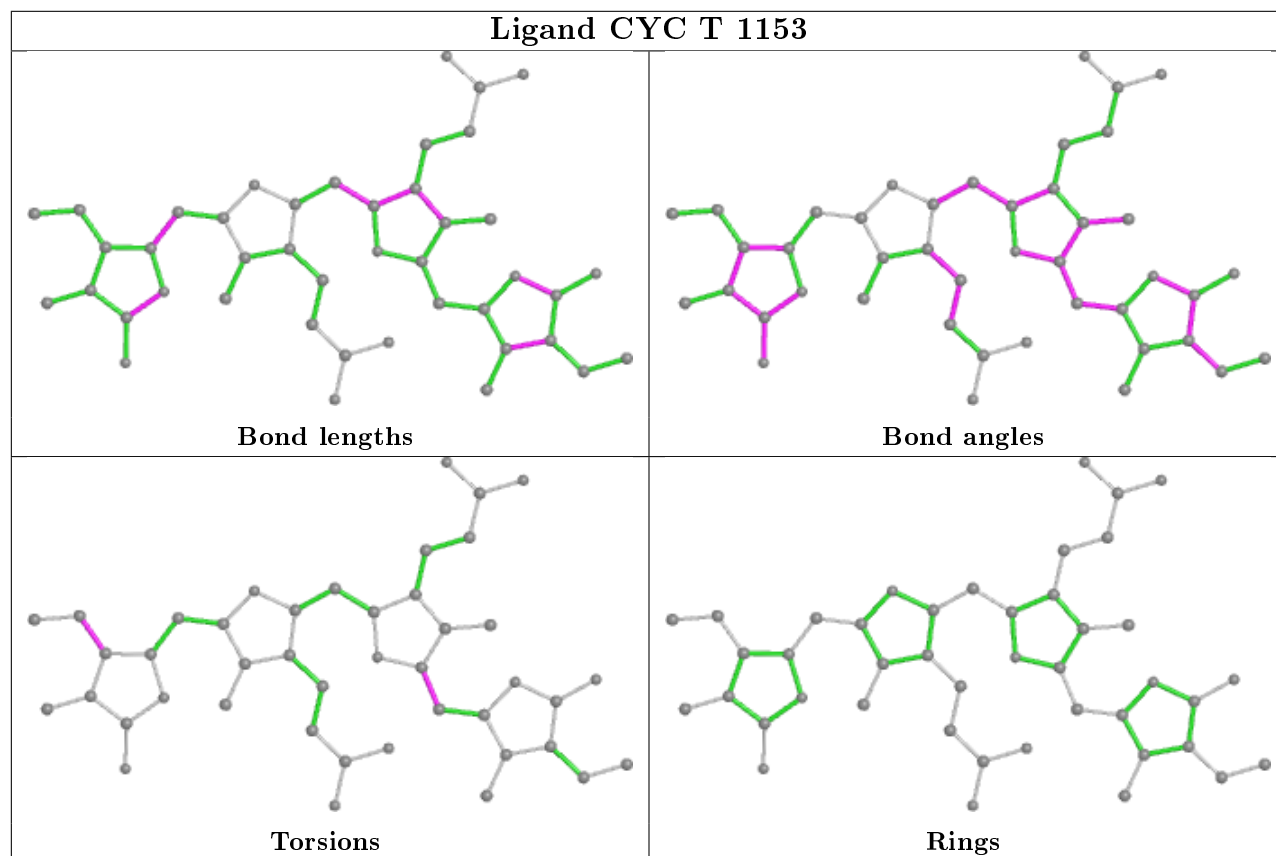
**Ligand CYC F 1153****Ligand CYC E 1084**

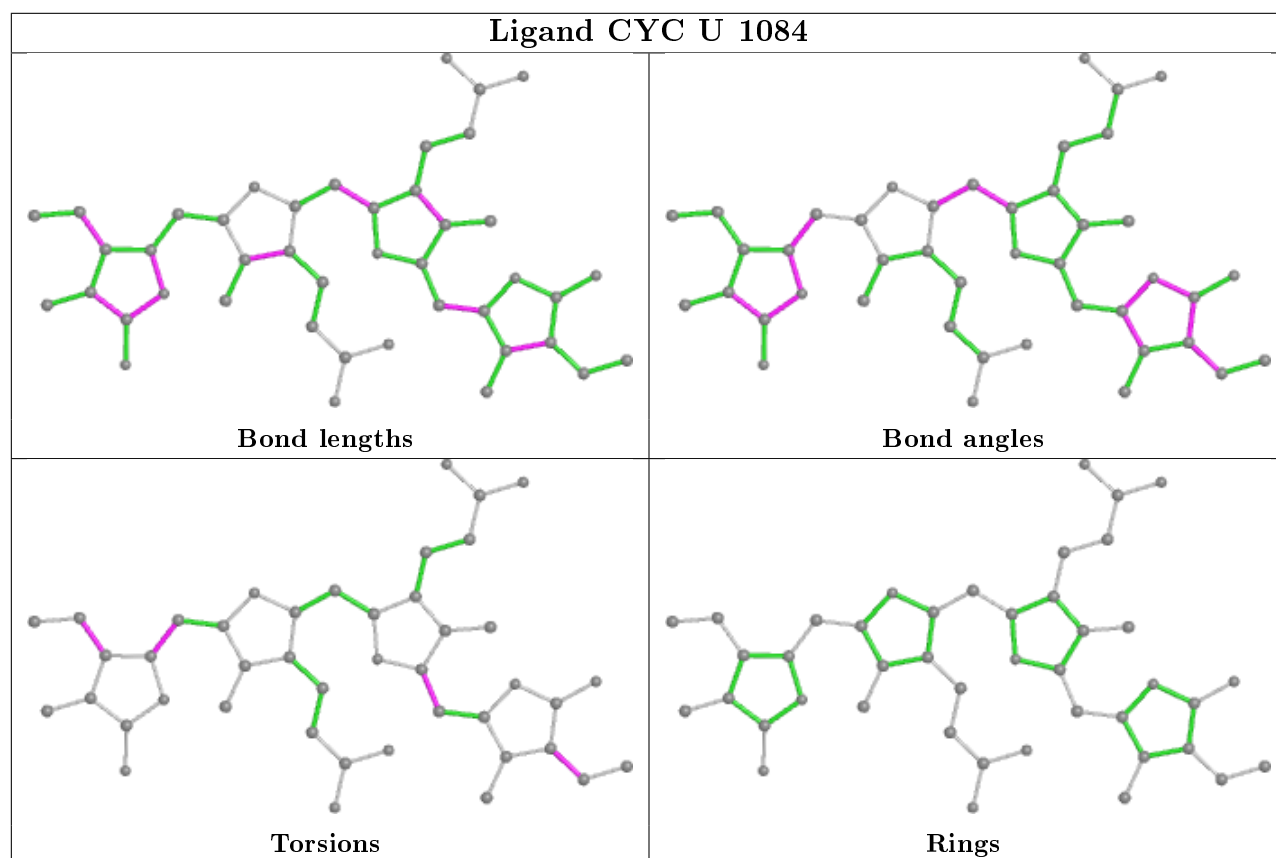
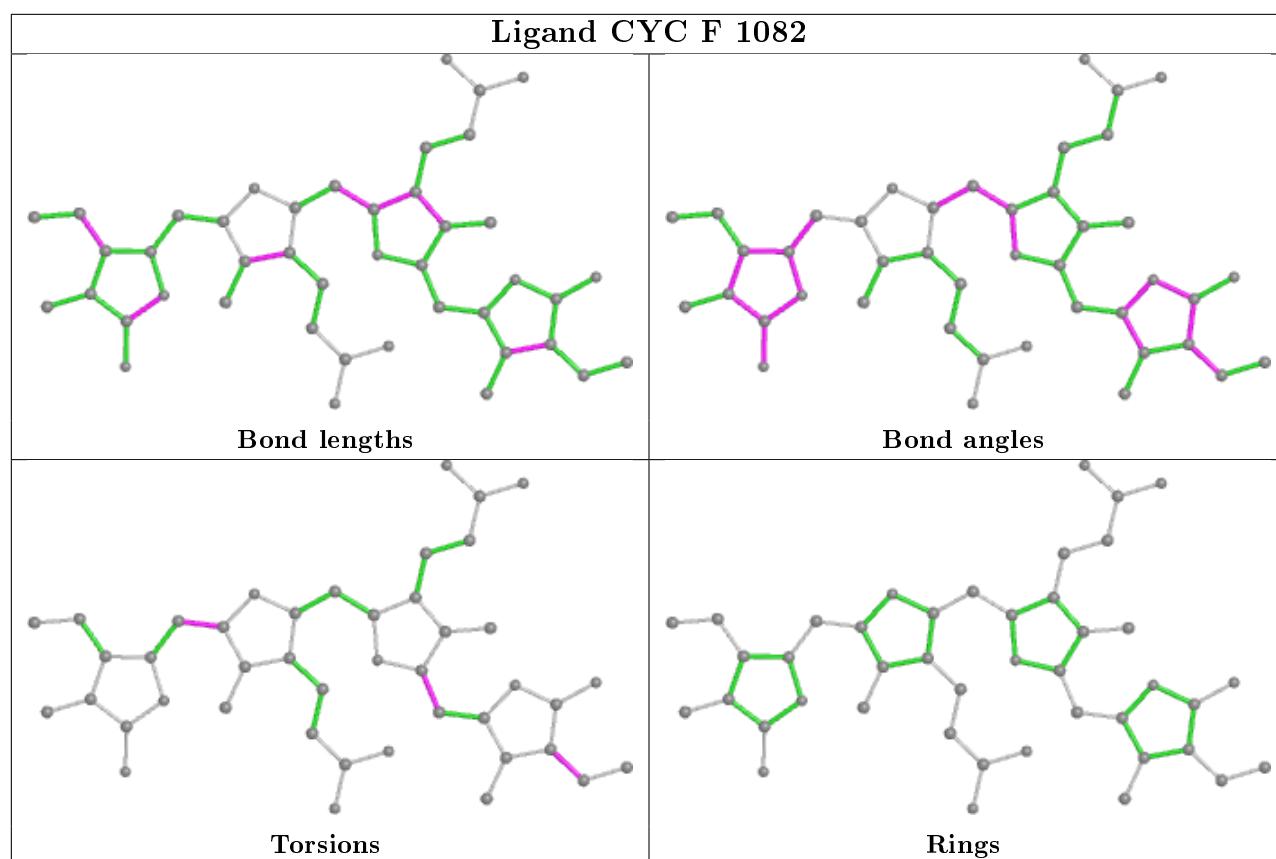
## Ligand CYC K 1084

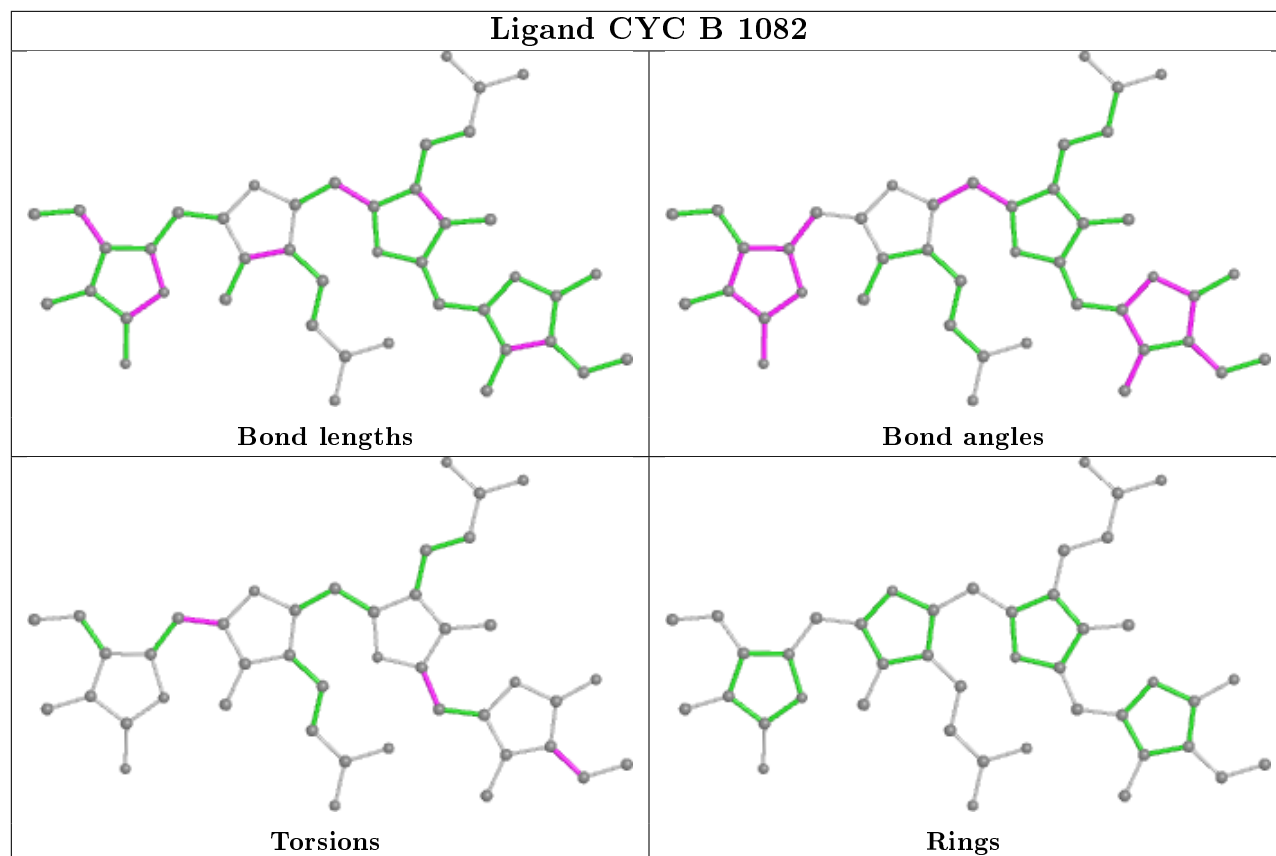
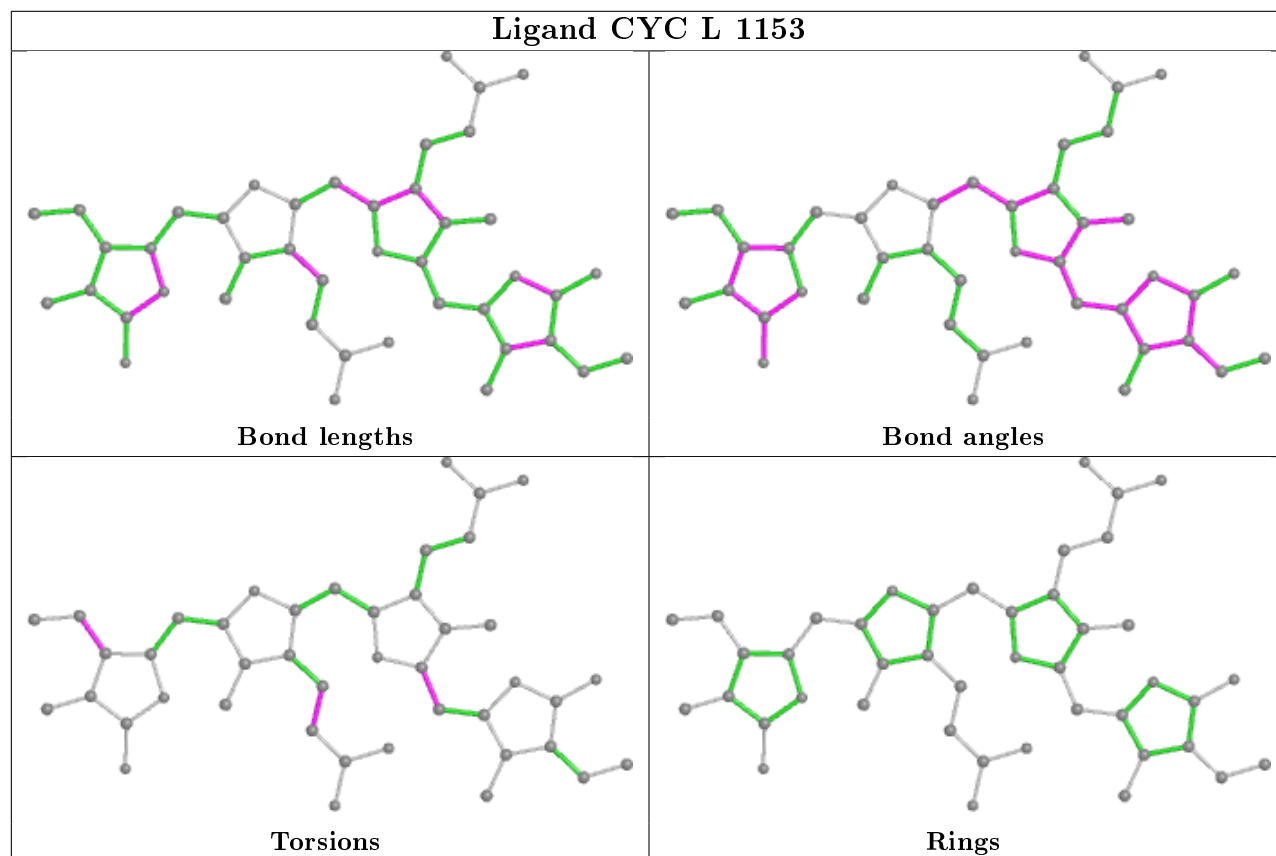


