



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:43 pm BST

PDB ID : 2UUM
Title : Crystal structure of C-phycocyanin from Phormidium, Lyngbya spp. (Marine) and Spirulina sp. (Fresh water) shows two different ways of energy transfer between two hexamers.
Authors : Satyanarayana, L.; Patel, A.; Mishra, S.; K Ghosh, P.; Suresh, C.G.
Deposited on : 2007-03-04
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

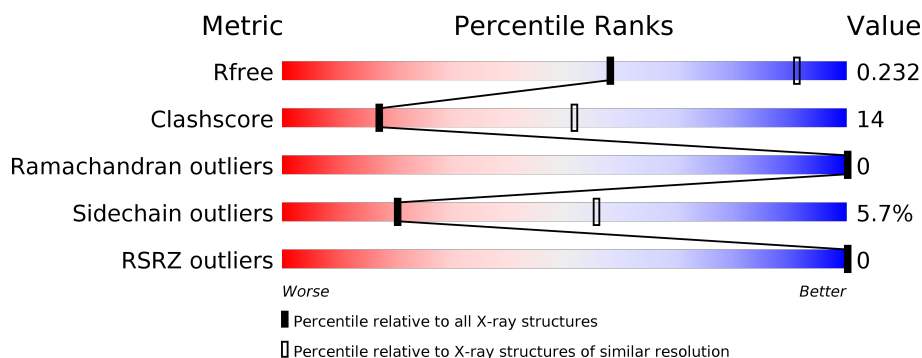
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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




















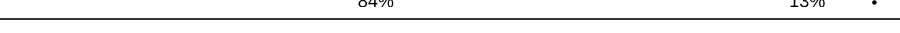
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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>83%</div> <div>16%</div> <div>.</div> </div>
1	C	162	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	E	162	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	G	162	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	I	162	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	K	162	<div> <div>85%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	162	 81% 18% .
1	O	162	 86% 12% .
1	Q	162	 87% 12% .
1	S	162	 86% 12% .
1	U	162	 88% 11% .
1	W	162	 81% 17% .
2	B	172	 84% 15% .
2	D	172	 83% 17% .
2	F	172	 86% 12% .
2	H	172	 85% 13% .
2	J	172	 82% 17% .
2	L	172	 81% 17% .
2	N	172	 83% 16% .
2	P	172	 83% 16% .
2	R	172	 84% 15% .
2	T	172	 85% 15% .
2	V	172	 84% 13% .
3	X	172	 81% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CYC	K	1084	-	-	X	-
4	CYC	M	1084	-	-	X	-
5	BLA	L	1153	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31610 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 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	1	0
			1235	780	207	242	6			
1	C	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	E	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	G	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	I	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	K	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	M	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	O	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	Q	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	S	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	U	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			
1	W	162	Total	C	N	O	S	0	0	0
			1233	778	207	242	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ILE	conflict	UNP P72509
A	148	VAL	THR	conflict	UNP P72509
C	11	VAL	ILE	conflict	UNP P72509
C	148	VAL	THR	conflict	UNP P72509
E	11	VAL	ILE	conflict	UNP P72509

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Chain	Residue	Modelled	Actual	Comment	Reference
E	148	VAL	THR	conflict	UNP P72509
G	11	VAL	ILE	conflict	UNP P72509
G	148	VAL	THR	conflict	UNP P72509
I	11	VAL	ILE	conflict	UNP P72509
I	148	VAL	THR	conflict	UNP P72509
K	11	VAL	ILE	conflict	UNP P72509
K	148	VAL	THR	conflict	UNP P72509
M	11	VAL	ILE	conflict	UNP P72509
M	148	VAL	THR	conflict	UNP P72509
O	11	VAL	ILE	conflict	UNP P72509
O	148	VAL	THR	conflict	UNP P72509
Q	11	VAL	ILE	conflict	UNP P72509
Q	148	VAL	THR	conflict	UNP P72509
S	11	VAL	ILE	conflict	UNP P72509
S	148	VAL	THR	conflict	UNP P72509
U	11	VAL	ILE	conflict	UNP P72509
U	148	VAL	THR	conflict	UNP P72509
W	11	VAL	ILE	conflict	UNP P72509
W	148	VAL	THR	conflict	UNP P72509