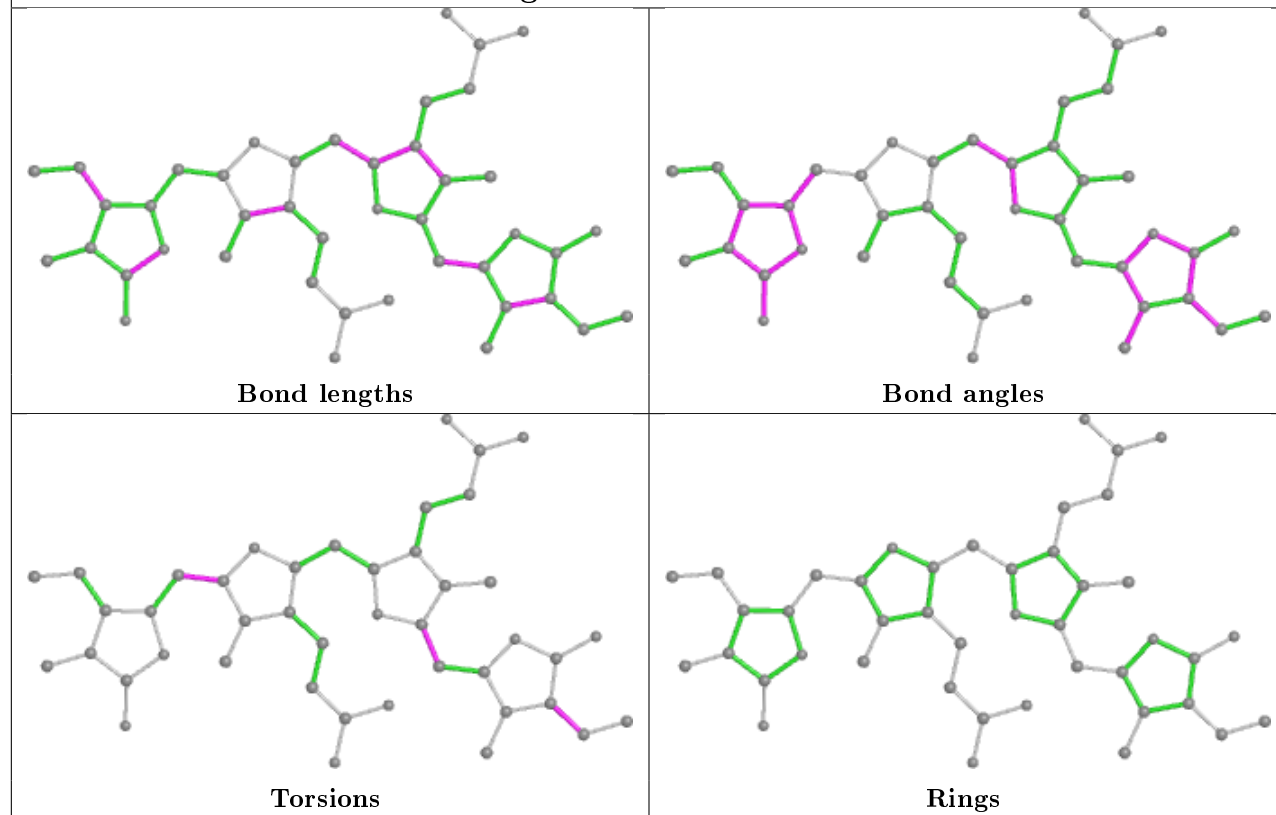
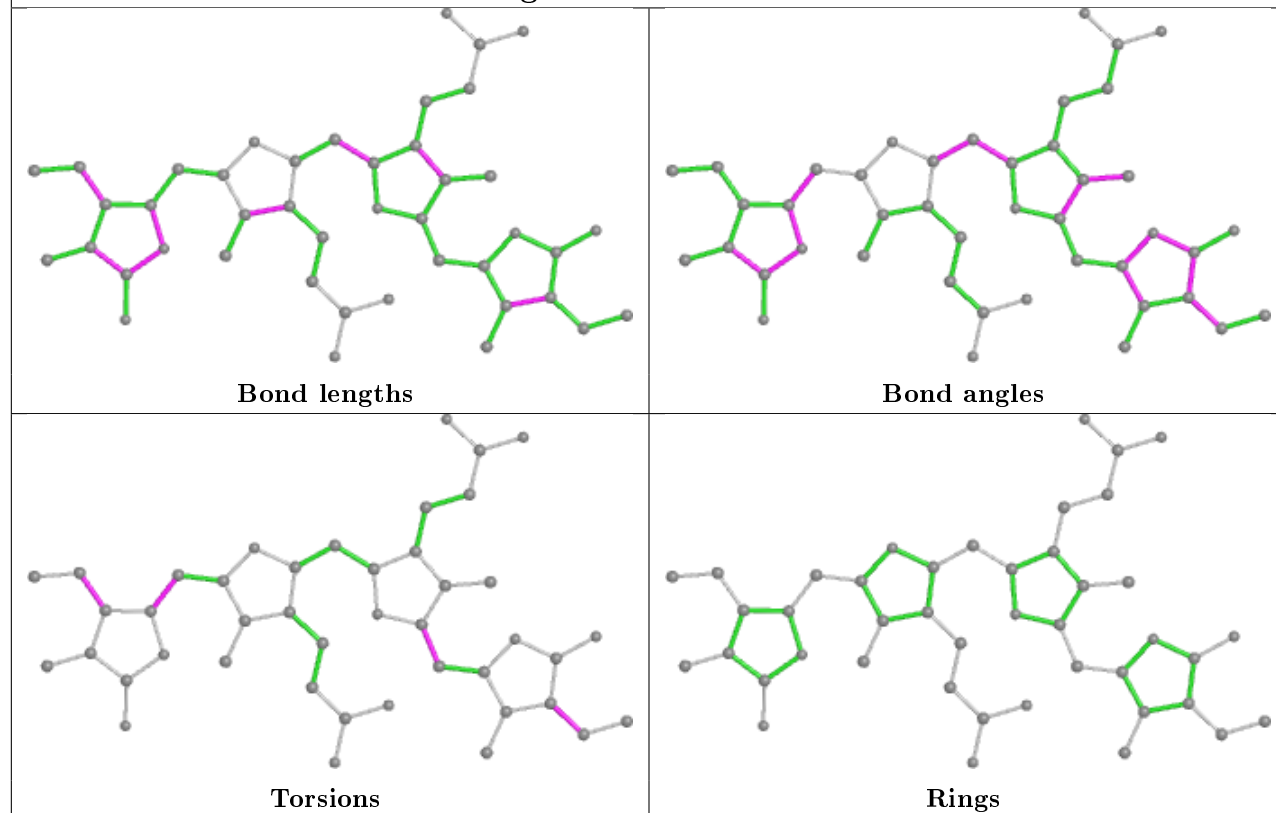
## Ligand CYC V 1153



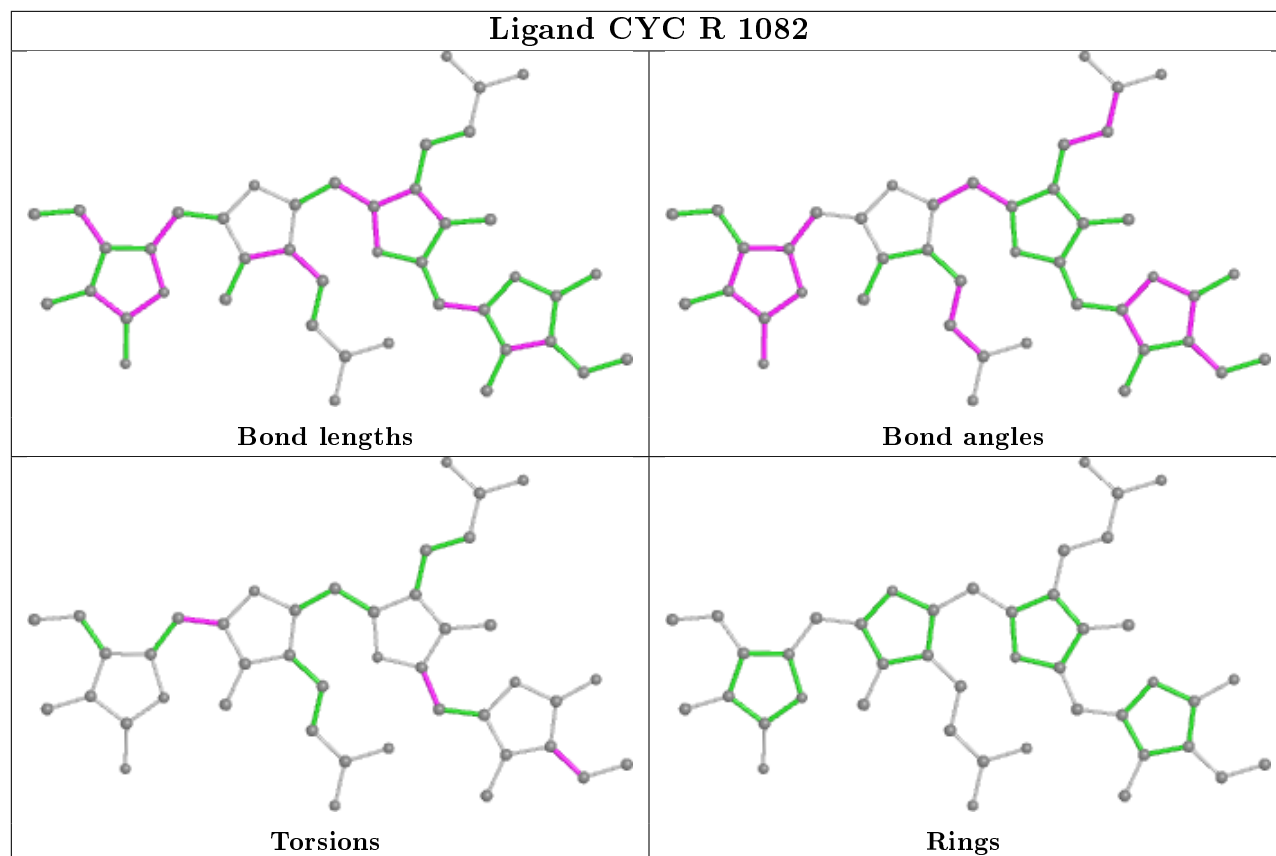
**Ligand CYC D 1082****Ligand CYC T 1153**



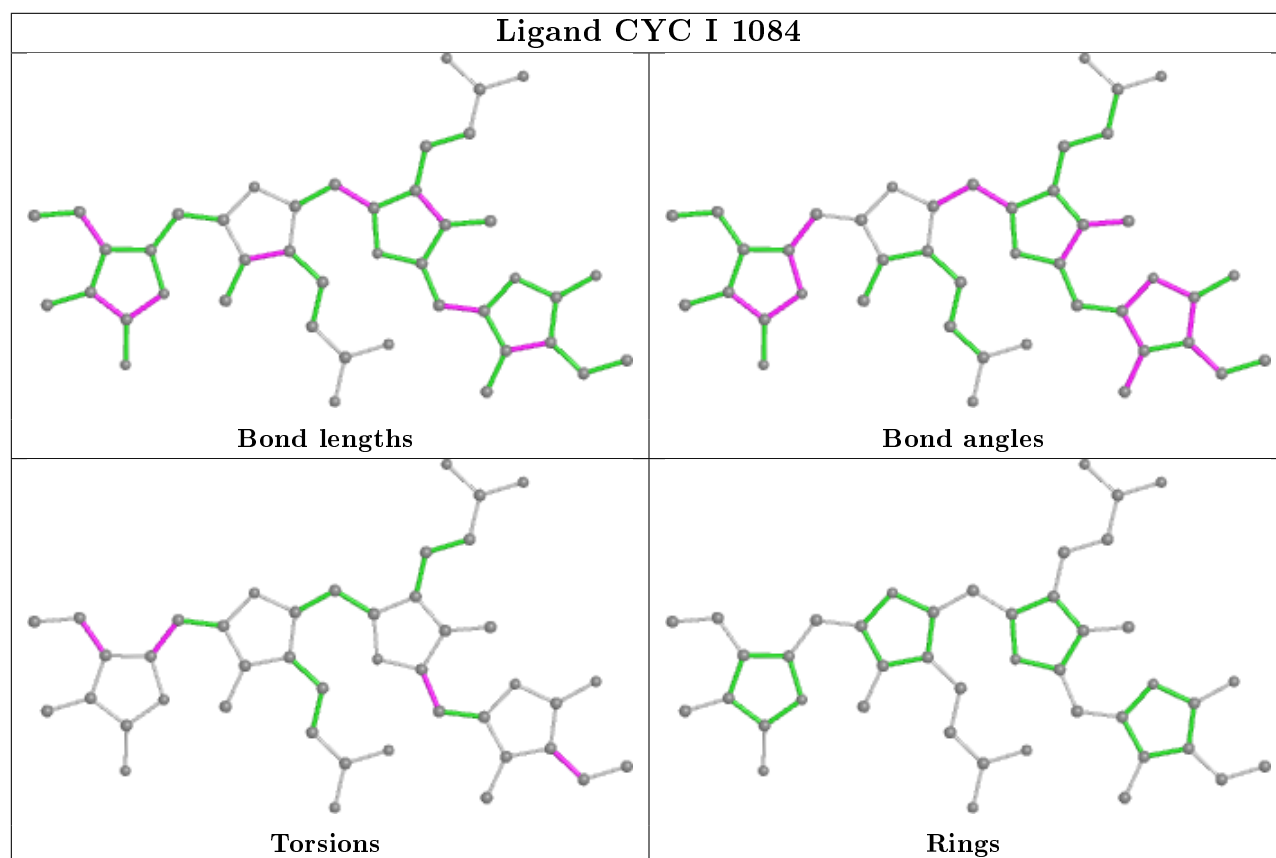
**Ligand CYC B 1082****Ligand CYC L 1153**

**Ligand CYC H 1082****Ligand CYC A 1084**

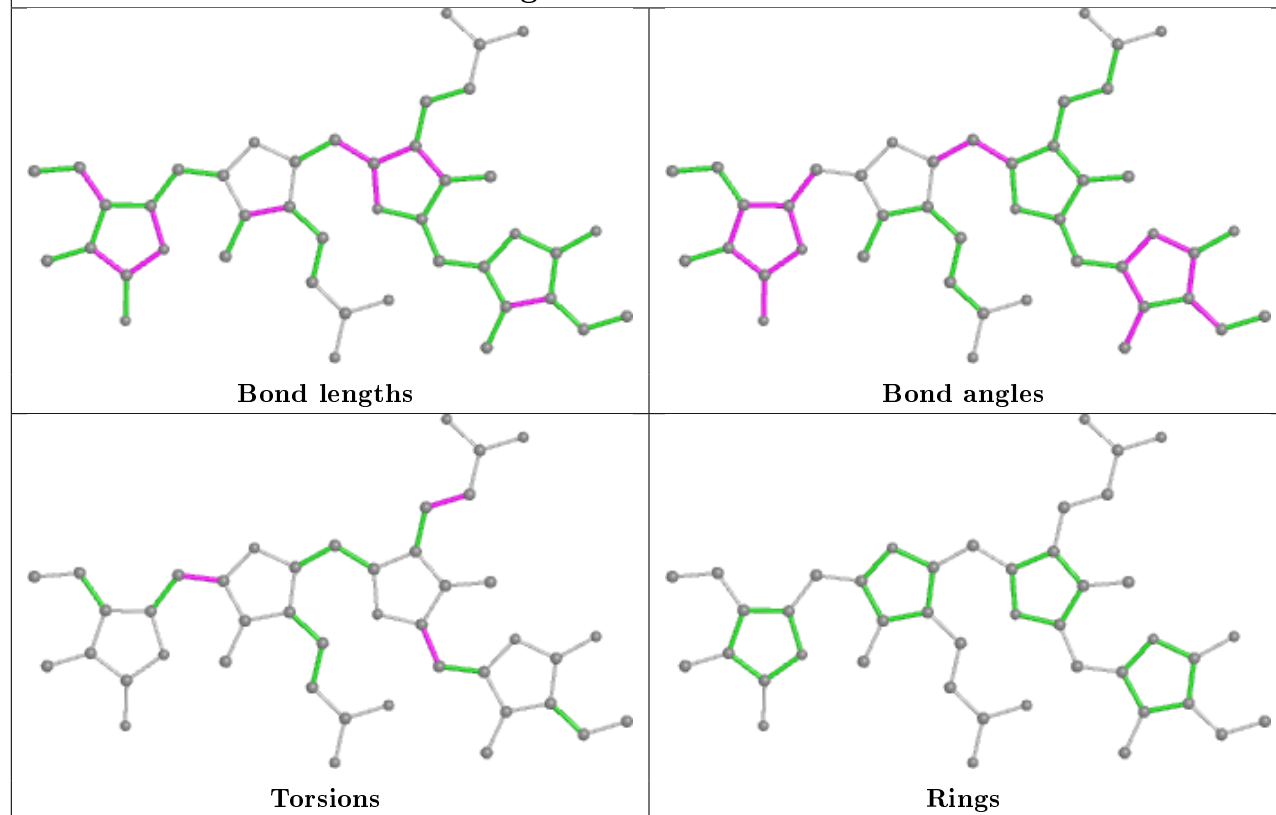
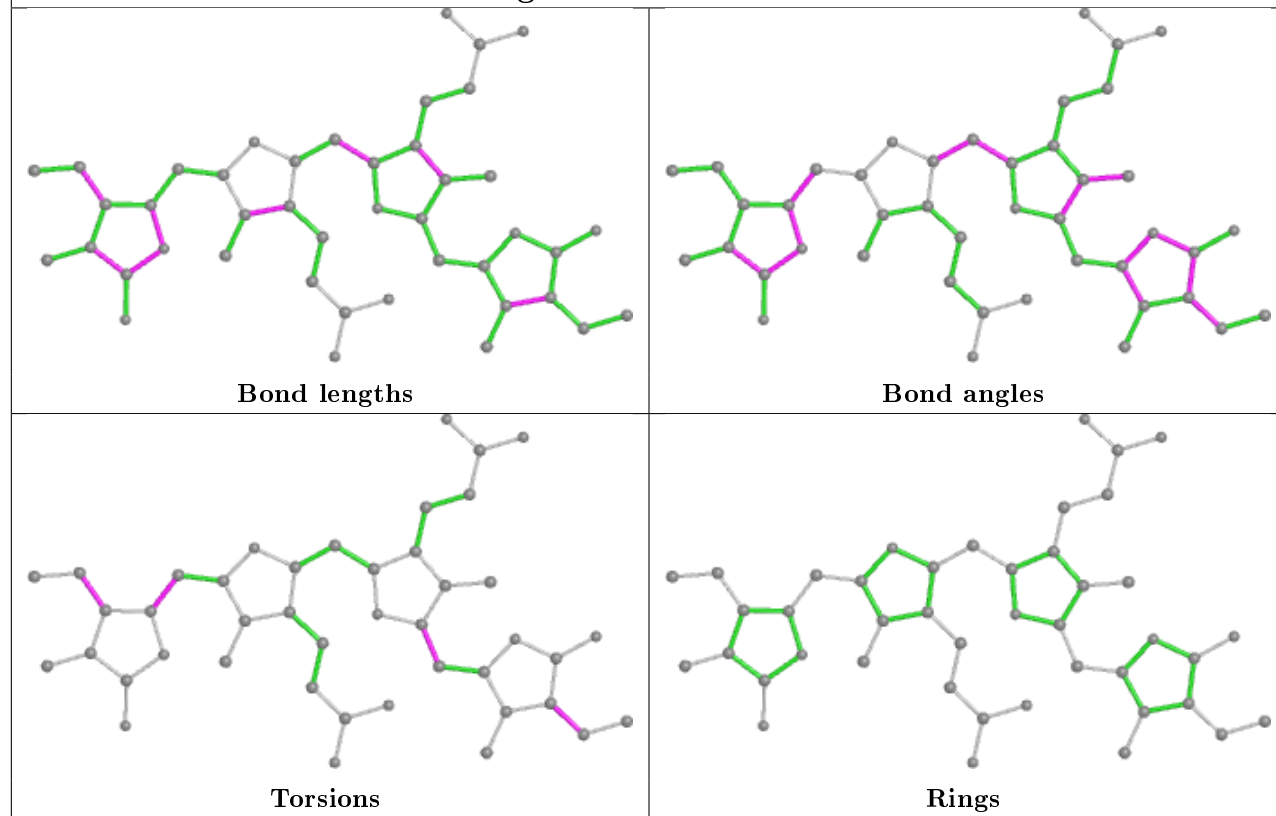
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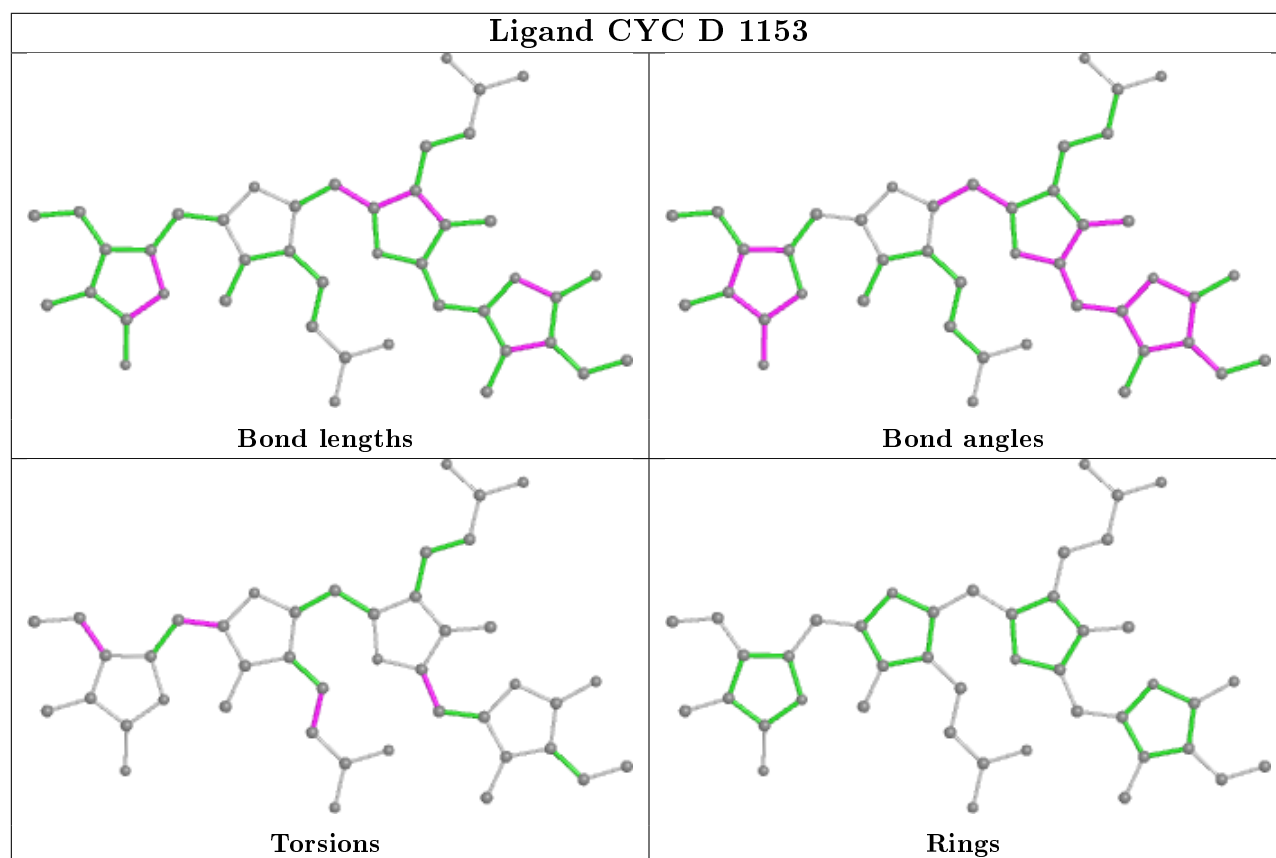
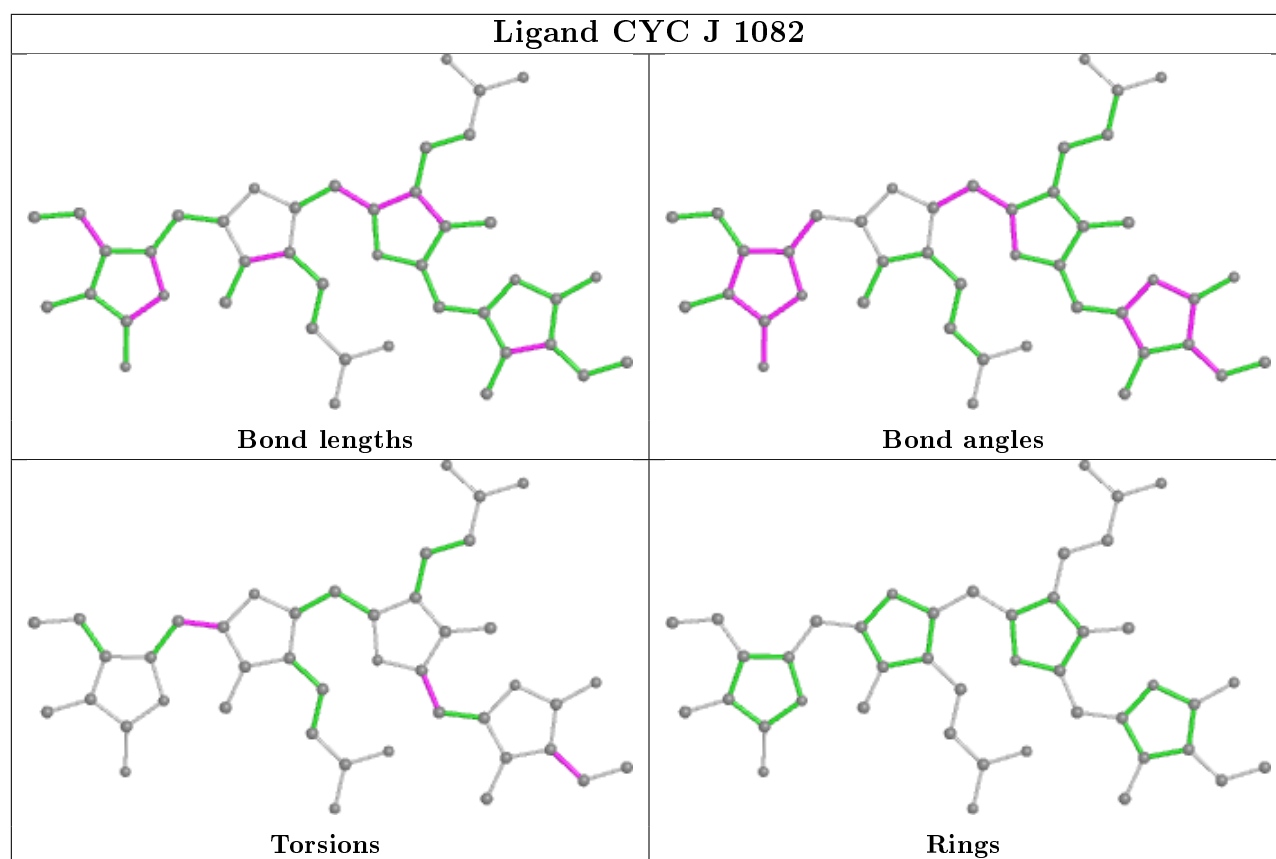