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	D	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	F	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	H	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	J	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	L	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	N	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	P	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	R	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0
2	T	172	Total 1258	C 779	N 218	O 252	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	172	Total	C	N	O	S	0	0	0
			1258	779	218	252	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	40	VAL	ALA	conflict	UNP P72508
B	77	THR	ARG	conflict	UNP P72508
D	40	VAL	ALA	conflict	UNP P72508
D	77	THR	ARG	conflict	UNP P72508
F	40	VAL	ALA	conflict	UNP P72508
F	77	THR	ARG	conflict	UNP P72508
H	40	VAL	ALA	conflict	UNP P72508
H	77	THR	ARG	conflict	UNP P72508
J	40	VAL	ALA	conflict	UNP P72508
J	77	THR	ARG	conflict	UNP P72508
L	40	VAL	ALA	conflict	UNP P72508
L	77	THR	ARG	conflict	UNP P72508
N	40	VAL	ALA	conflict	UNP P72508
N	77	THR	ARG	conflict	UNP P72508
P	40	VAL	ALA	conflict	UNP P72508
P	77	THR	ARG	conflict	UNP P72508
R	40	VAL	ALA	conflict	UNP P72508
R	77	THR	ARG	conflict	UNP P72508
T	40	VAL	ALA	conflict	UNP P72508
T	77	THR	ARG	conflict	UNP P72508
V	40	VAL	ALA	conflict	UNP P72508
V	77	THR	ARG	conflict	UNP P72508

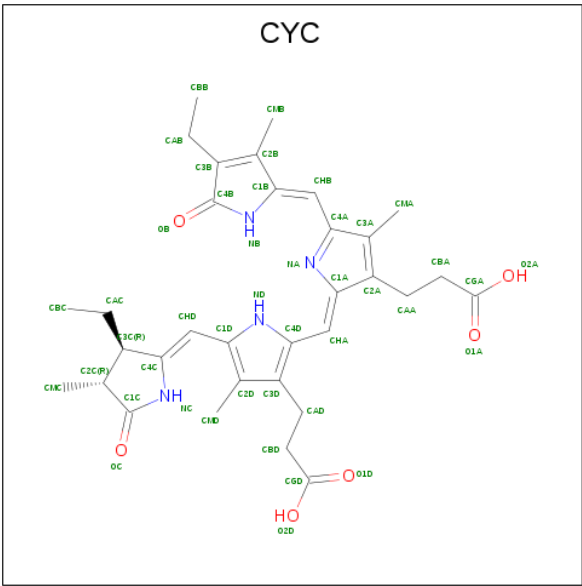
- Molecule 3 is a protein called C-PHYCOCYANIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	172	Total	C	N	O	S	0	0	0
			1263	783	219	252	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	40	VAL	ALA	conflict	UNP P72508
X	77	THR	ARG	conflict	UNP P72508
X	132	LYS	GLY	conflict	UNP P72508

- Molecule 4 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	4	6		
4	C	1	Total	C	N	O	0	0
			43	33	4	6		
4	E	1	Total	C	N	O	0	0
			43	33	4	6		
4	G	1	Total	C	N	O	0	0
			43	33	4	6		
4	K	1	Total	C	N	O	0	0
			43	33	4	6		
4	M	1	Total	C	N	O	0	0
			43	33	4	6		
4	O	1	Total	C	N	O	0	0
			43	33	4	6		
4	Q	1	Total	C	N	O	0	0
			43	33	4	6		
4	R	1	Total	C	N	O	0	0
			43	33	4	6		
4	S	1	Total	C	N	O	0	0
			43	33	4	6		
4	U	1	Total	C	N	O	0	0
			43	33	4	6		
4	W	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			43	33	4	6		
5	P	1	Total	C	N	O	0	0
			43	33	4	6		
5	P	1	Total	C	N	O	0	0
			43	33	4	6		
5	R	1	Total	C	N	O	0	0
			43	33	4	6		
5	T	1	Total	C	N	O	0	0
			43	33	4	6		
5	T	1	Total	C	N	O	0	0
			43	33	4	6		
5	V	1	Total	C	N	O	0	0
			43	33	4	6		
5	V	1	Total	C	N	O	0	0
			43	33	4	6		
5	X	1	Total	C	N	O	0	0
			43	33	4	6		
5	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	C	10	Total	O	0	0
			10	10		
6	D	21	Total	O	0	0
			21	21		
6	F	6	Total	O	0	0
			6	6		
6	G	5	Total	O	0	0
			5	5		
6	I	13	Total	O	0	0
			13	13		
6	J	17	Total	O	0	0
			17	17		
6	L	5	Total	O	0	0
			5	5		
6	M	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	16	Total 16	O 16	0	0
6	P	7	Total 7	O 7	0	0
6	Q	6	Total 6	O 6	0	0
6	S	2	Total 2	O 2	0	0
6	T	2	Total 2	O 2	0	0
6	U	5	Total 5	O 5	0	0
6	W	13	Total 13	O 13	0	0
6	X	15	Total 15	O 15	0	0

3 Residue-property plots [i](#)


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 CHAIN

Chain A: 




- Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain C: 




- Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain E: 




- Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain G: 




- Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain I: 



- Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain K: 