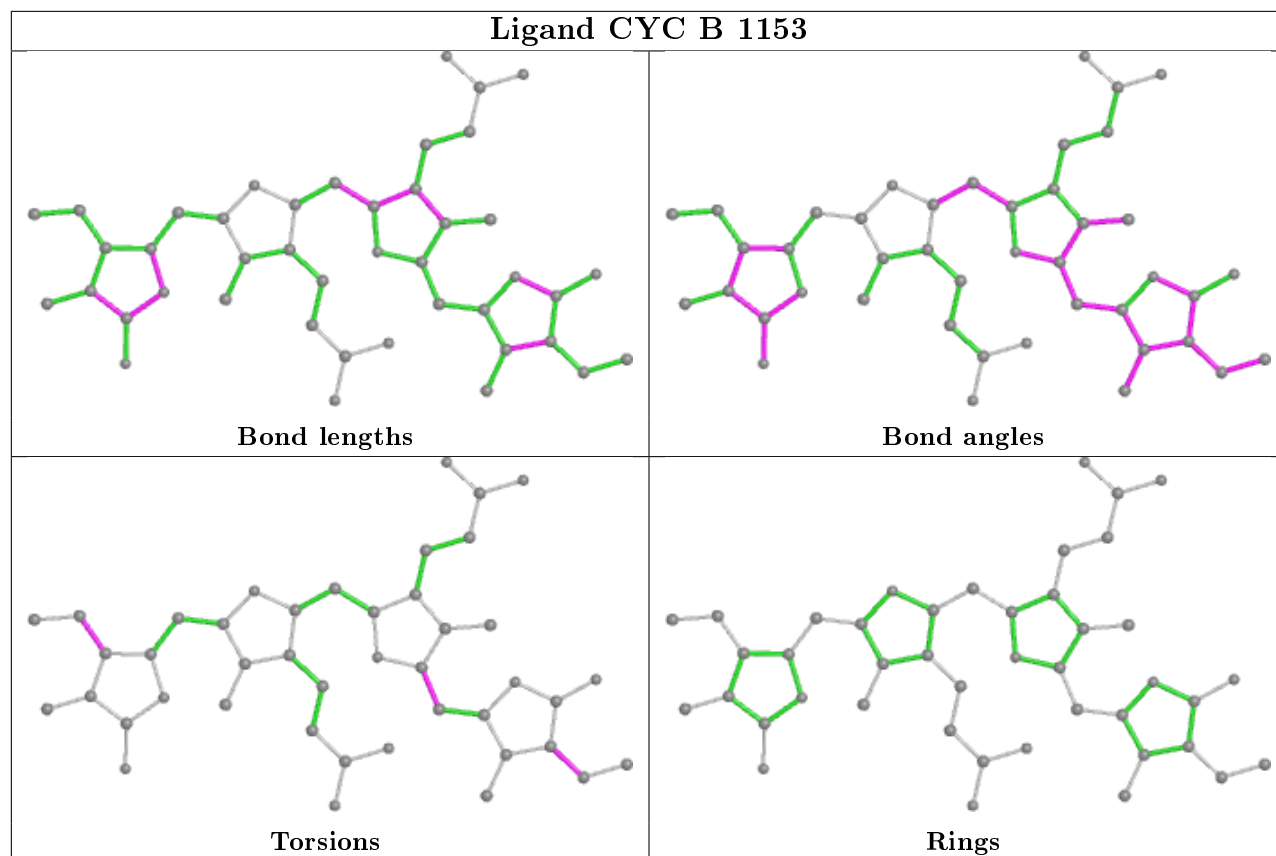
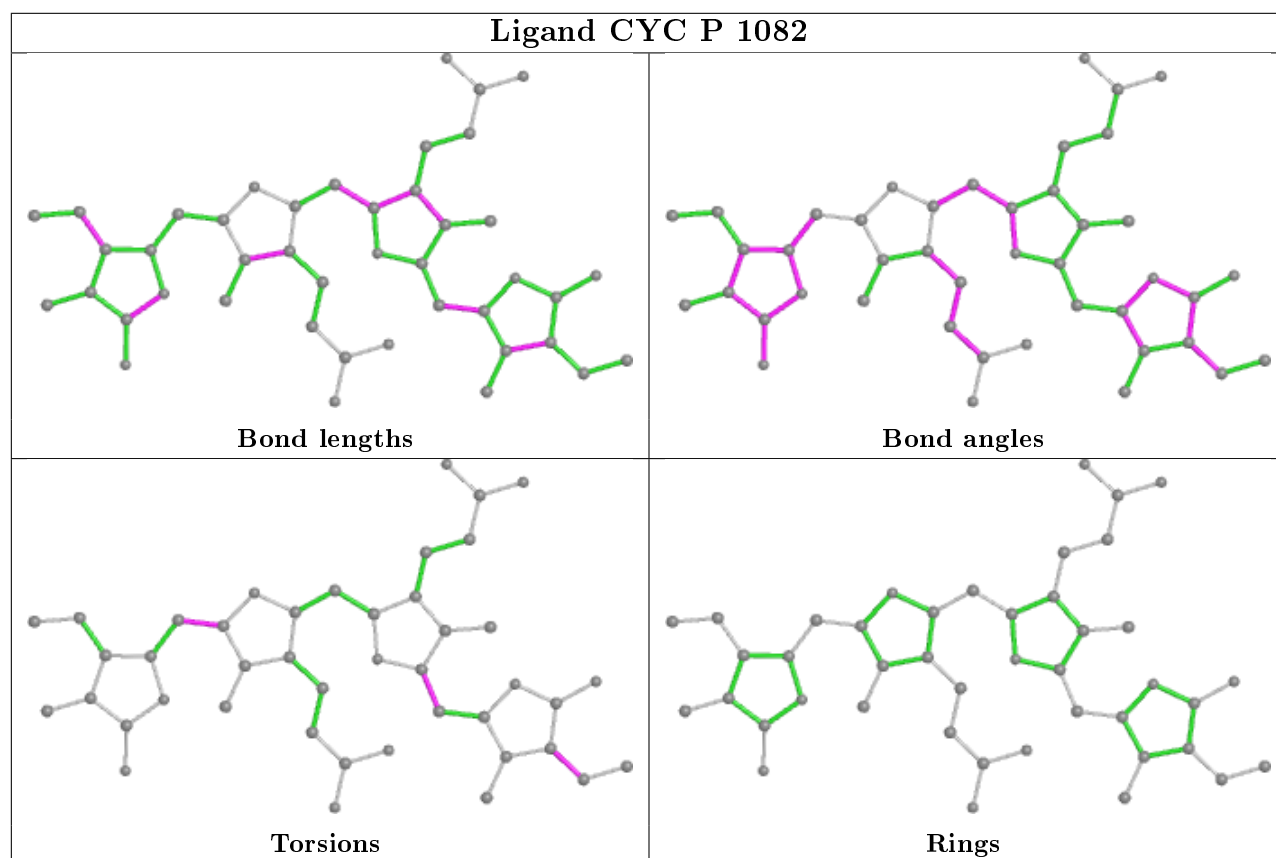
## Ligand CYC I 1084





**Ligand CYC X 1082****Ligand CYC M 1084**



**Ligand CYC B 1153****Ligand CYC P 1082**

## 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<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	162/162 (100%)	-0.77	0 100 100	10, 17, 32, 43	2 (1%)
1	C	162/162 (100%)	-0.69	0 100 100	12, 21, 34, 47	3 (1%)
1	E	162/162 (100%)	-0.80	0 100 100	8, 17, 30, 39	1 (0%)
1	G	162/162 (100%)	-0.71	0 100 100	12, 20, 34, 41	2 (1%)
1	I	162/162 (100%)	-0.72	0 100 100	12, 20, 34, 43	1 (0%)
1	K	162/162 (100%)	-0.76	0 100 100	10, 17, 29, 43	1 (0%)
1	M	162/162 (100%)	-0.55	1 (0%) 89 88	12, 23, 37, 52	1 (0%)
1	O	162/162 (100%)	-0.73	0 100 100	12, 21, 34, 44	3 (1%)
1	Q	162/162 (100%)	-0.74	0 100 100	11, 18, 32, 45	1 (0%)
1	S	162/162 (100%)	-0.75	0 100 100	12, 19, 33, 45	2 (1%)
1	U	162/162 (100%)	-0.64	0 100 100	13, 22, 37, 44	1 (0%)
1	W	162/162 (100%)	-0.72	0 100 100	13, 20, 32, 45	1 (0%)
2	B	171/172 (99%)	-0.80	0 100 100	8, 17, 32, 39	0
2	D	171/172 (99%)	-0.68	0 100 100	12, 22, 37, 44	0
2	F	171/172 (99%)	-0.57	1 (0%) 89 88	13, 24, 36, 50	1 (0%)
2	H	171/172 (99%)	-0.65	0 100 100	11, 21, 35, 45	1 (0%)
2	J	171/172 (99%)	-0.61	0 100 100	13, 22, 35, 49	0
2	L	171/172 (99%)	-0.64	1 (0%) 89 88	11, 20, 35, 56	0
2	N	171/172 (99%)	-0.67	0 100 100	10, 20, 35, 49	0
2	P	171/172 (99%)	-0.43	1 (0%) 89 88	17, 28, 41, 57	0
2	R	171/172 (99%)	-0.59	0 100 100	13, 23, 38, 43	1 (0%)
2	T	171/172 (99%)	-0.61	0 100 100	14, 23, 36, 47	1 (0%)
2	V	171/172 (99%)	-0.74	0 100 100	9, 19, 33, 42	1 (0%)
2	X	171/172 (99%)	-0.48	0 100 100	15, 25, 38, 49	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3996/4008 (99%)	-0.67	4 (0%) 95 95	8, 21, 36, 57	25 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	70	GLN	2.5
2	F	172	SER	2.3
2	P	172	SER	2.2
2	L	29	GLN	2.1

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

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
2	MEN	P	72	9/10	0.91	0.11	26,28,33,36	0
2	MEN	X	72	9/10	0.94	0.09	22,24,31,31	0
2	MEN	J	72	9/10	0.96	0.07	21,23,23,27	0
2	MEN	T	72	9/10	0.96	0.08	21,24,26,30	0
2	MEN	B	72	9/10	0.96	0.08	14,16,19,21	0
2	MEN	H	72	9/10	0.96	0.09	17,19,25,25	0
2	MEN	F	72	9/10	0.96	0.08	18,19,21,23	0
2	MEN	N	72	9/10	0.97	0.07	16,18,25,27	0
2	MEN	D	72	9/10	0.97	0.08	15,18,26,28	0
2	MEN	V	72	9/10	0.97	0.08	16,18,21,22	0
2	MEN	L	72	9/10	0.98	0.06	16,19,22,24	0
2	MEN	R	72	9/10	0.98	0.07	20,21,27,27	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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,

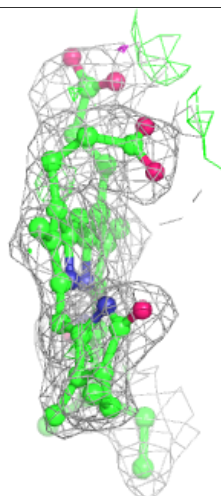
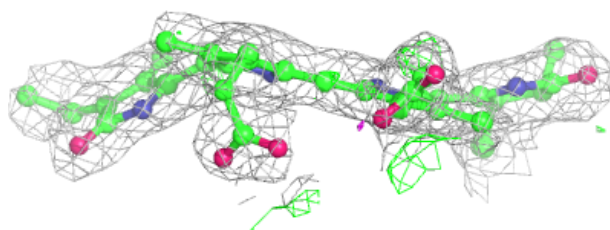
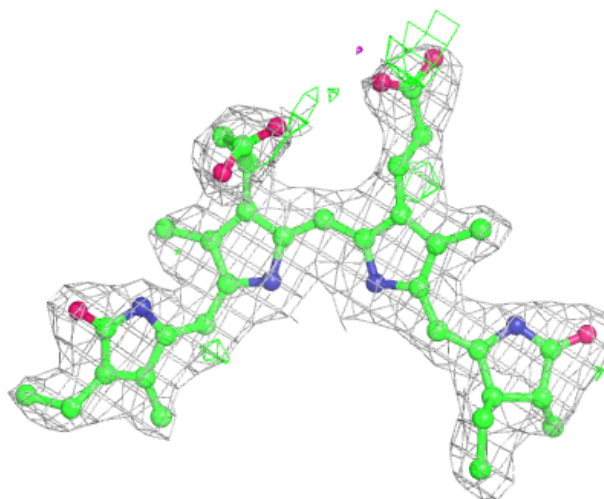
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CYC	P	1082	43/43	0.85	0.16	26,39,47,49	0
3	CYC	J	1082	43/43	0.86	0.15	18,29,37,42	0
3	CYC	T	1082	43/43	0.87	0.16	20,30,37,39	0
3	CYC	X	1082	43/43	0.87	0.14	20,30,39,43	0
3	CYC	R	1082	43/43	0.88	0.15	18,28,34,43	0
3	CYC	F	1082	43/43	0.88	0.15	18,29,39,42	0
3	CYC	L	1082	43/43	0.89	0.13	13,23,33,37	0
3	CYC	H	1082	43/43	0.90	0.13	11,25,31,37	0
3	CYC	X	1153	43/43	0.90	0.12	23,29,40,45	0
3	CYC	N	1082	43/43	0.90	0.13	17,27,35,37	0
3	CYC	V	1082	43/43	0.90	0.14	12,24,30,36	0
3	CYC	B	1082	43/43	0.90	0.14	1,23,30,36	0
3	CYC	D	1082	43/43	0.91	0.13	17,28,32,35	0
3	CYC	L	1153	43/43	0.92	0.11	18,25,37,44	0
3	CYC	R	1153	43/43	0.92	0.12	17,23,32,39	0
3	CYC	T	1153	43/43	0.93	0.11	17,22,32,39	0
3	CYC	P	1153	43/43	0.93	0.11	19,27,40,44	0
3	CYC	U	1084	43/43	0.93	0.13	15,21,23,25	0
3	CYC	F	1153	43/43	0.93	0.11	17,22,34,42	0
3	CYC	D	1153	43/43	0.93	0.12	17,21,28,36	0
3	CYC	B	1153	43/43	0.93	0.11	11,16,23,30	0
3	CYC	N	1153	43/43	0.93	0.11	15,18,26,32	0
3	CYC	H	1153	43/43	0.94	0.10	12,18,30,36	0
3	CYC	M	1084	43/43	0.94	0.13	18,21,25,28	0
3	CYC	J	1153	43/43	0.94	0.11	15,21,28,34	0
3	CYC	W	1084	43/43	0.95	0.11	11,17,21,24	0
3	CYC	V	1153	43/43	0.95	0.10	9,17,25,30	0
3	CYC	I	1084	43/43	0.95	0.13	7,14,17,19	0
3	CYC	C	1084	43/43	0.96	0.11	13,19,22,23	0
3	CYC	Q	1084	43/43	0.96	0.09	5,13,16,19	0
3	CYC	G	1084	43/43	0.96	0.11	8,16,20,23	0
3	CYC	K	1084	43/43	0.96	0.11	7,13,15,18	0
3	CYC	O	1084	43/43	0.96	0.12	12,15,18,19	0
3	CYC	A	1084	43/43	0.97	0.11	11,14,18,20	0
3	CYC	E	1084	43/43	0.97	0.10	5,10,14,15	0
3	CYC	S	1084	43/43	0.97	0.10	11,13,16,17	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 CYC P 1082:**

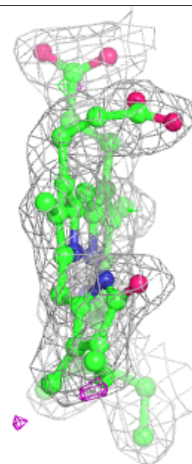
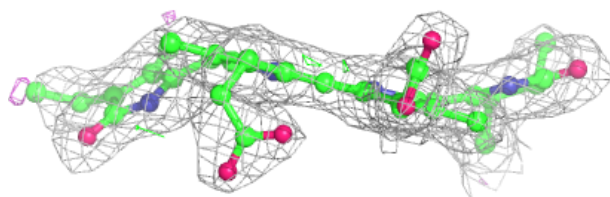
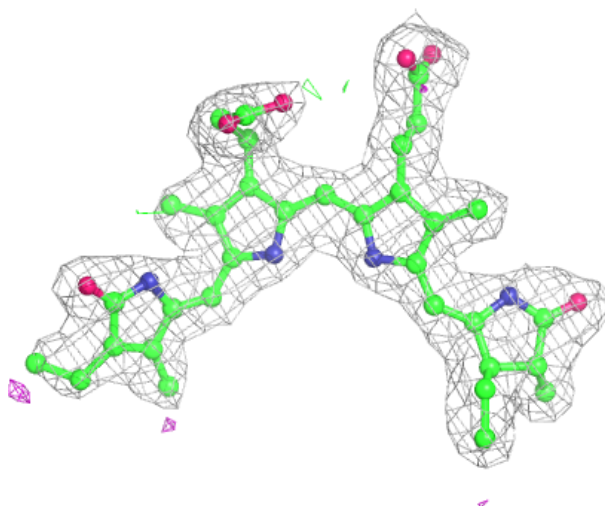
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





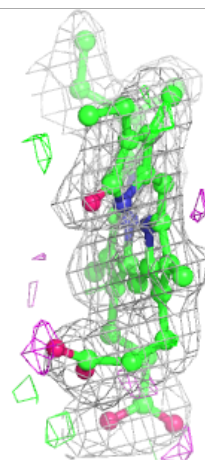
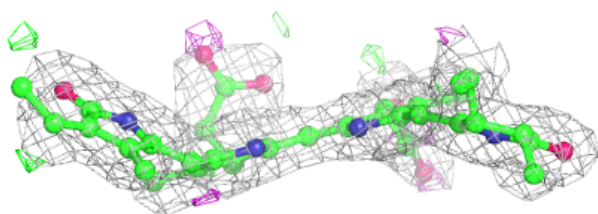
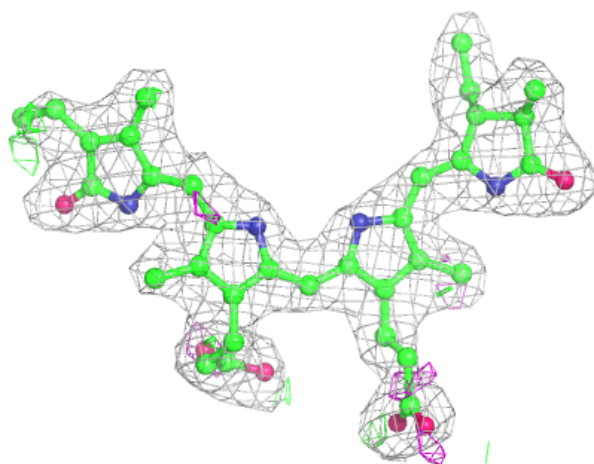
**Electron density around CYC J 1082:**

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



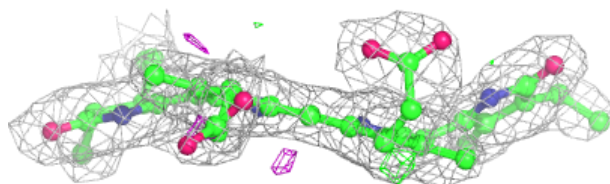
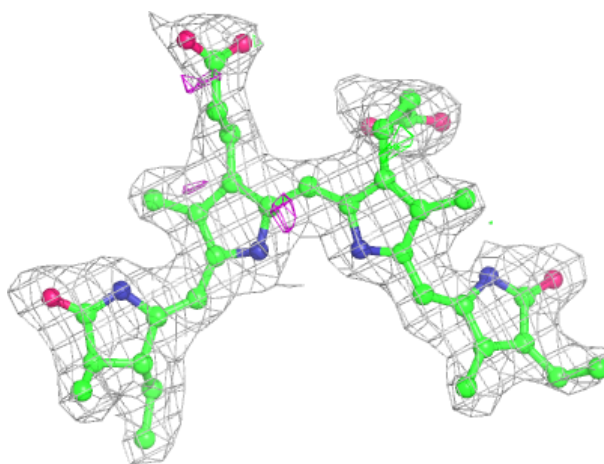
**Electron density around CYC T 1082:**

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



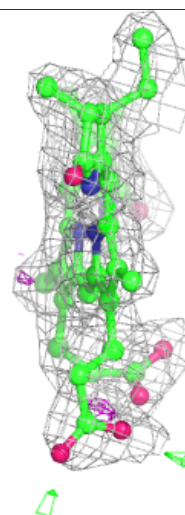
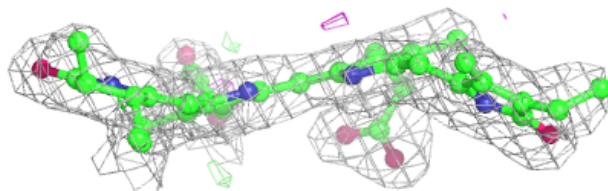
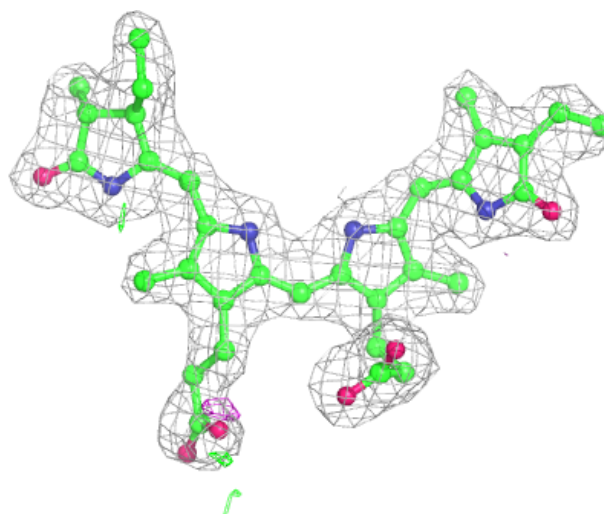
**Electron density around CYC X 1082:**

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



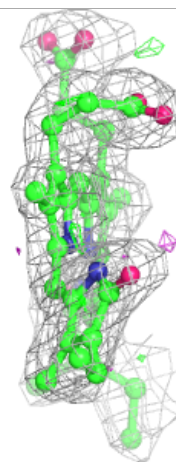
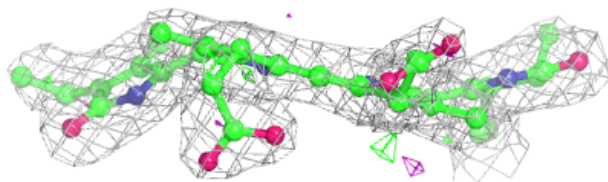
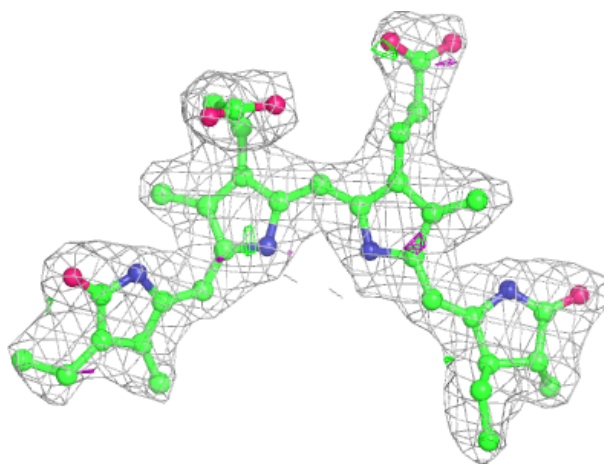
**Electron density around CYC R 1082:**

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



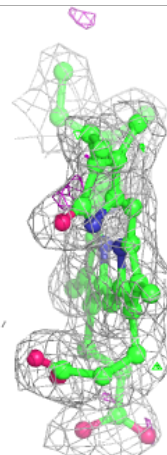
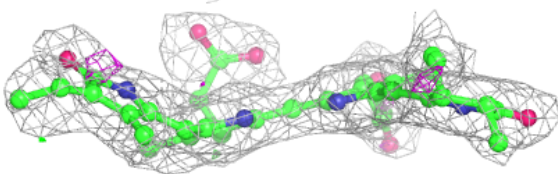
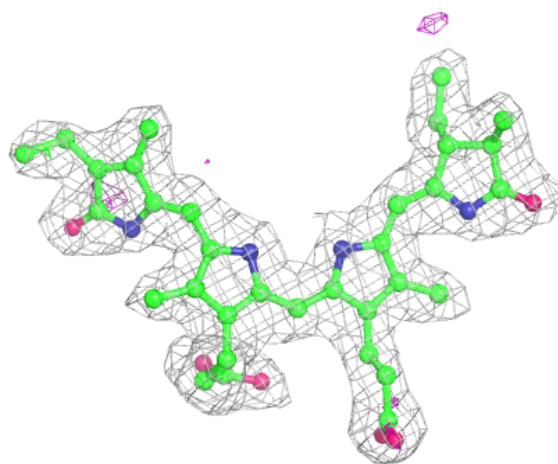
**Electron density around CYC F 1082:**

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



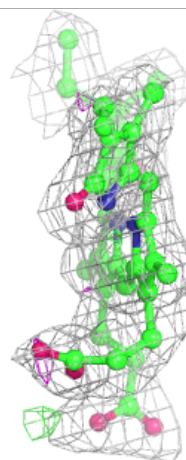
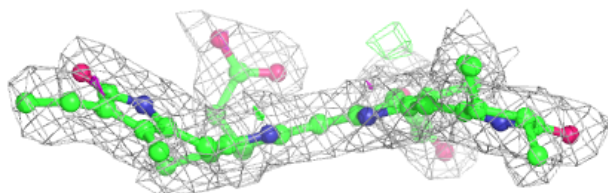
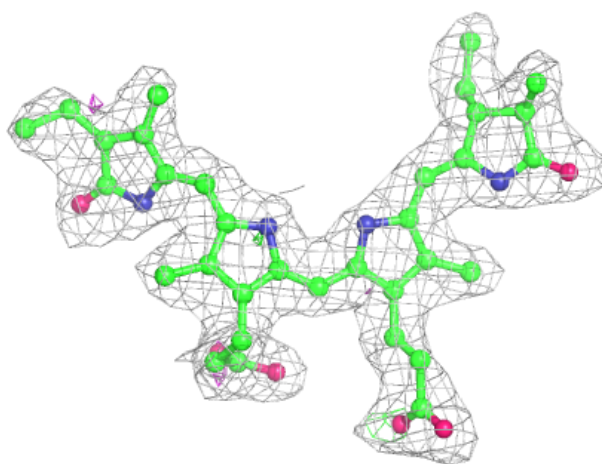
**Electron density around CYC L 1082:**

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



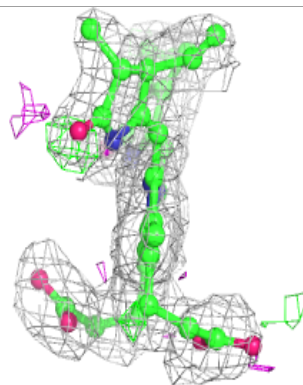
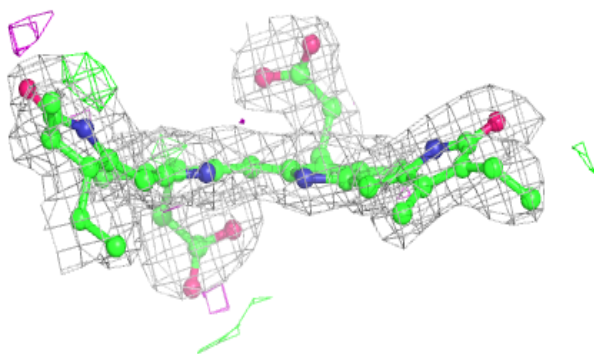
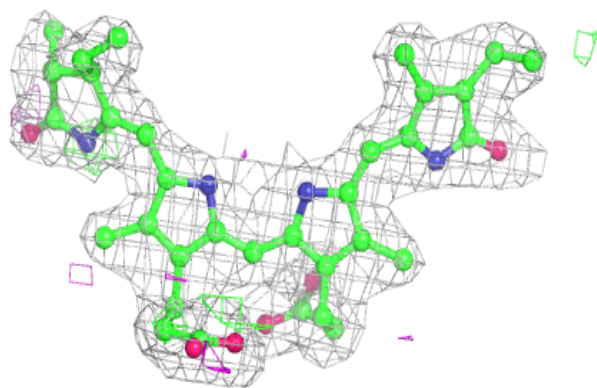
**Electron density around CYC H 1082:**

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



**Electron density around CYC X 1153:**

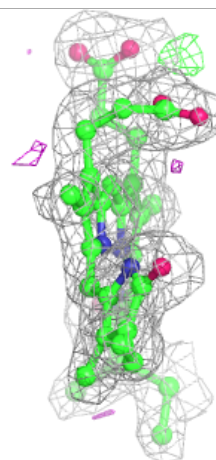
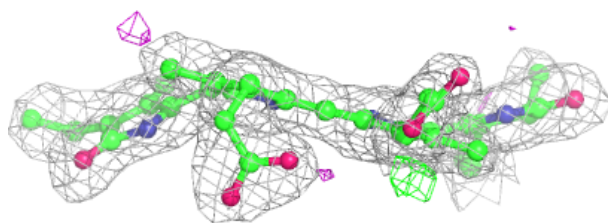
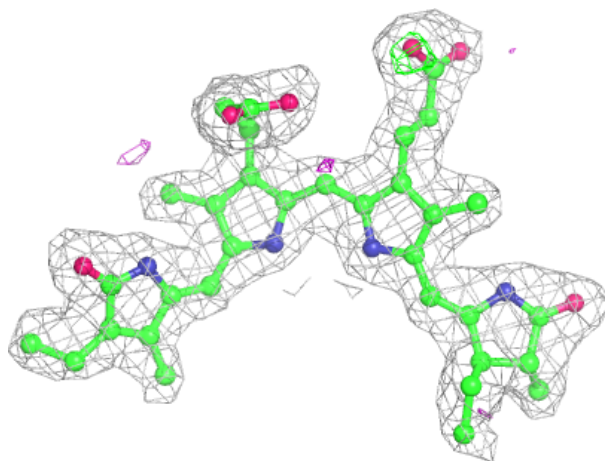
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





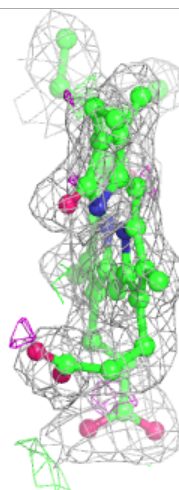
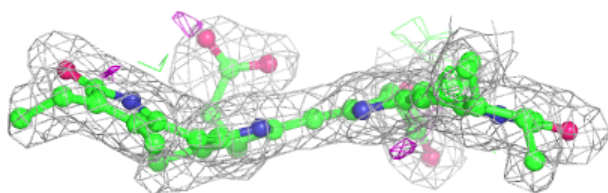
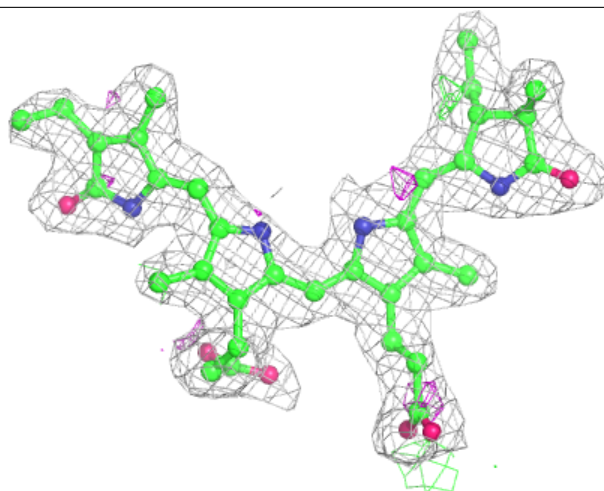
**Electron density around CYC N 1082:**

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



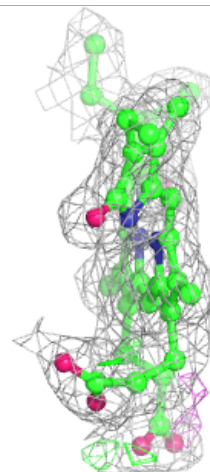
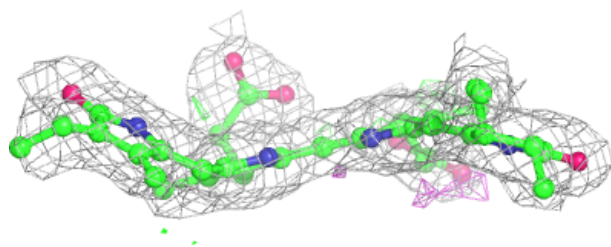
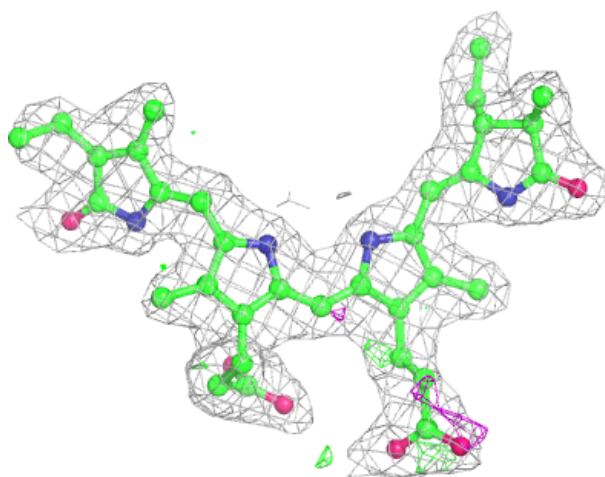
**Electron density around CYC V 1082:**