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain M: 81% 18%



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain O: 86% 12%



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain Q: 87% 12%



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain S: 86% 12%



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain U: 88% 11%



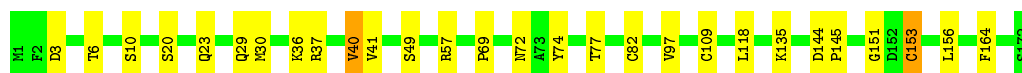
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain W: 81% 17%



• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain B: 84% 15%



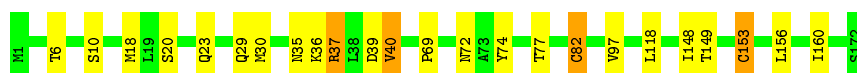
- Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain D: 83% 17%



- Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain F: 86% 12%



- Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain H: 85% 13%



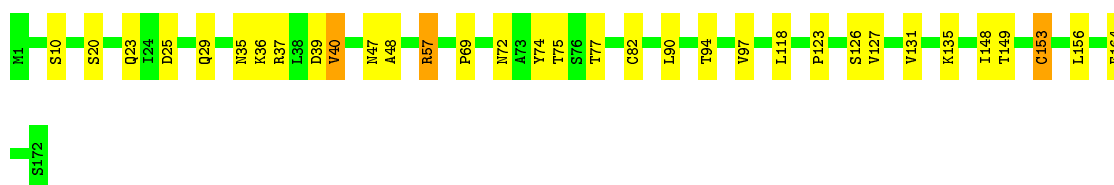
- Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain J: 82% 17%



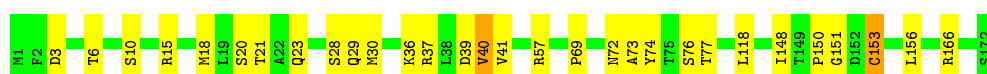
- Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain L: 81% 17%