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



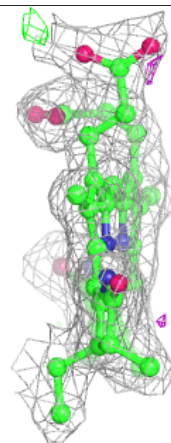
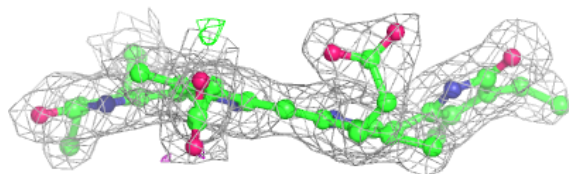
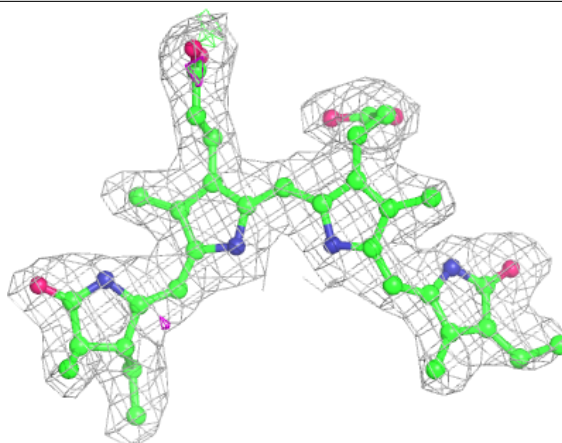
**Electron density around CYC B 1082:**

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

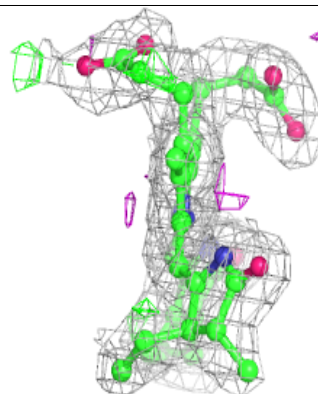
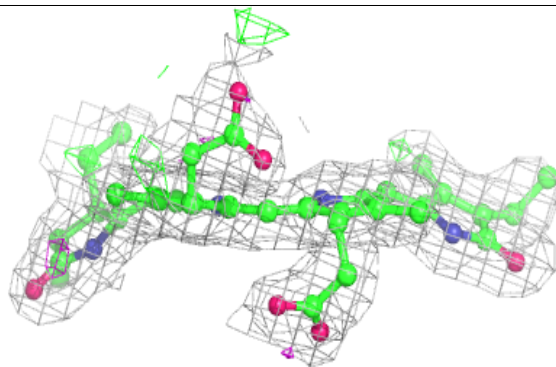
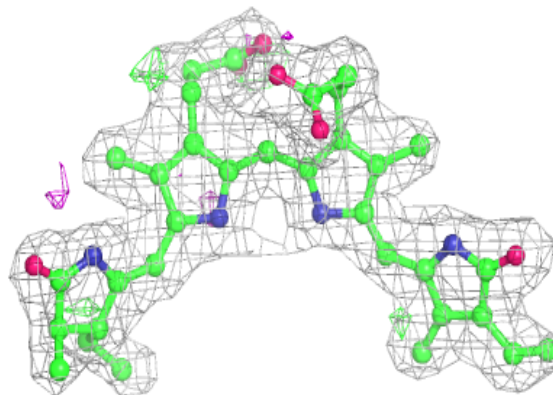


**Electron density around CYC D 1082:**

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

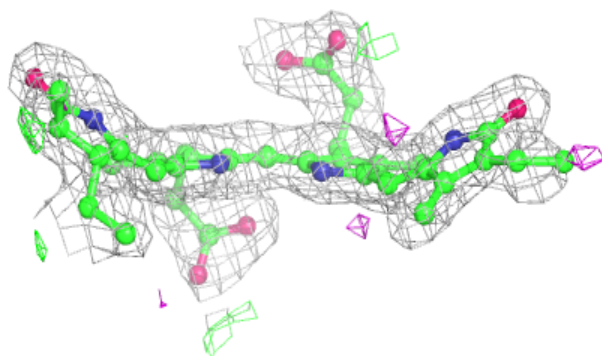
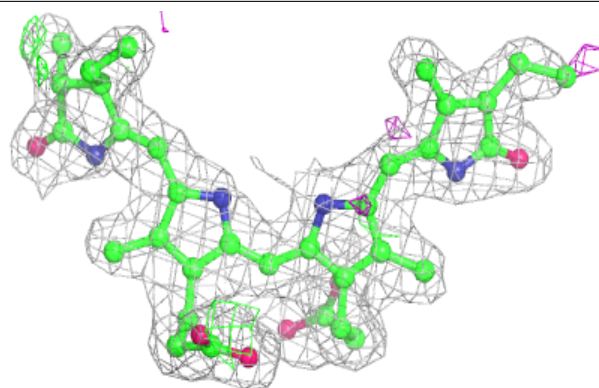
**Electron density around CYC L 1153:**

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

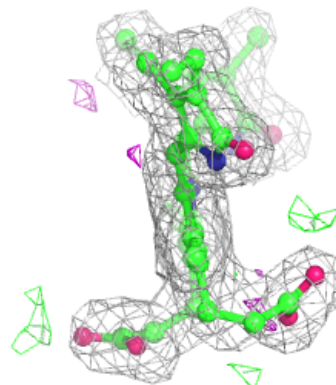
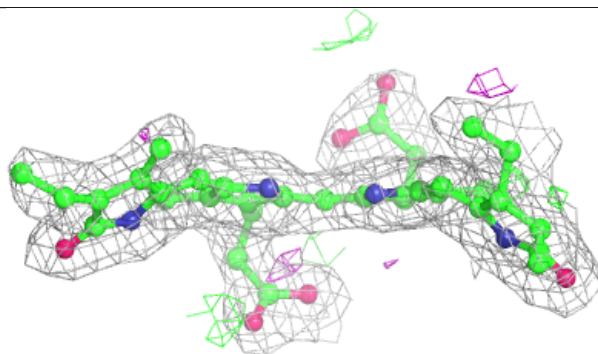
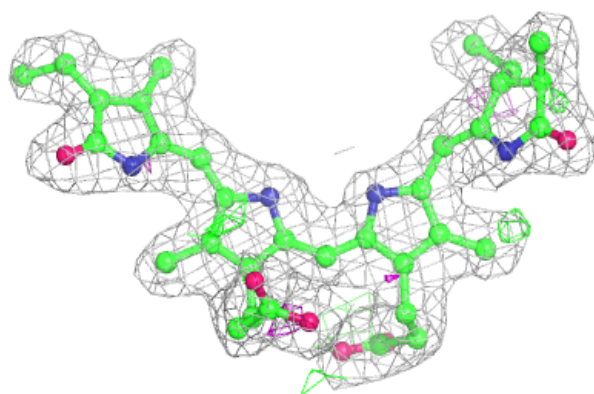


**Electron density around CYC R 1153:**

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

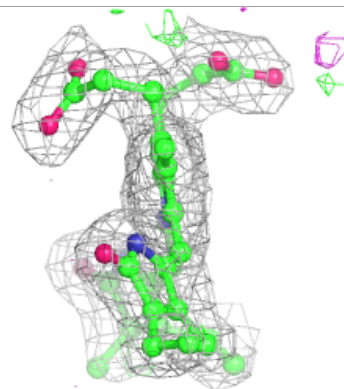
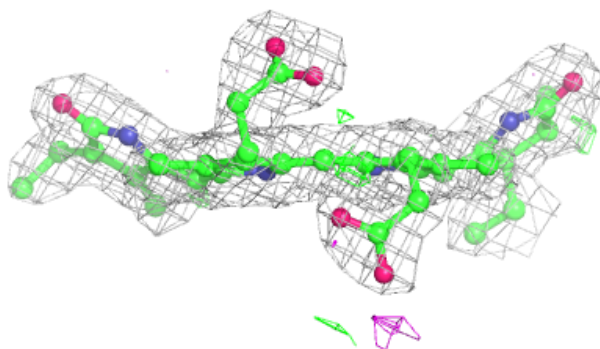
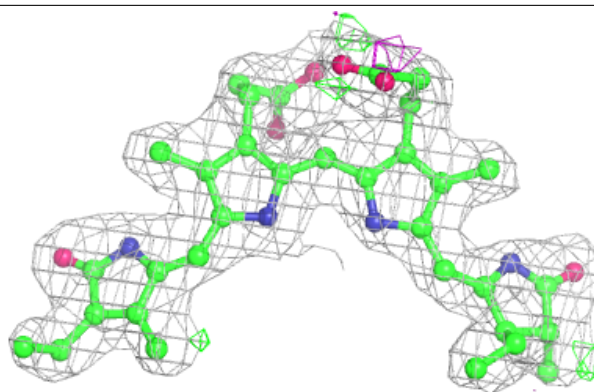
**Electron density around CYC T 1153:**

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



**Electron density around CYC P 1153:**

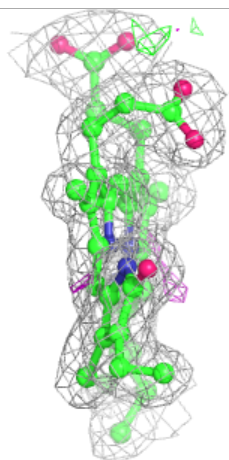
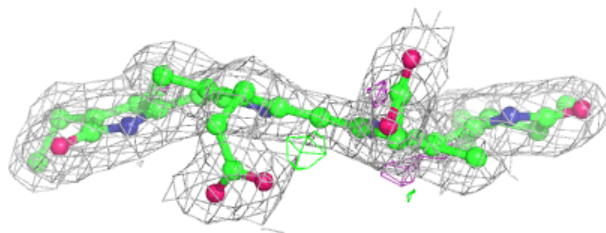
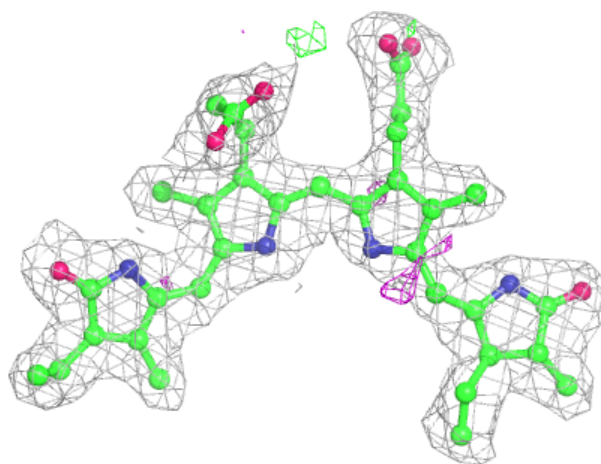
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





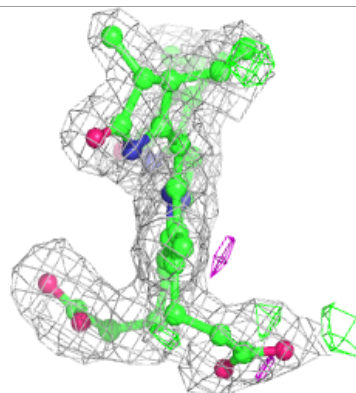
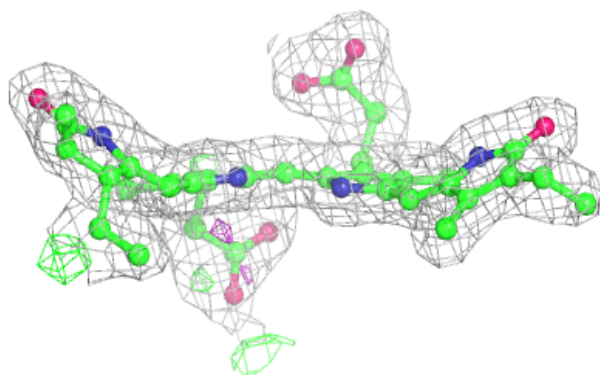
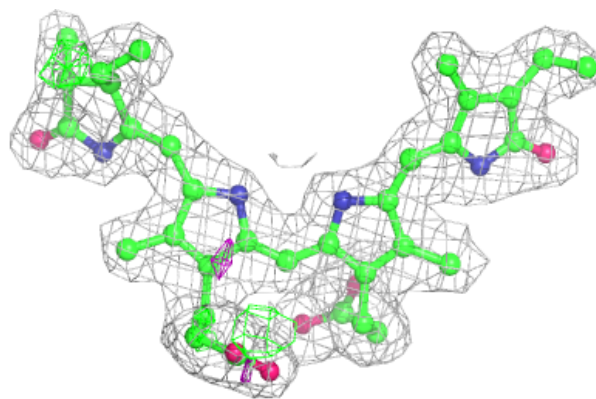
**Electron density around CYC U 1084:**

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

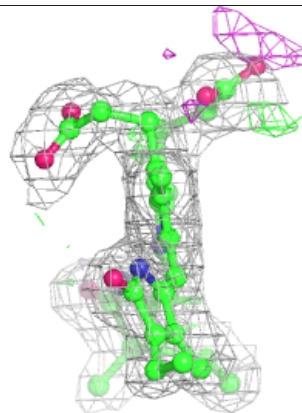
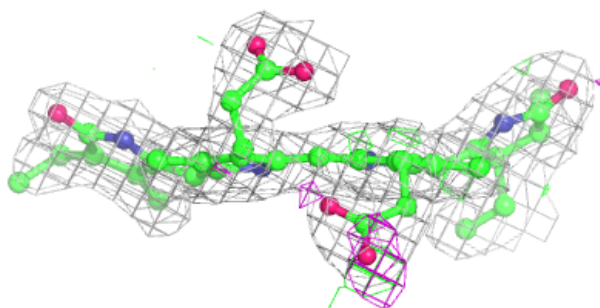
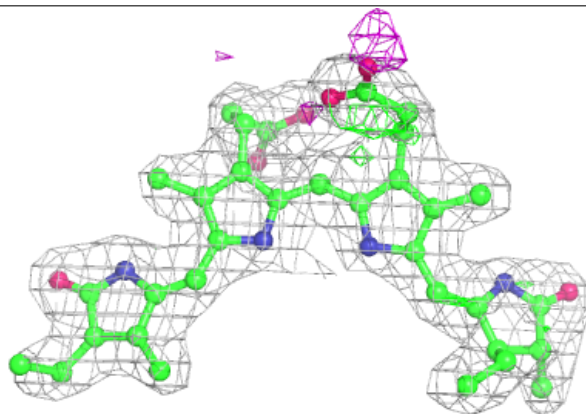