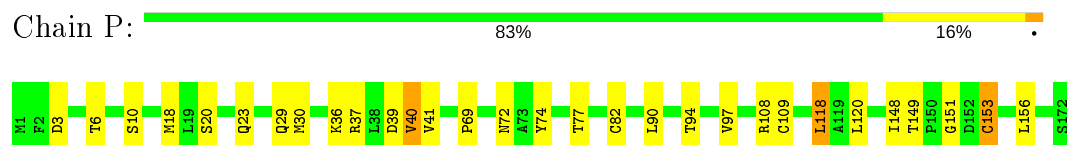


- Molecule 2: C-PHYCOCYANIN BETA CHAIN

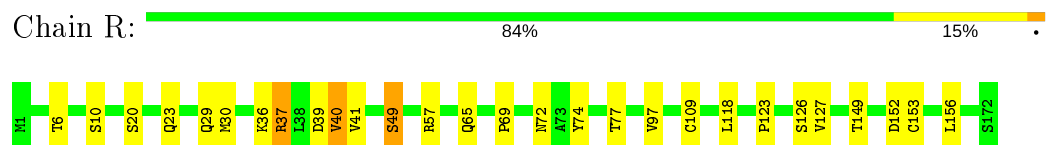
Chain N: 83% 16%



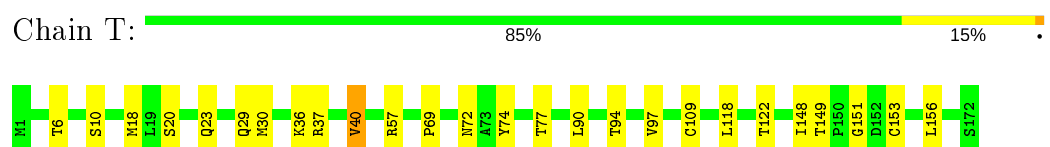
- Molecule 2: C-PHYCOCYANIN BETA CHAIN



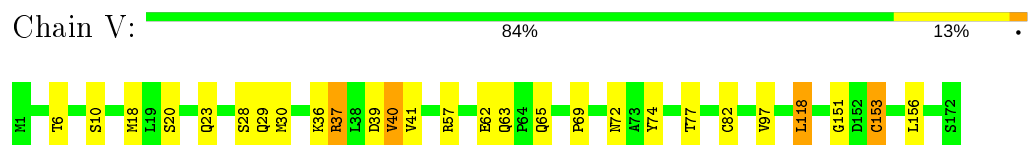
- Molecule 2: C-PHYCOCYANIN BETA CHAIN



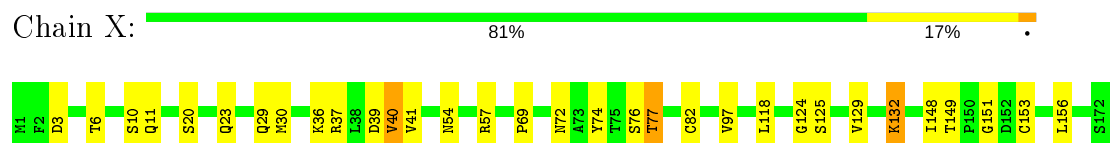
- Molecule 2: C-PHYCOCYANIN BETA CHAIN



- Molecule 2: C-PHYCOCYANIN BETA CHAIN



- Molecule 3: C-PHYCOCYANIN BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.33Å 115.64Å 183.26Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	182.57 – 3.00 39.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (182.57-3.00) 96.6 (39.60-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.242 0.193 , 0.232	Depositor DCC
R_{free} test set	4331 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31610	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.94	0/1264	0.81	0/1710
1	C	0.99	1/1256 (0.1%)	0.89	3/1699 (0.2%)
1	E	1.01	1/1256 (0.1%)	0.84	0/1699
1	G	0.98	1/1256 (0.1%)	0.83	0/1699
1	I	0.98	0/1256	0.85	1/1699 (0.1%)
1	K	0.97	2/1256 (0.2%)	0.87	1/1699 (0.1%)
1	M	0.99	0/1256	0.90	1/1699 (0.1%)
1	O	1.03	3/1256 (0.2%)	0.85	0/1699
1	Q	0.99	1/1256 (0.1%)	0.84	1/1699 (0.1%)
1	S	1.00	2/1256 (0.2%)	0.83	1/1699 (0.1%)
1	U	0.98	0/1256	0.83	0/1699
1	W	0.97	2/1256 (0.2%)	0.83	1/1699 (0.1%)
2	B	0.92	2/1272 (0.2%)	0.83	1/1724 (0.1%)
2	D	0.93	0/1272	0.87	0/1724
2	F	0.90	3/1272 (0.2%)	0.84	1/1724 (0.1%)
2	H	0.94	0/1272	0.87	1/1724 (0.1%)
2	J	0.96	1/1272 (0.1%)	0.89	0/1724
2	L	0.93	2/1272 (0.2%)	0.84	1/1724 (0.1%)
2	N	1.02	1/1272 (0.1%)	0.87	0/1724
2	P	0.98	3/1272 (0.2%)	0.85	0/1724
2	R	0.92	3/1272 (0.2%)	0.87	2/1724 (0.1%)
2	T	0.92	0/1272	0.85	0/1724
2	V	0.95	2/1272 (0.2%)	0.88	1/1724 (0.1%)
3	X	0.97	1/1277 (0.1%)	0.89	0/1730
All	All	0.97	31/30349 (0.1%)	0.86	16/41093 (0.0%)

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	CYS	CB-SG	-9.10	1.66	1.82
2	V	153	CYS	CB-SG	-7.33	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	153	CYS	CB-SG	-7.31	1.69	1.82
3	X	77	THR	CA-CB	7.24	1.72	1.53
1	W	84	CYS	CB-SG	-7.20	1.70	1.82

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	57	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	F	37	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	30	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	I	77	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	93	ARG	NE-CZ-NH1	6.47	123.54	120.30

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	1235	0	1210	17	1
1	C	1233	0	1205	25	0
1	E	1233	0	1205	19	0
1	G	1233	0	1205	20	0
1	I	1233	0	1205	18	1
1	K	1233	0	1205	19	2
1	M	1233	0	1205	28	0
1	O	1233	0	1205	13	1
1	Q	1233	0	1205	16	1
1	S	1233	0	1205	14	1
1	U	1233	0	1205	10	0
1	W	1233	0	1205	23	1
2	B	1258	0	1255	29	0
2	D	1258	0	1254	37	1
2	F	1258	0	1254	23	0
2	H	1258	0	1255	33	0
2	J	1258	0	1255	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1258	0	1255	35	0
2	N	1258	0	1254	31	0
2	P	1258	0	1255	32	0
2	R	1258	0	1254	26	0
2	T	1258	0	1254	27	0
2	V	1258	0	1254	28	1
3	X	1263	0	1265	42	0
4	A	43	0	36	15	0
4	C	43	0	37	15	0
4	E	43	0	37	12	0
4	G	43	0	35	12	0
4	K	43	0	37	21	0
4	M	43	0	36	22	0
4	O	43	0	37	18	0
4	Q	43	0	37	16	0
4	R	43	0	37	13	0
4	S	43	0	36	12	0
4	U	43	0	35	15	0
4	W	43	0	37	14	0
5	B	86	0	64	26	0
5	D	86	0	64	31	0
5	F	86	0	63	26	0
5	H	86	0	64	34	0
5	I	43	0	31	17	0
5	J	86	0	64	37	0
5	L	86	0	64	40	0
5	N	86	0	63	34	0
5	P	86	0	64	29	0
5	R	43	0	32	15	0
5	T	86	0	63	27	0
5	V	86	0	63	29	0
5	X	86	0	64	34	0
6	A	8	0	0	1	0
6	C	10	0	0	4	0
6	D	21	0	0	2	0
6	F	6	0	0	0	0
6	G	5	0	0	1	0
6	I	13	0	0	2	0
6	J	17	0	0	3	0
6	L	5	0	0	0	0
6	M	12	0	0	3	0
6	N	16	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	7	0	0	1	0
6	Q	6	0	0	1	0
6	S	2	0	0	0	0
6	T	2	0	0	0	0
6	U	5	0	0	1	0
6	W	13	0	0	7	0
6	X	15	0	0	9	0
All	All	31610	0	30729	856	5

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 14.

The worst 5 of 856 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)
2:L:153:CYS:SG	5:L:1153:BLA:HAC	1.44	1.53
2:V:153:CYS:SG	5:V:1153:BLA:HBC1	1.59	1.40
2:D:153:CYS:SG	5:D:1153:BLA:CBC	2.13	1.36
2:B:82:CYS:SG	5:B:1082:BLA:CAC	2.13	1.36
2:P:82:CYS:SG	5:P:1082:BLA:CAC	2.15	1.35

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:SER:OG	2:V:62:GLU:OE1[2_656]	2.03	0.17
1:I:68:GLN:NE2	1:W:68:GLN:NE2[1_655]	2.06	0.14
1:K:67:THR:O	1:S:61:ASN:CG[1_656]	2.08	0.12
1:A:60:TYR:O	1:Q:68:GLN:OE1[1_655]	2.11	0.09
1:K:61:ASN:CG	1:O:68:GLN:NE2[1_656]	2.17	0.03

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	161/162 (99%)	158 (98%)	3 (2%)	0	100	100
1	C	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	E	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	G	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	I	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	K	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	M	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
1	O	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	Q	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	S	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	U	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	W	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
2	B	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	D	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	F	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	H	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	J	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	L	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	N	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	P	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	R	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	T	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	V	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	X	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
All	All	3961/4008 (99%)	3851 (97%)	110 (3%)	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	125/125 (100%)	117 (94%)	8 (6%)	17	51
1	C	124/125 (99%)	116 (94%)	8 (6%)	17	50
1	E	124/125 (99%)	115 (93%)	9 (7%)	14	44
1	G	124/125 (99%)	115 (93%)	9 (7%)	14	44
1	I	124/125 (99%)	115 (93%)	9 (7%)	14	44
1	K	124/125 (99%)	116 (94%)	8 (6%)	17	50
1	M	124/125 (99%)	118 (95%)	6 (5%)	25	62
1	O	124/125 (99%)	115 (93%)	9 (7%)	14	44
1	Q	124/125 (99%)	116 (94%)	8 (6%)	17	50
1	S	124/125 (99%)	115 (93%)	9 (7%)	14	44
1	U	124/125 (99%)	114 (92%)	10 (8%)	11	40
1	W	124/125 (99%)	117 (94%)	7 (6%)	21	56
2	B	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	D	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	F	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	H	131/133 (98%)	124 (95%)	7 (5%)	22	58
2	J	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	L	131/133 (98%)	127 (97%)	4 (3%)	40	75
2	N	131/133 (98%)	123 (94%)	8 (6%)	18	53
2	P	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	R	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	T	131/133 (98%)	125 (95%)	6 (5%)	27	64
2	V	131/133 (98%)	124 (95%)	7 (5%)	22	58
3	X	132/134 (98%)	126 (96%)	6 (4%)	27	64
All	All	3062/3097 (99%)	2888 (94%)	174 (6%)	20	56

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	42	LYS
2	N	40	VAL
2	V	118	LEU