**Electron density around CYC F 1153:**

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

**Electron density around CYC D 1153:**

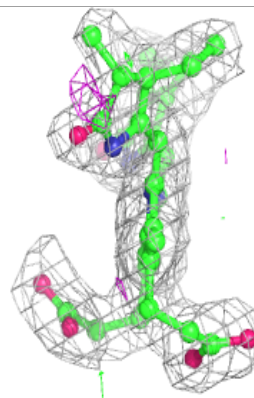
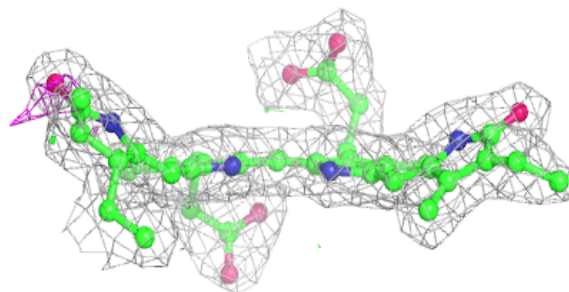
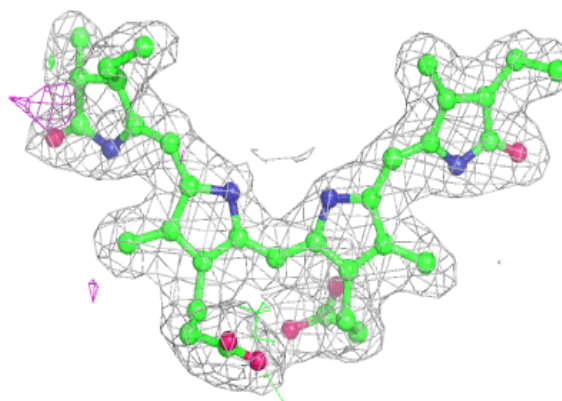
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



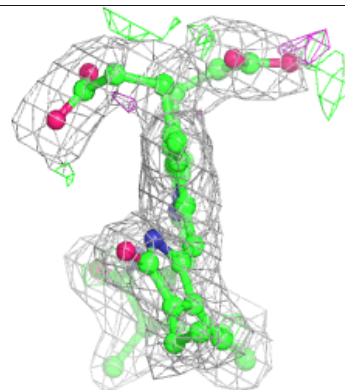
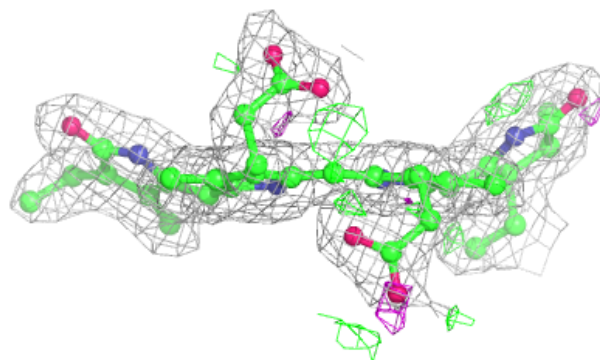
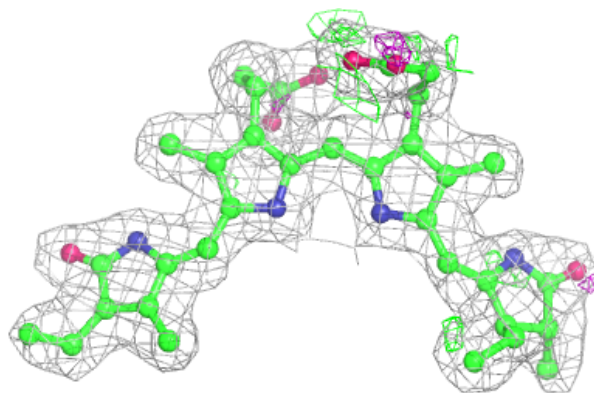


**Electron density around CYC B 1153:**

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

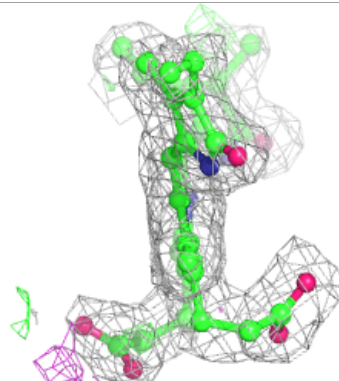
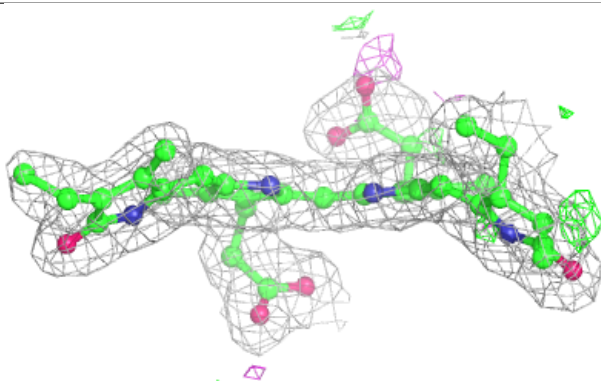
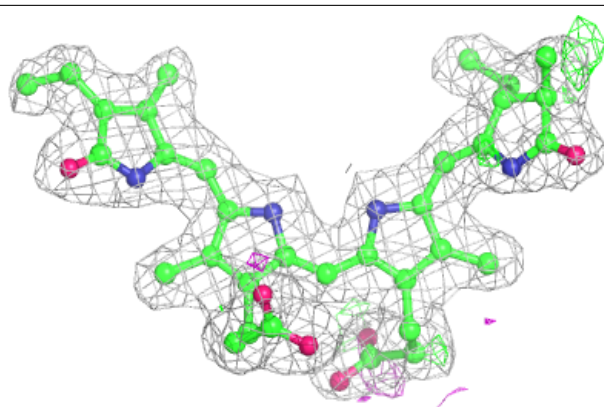
**Electron density around CYC N 1153:**

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

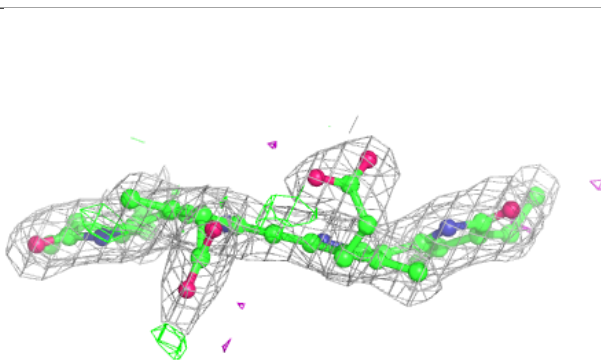
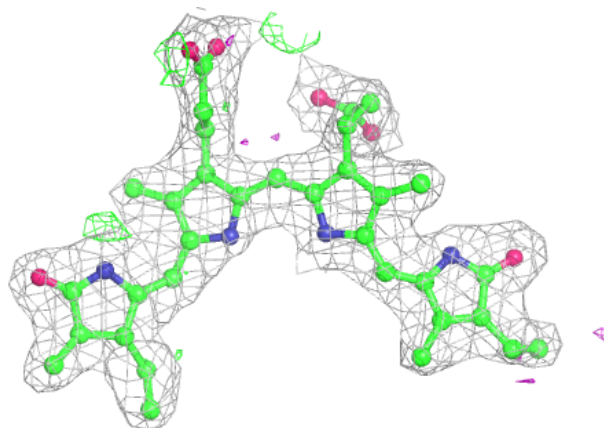


**Electron density around CYC H 1153:**

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

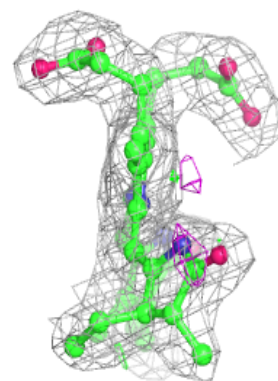
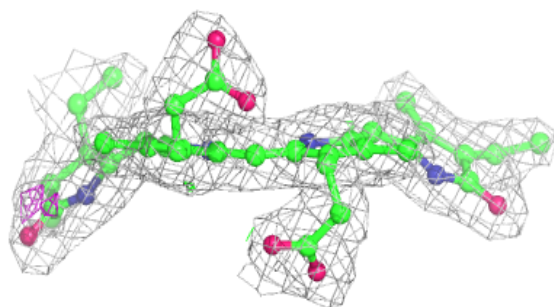
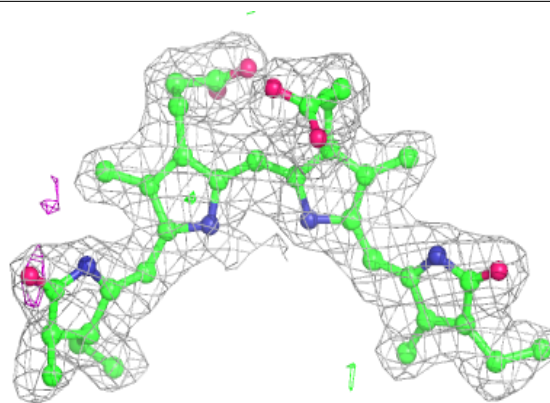
**Electron density around CYC M 1084:**

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



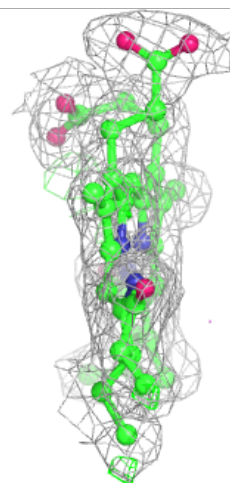
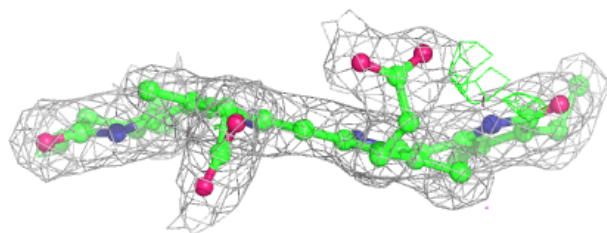
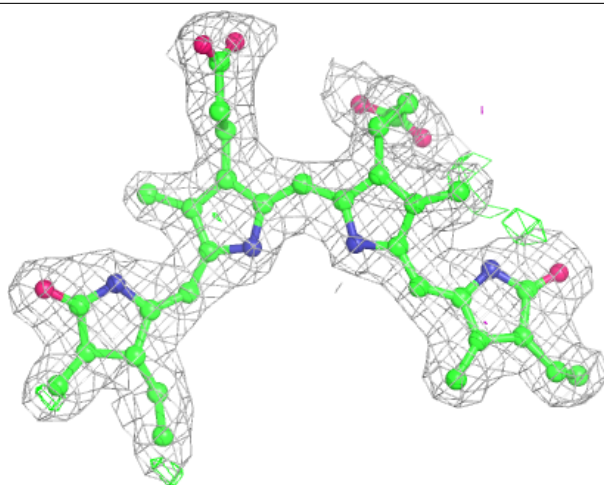
**Electron density around CYC J 1153:**

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



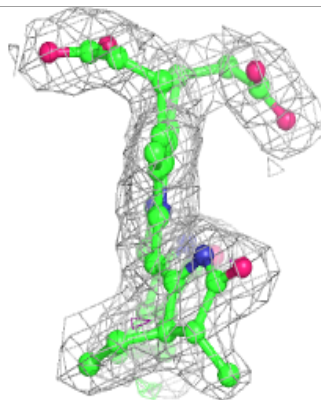
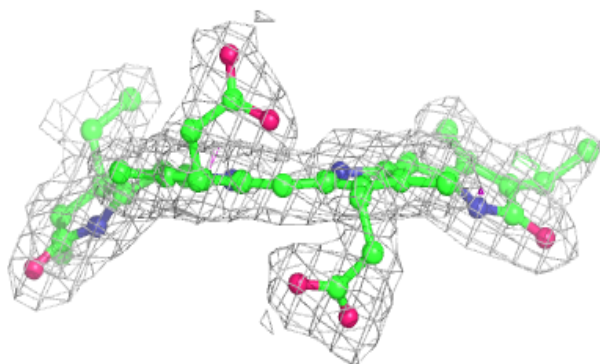
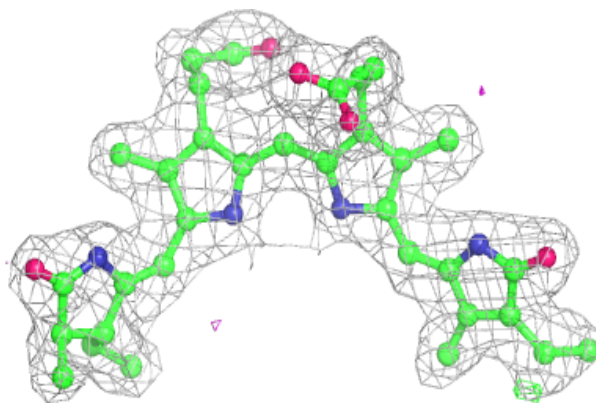
**Electron density around CYC W 1084:**

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



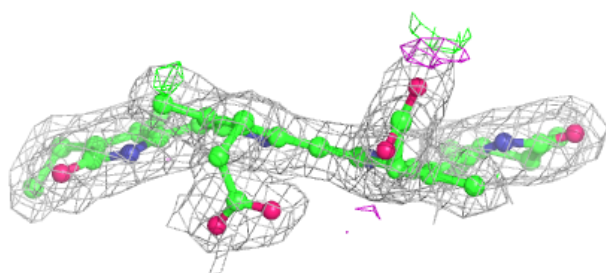
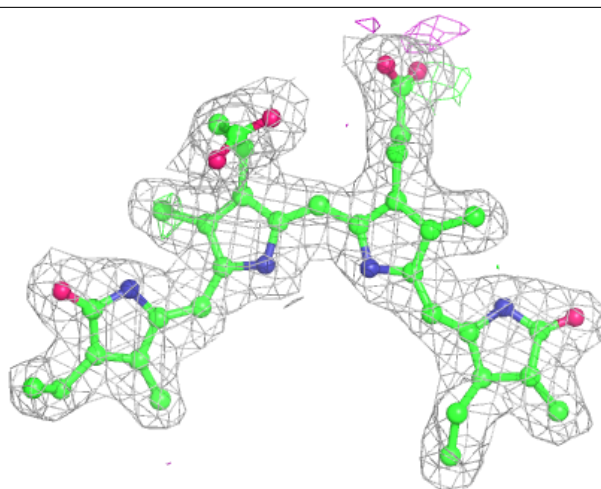
**Electron density around CYC V 1153:**

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



**Electron density around CYC I 1084:**

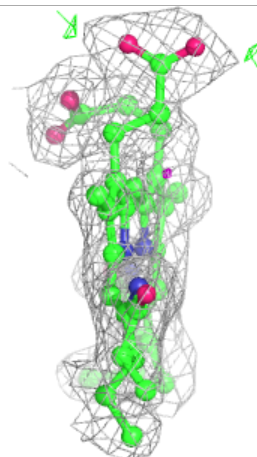
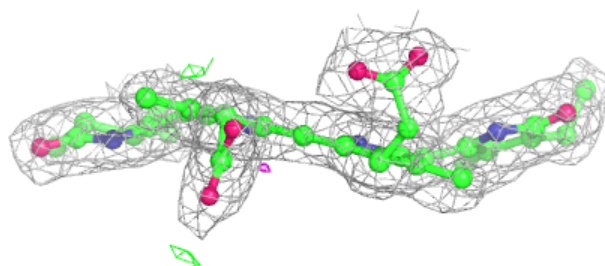
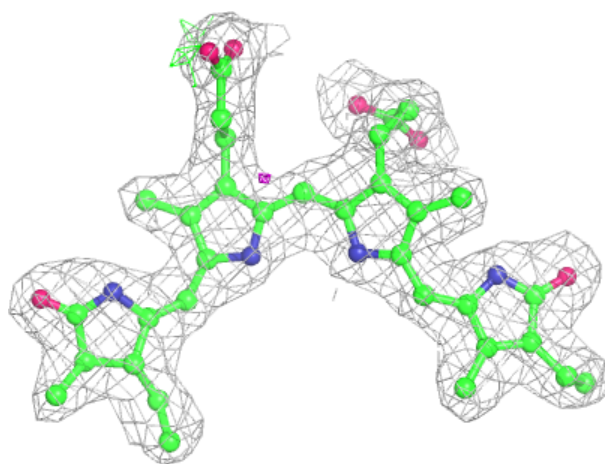
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