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Mol	Chain	Res	Type
1	K	68	GLN
1	M	32	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	23	GLN
1	O	68	GLN
1	W	139	ASN
1	M	139	ASN
2	N	23	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
4	CYC	S	1084	1	36,46,46	3.31	13 (36%)	44,67,67	4.28	22 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BLA	N	1082	2	36,46,46	3.84	14 (38%)	47,67,67	3.99	26 (55%)
5	BLA	D	1153	-	36,46,46	3.69	15 (41%)	47,67,67	3.77	21 (44%)
5	BLA	P	1082	-	36,46,46	3.47	15 (41%)	47,67,67	3.72	26 (55%)
5	BLA	B	1153	-	36,46,46	3.79	18 (50%)	47,67,67	4.12	25 (53%)
4	CYC	O	1084	1	36,46,46	3.15	14 (38%)	44,67,67	3.90	18 (40%)
4	CYC	M	1084	1	36,46,46	3.83	14 (38%)	44,67,67	3.53	25 (56%)
4	CYC	C	1084	1	36,46,46	3.04	13 (36%)	44,67,67	4.36	28 (63%)
4	CYC	A	1084	1	36,46,46	3.22	11 (30%)	44,67,67	3.89	20 (45%)
5	BLA	D	1082	2	36,46,46	3.97	16 (44%)	47,67,67	3.97	28 (59%)
5	BLA	L	1153	-	36,46,46	3.59	16 (44%)	47,67,67	3.81	20 (42%)
5	BLA	L	1082	2	36,46,46	3.87	14 (38%)	47,67,67	3.73	27 (57%)
4	CYC	W	1084	1	36,46,46	3.27	10 (27%)	44,67,67	3.75	24 (54%)
4	CYC	U	1084	1	36,46,46	3.32	13 (36%)	44,67,67	3.41	21 (47%)
4	CYC	K	1084	1	36,46,46	3.46	14 (38%)	44,67,67	3.70	18 (40%)
5	BLA	F	1153	2	36,46,46	3.28	15 (41%)	47,67,67	3.68	21 (44%)
4	CYC	R	1082	2	36,46,46	4.18	14 (38%)	44,67,67	4.22	24 (54%)
4	CYC	E	1084	1	36,46,46	3.34	13 (36%)	44,67,67	4.33	22 (50%)
5	BLA	B	1082	-	36,46,46	3.92	17 (47%)	47,67,67	3.62	25 (53%)
5	BLA	H	1153	-	36,46,46	3.51	14 (38%)	47,67,67	3.94	25 (53%)
5	BLA	I	1084	1	36,46,46	3.45	14 (38%)	47,67,67	3.70	23 (48%)
5	BLA	J	1082	2	36,46,46	3.97	15 (41%)	47,67,67	3.45	26 (55%)
4	CYC	Q	1084	1	36,46,46	3.52	10 (27%)	44,67,67	3.16	20 (45%)
5	BLA	N	1153	-	36,46,46	3.67	19 (52%)	47,67,67	3.98	25 (53%)
5	BLA	T	1082	2	36,46,46	3.40	14 (38%)	47,67,67	3.86	28 (59%)
5	BLA	V	1082	2	36,46,46	3.56	14 (38%)	47,67,67	3.80	24 (51%)
5	BLA	V	1153	-	36,46,46	3.73	16 (44%)	47,67,67	3.81	20 (42%)
5	BLA	F	1082	2	36,46,46	3.75	13 (36%)	47,67,67	3.72	26 (55%)
5	BLA	J	1153	-	36,46,46	3.34	15 (41%)	47,67,67	4.05	26 (55%)
5	BLA	X	1153	-	36,46,46	3.83	17 (47%)	47,67,67	3.28	21 (44%)
5	BLA	P	1153	-	36,46,46	3.42	13 (36%)	47,67,67	3.72	21 (44%)
5	BLA	X	1082	-	36,46,46	4.14	16 (44%)	47,67,67	3.24	20 (42%)
4	CYC	G	1084	1	36,46,46	3.13	12 (33%)	44,67,67	3.41	25 (56%)
5	BLA	T	1153	-	36,46,46	3.29	16 (44%)	47,67,67	3.99	24 (51%)
5	BLA	R	1153	-	36,46,46	3.32	18 (50%)	47,67,67	3.72	23 (48%)
5	BLA	H	1082	-	36,46,46	3.79	15 (41%)	47,67,67	3.27	23 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYC	S	1084	1	-	7/21/74/74	0/4/4/4
5	BLA	N	1082	2	-	10/22/74/74	0/4/4/4
5	BLA	D	1153	-	-	6/22/74/74	0/4/4/4
5	BLA	P	1082	-	-	12/22/74/74	0/4/4/4
5	BLA	B	1153	-	-	7/22/74/74	0/4/4/4
4	CYC	O	1084	1	-	12/21/74/74	0/4/4/4
4	CYC	M	1084	1	-	10/21/74/74	0/4/4/4
4	CYC	C	1084	1	-	10/21/74/74	0/4/4/4
4	CYC	A	1084	1	-	12/21/74/74	0/4/4/4
5	BLA	D	1082	2	-	9/22/74/74	0/4/4/4
5	BLA	L	1153	-	-	8/22/74/74	0/4/4/4
5	BLA	L	1082	2	-	9/22/74/74	0/4/4/4
4	CYC	W	1084	1	-	6/21/74/74	0/4/4/4
4	CYC	U	1084	1	-	10/21/74/74	0/4/4/4
4	CYC	K	1084	1	-	8/21/74/74	0/4/4/4
5	BLA	F	1153	2	-	5/22/74/74	0/4/4/4
4	CYC	R	1082	2	-	7/21/74/74	0/4/4/4
4	CYC	E	1084	1	-	9/21/74/74	0/4/4/4
5	BLA	B	1082	-	-	8/22/74/74	0/4/4/4
5	BLA	H	1153	-	-	5/22/74/74	0/4/4/4
5	BLA	I	1084	1	-	9/22/74/74	0/4/4/4
5	BLA	J	1082	2	-	9/22/74/74	0/4/4/4
4	CYC	Q	1084	1	-	10/21/74/74	0/4/4/4
5	BLA	N	1153	-	-	6/22/74/74	0/4/4/4
5	BLA	T	1082	2	-	11/22/74/74	0/4/4/4
5	BLA	V	1082	2	-	11/22/74/74	0/4/4/4
5	BLA	V	1153	-	-	6/22/74/74	0/4/4/4
5	BLA	F	1082	2	-	10/22/74/74	0/4/4/4
5	BLA	J	1153	-	-	8/22/74/74	0/4/4/4
5	BLA	X	1153	-	-	9/22/74/74	0/4/4/4
5	BLA	P	1153	-	-	5/22/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BLA	X	1082	-	-	7/22/74/74	0/4/4/4
4	CYC	G	1084	1	-	10/21/74/74	0/4/4/4
5	BLA	T	1153	-	-	7/22/74/74	0/4/4/4
5	BLA	R	1153	-	-	5/22/74/74	0/4/4/4
5	BLA	H	1082	-	-	11/22/74/74	0/4/4/4

The worst 5 of 520 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1082	CYC	CHA-C1A	19.72	1.51	1.35
4	M	1084	CYC	CHA-C1A	18.65	1.50	1.35
5	X	1082	BLA	CHA-C4D	18.13	1.50	1.35
5	D	1082	BLA	CHA-C4D	17.62	1.49	1.35
5	J	1082	BLA	CHA-C4D	17.34	1.49	1.35

The worst 5 of 841 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1084	CYC	CAA-CBA-CGA	-18.55	81.56	112.67
4	O	1084	CYC	CAA-CBA-CGA	-17.32	83.61	112.67
4	C	1084	CYC	CAA-CBA-CGA	-14.84	87.78	112.67
4	R	1082	CYC	C3B-C4B-NB	14.10	118.17	106.78
4	K	1084	CYC	CAA-CBA-CGA	-13.44	90.11	112.67

There are no chirality outliers.

5 of 304 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	1084	CYC	C3A-C2A-CAA-CBA
4	S	1084	CYC	NA-C4A-CHB-C1B
4	S	1084	CYC	C3A-C4A-CHB-C1B
4	S	1084	CYC	C4C-C3C-CAC-CBC
4	S	1084	CYC	ND-C1D-CHD-C4C

There are no ring outliers.

36 monomers are involved in 564 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1084	CYC	12	0
5	N	1082	BLA	15	0