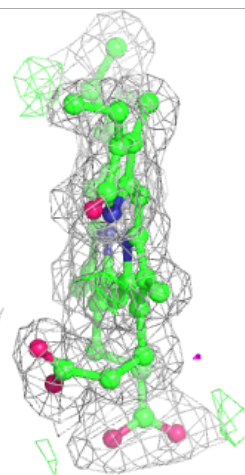
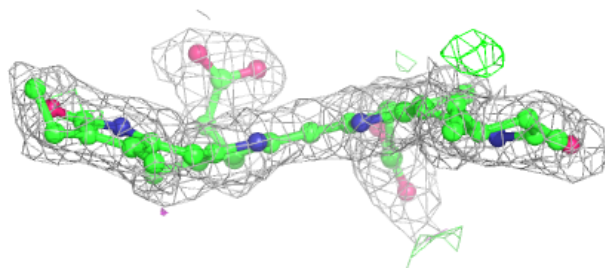
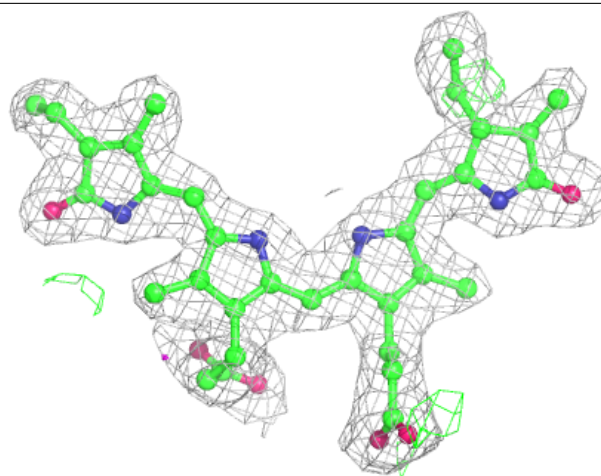
**Electron density around CYC C 1084:**

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



**Electron density around CYC Q 1084:**

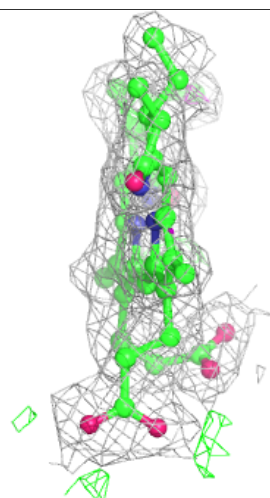
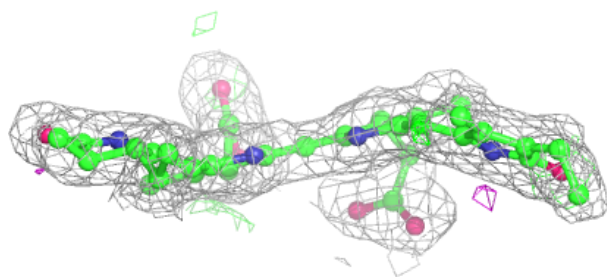
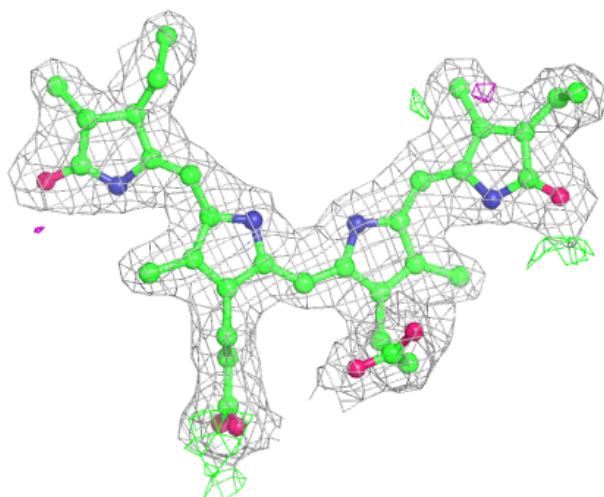
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





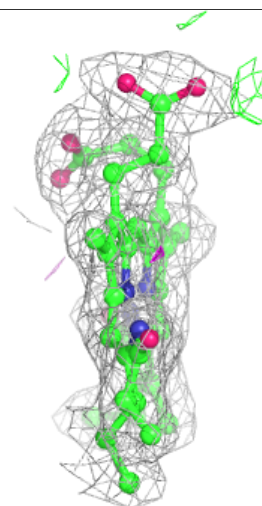
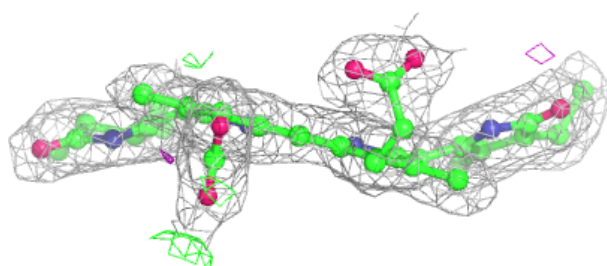
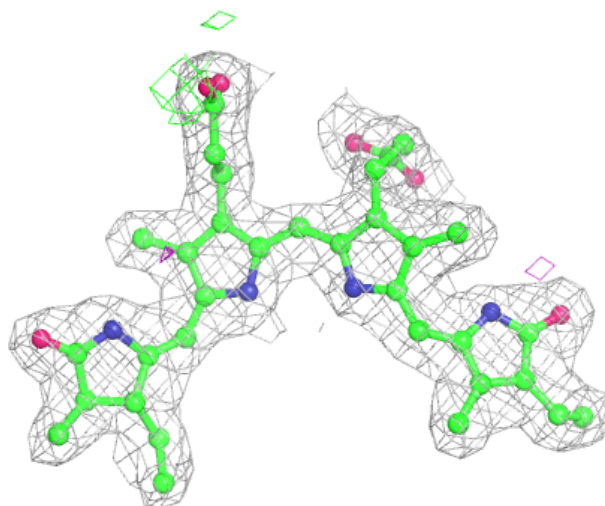
**Electron density around CYC G 1084:**

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



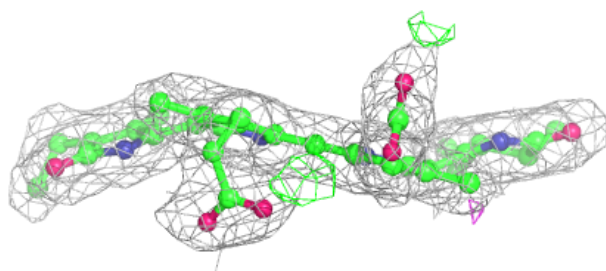
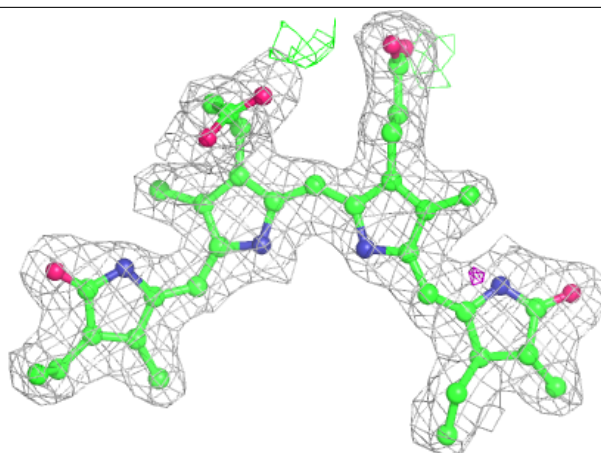
**Electron density around CYC K 1084:**

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



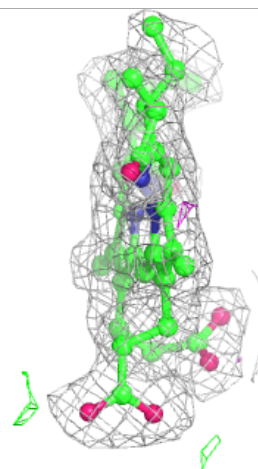
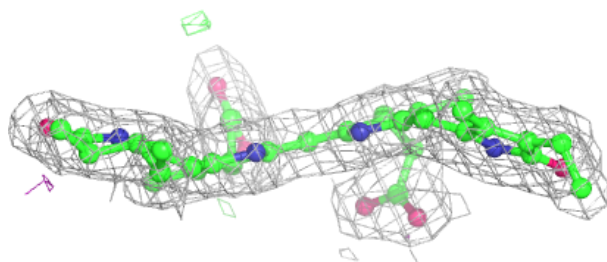
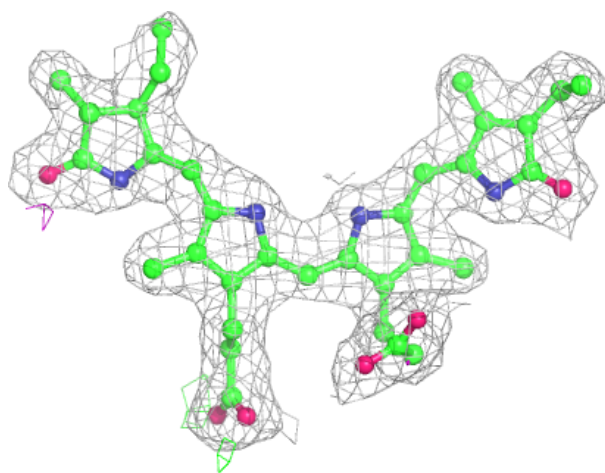
**Electron density around CYC O 1084:**

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



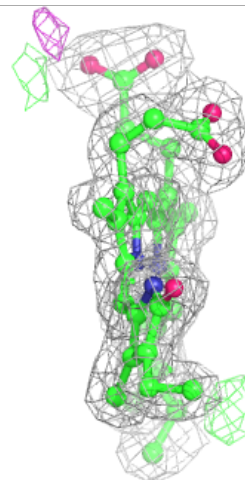
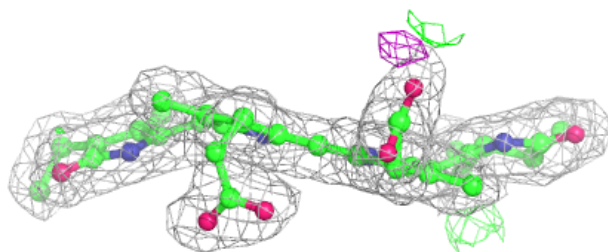
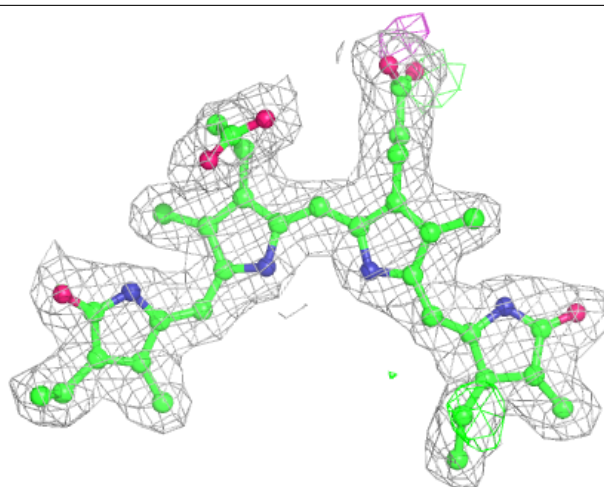
**Electron density around CYC A 1084:**

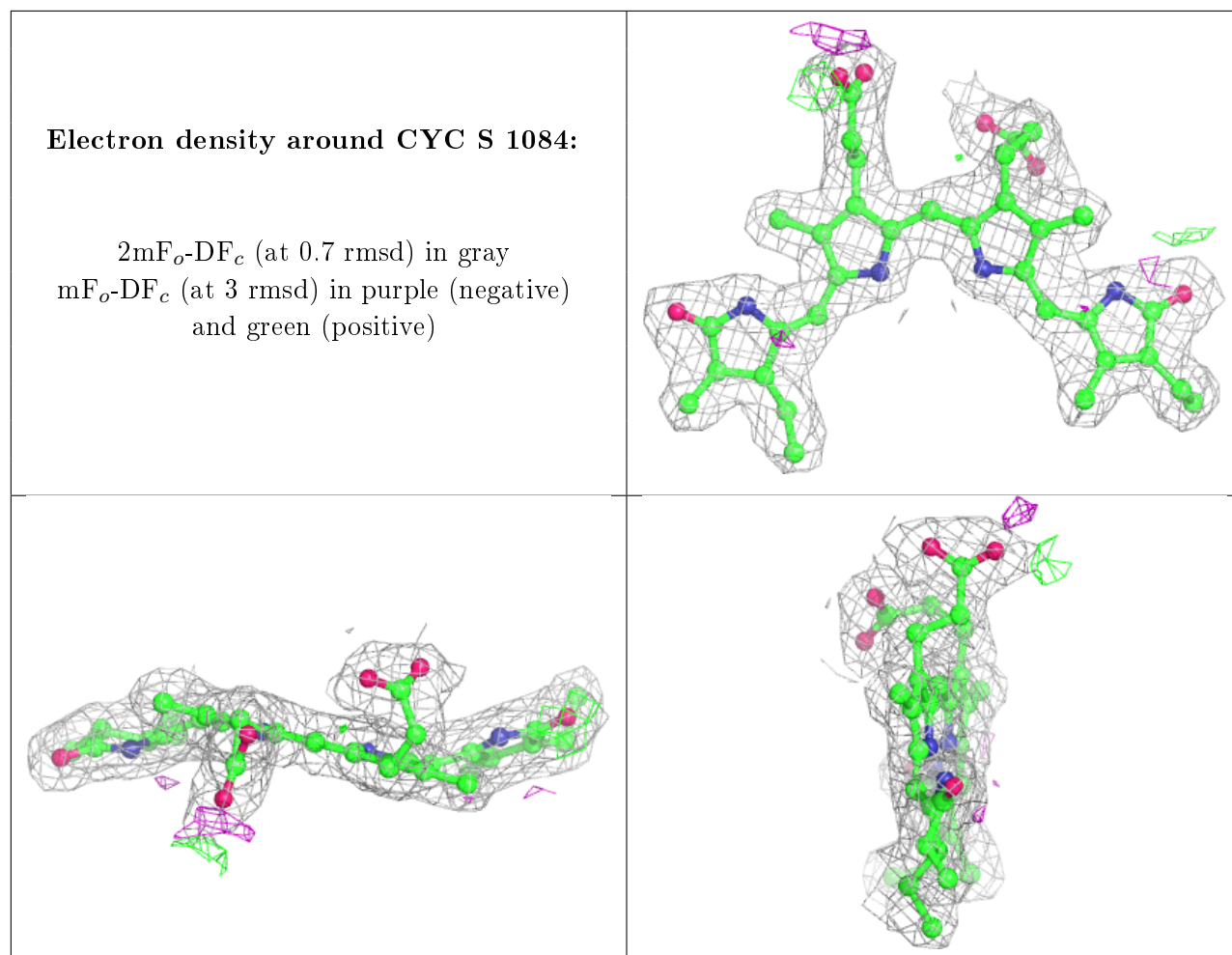
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CYC E 1084:**

$2mF_o-DF_c$  (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.