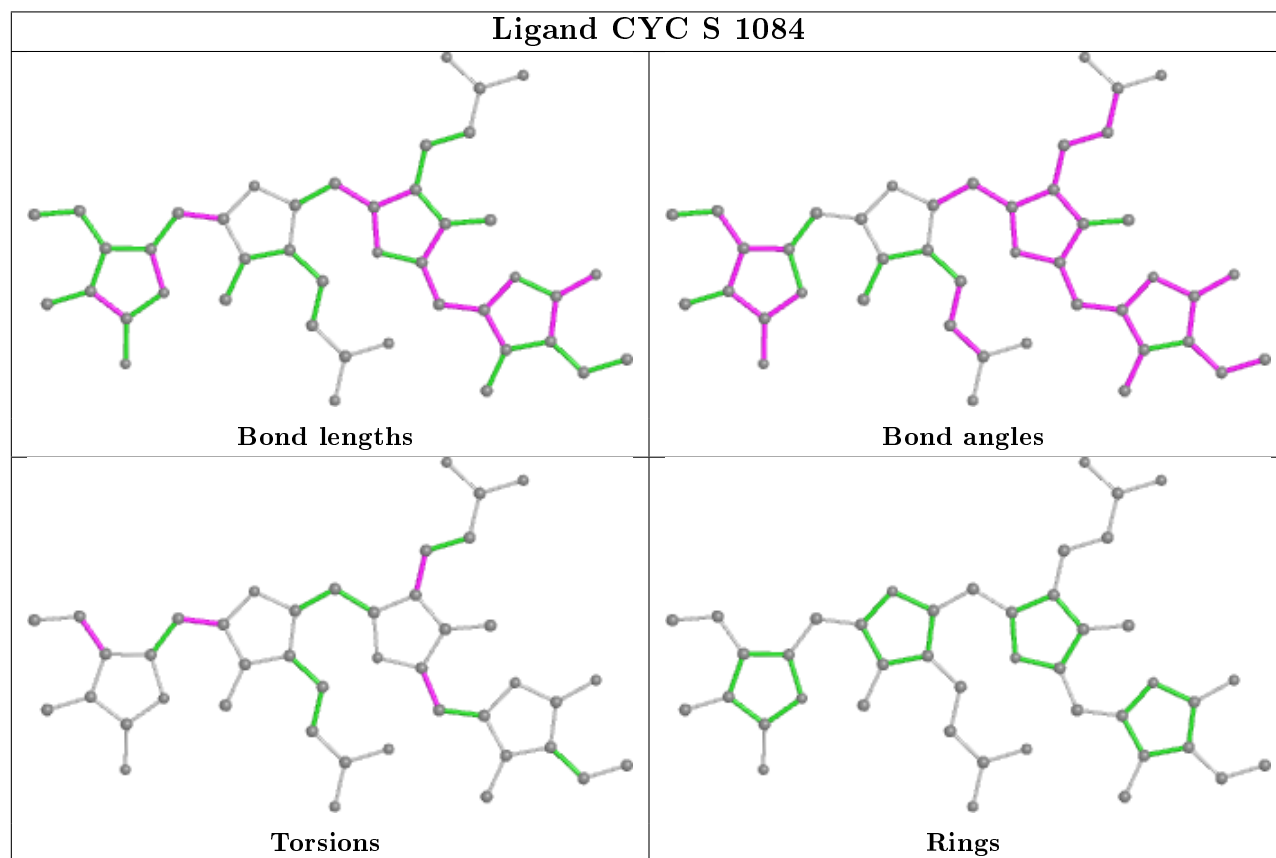
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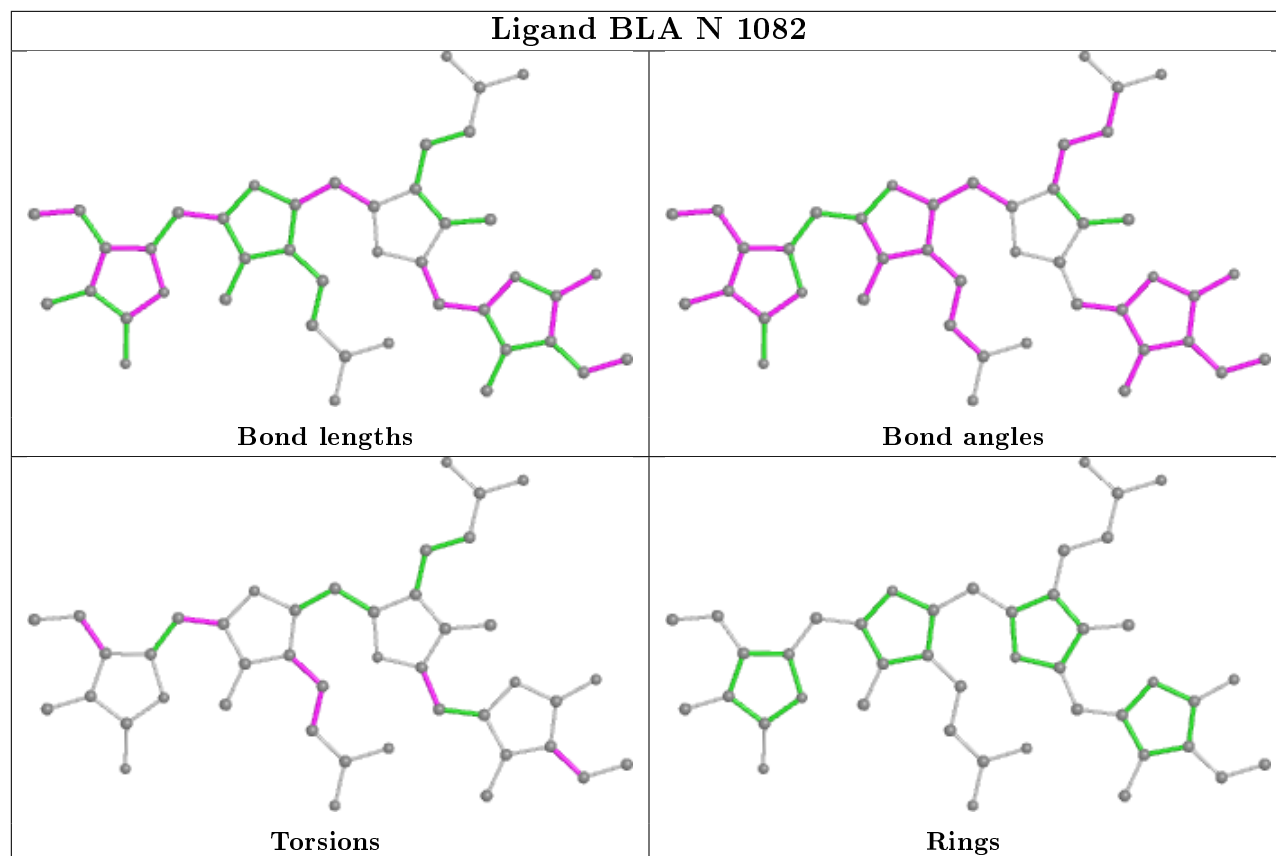
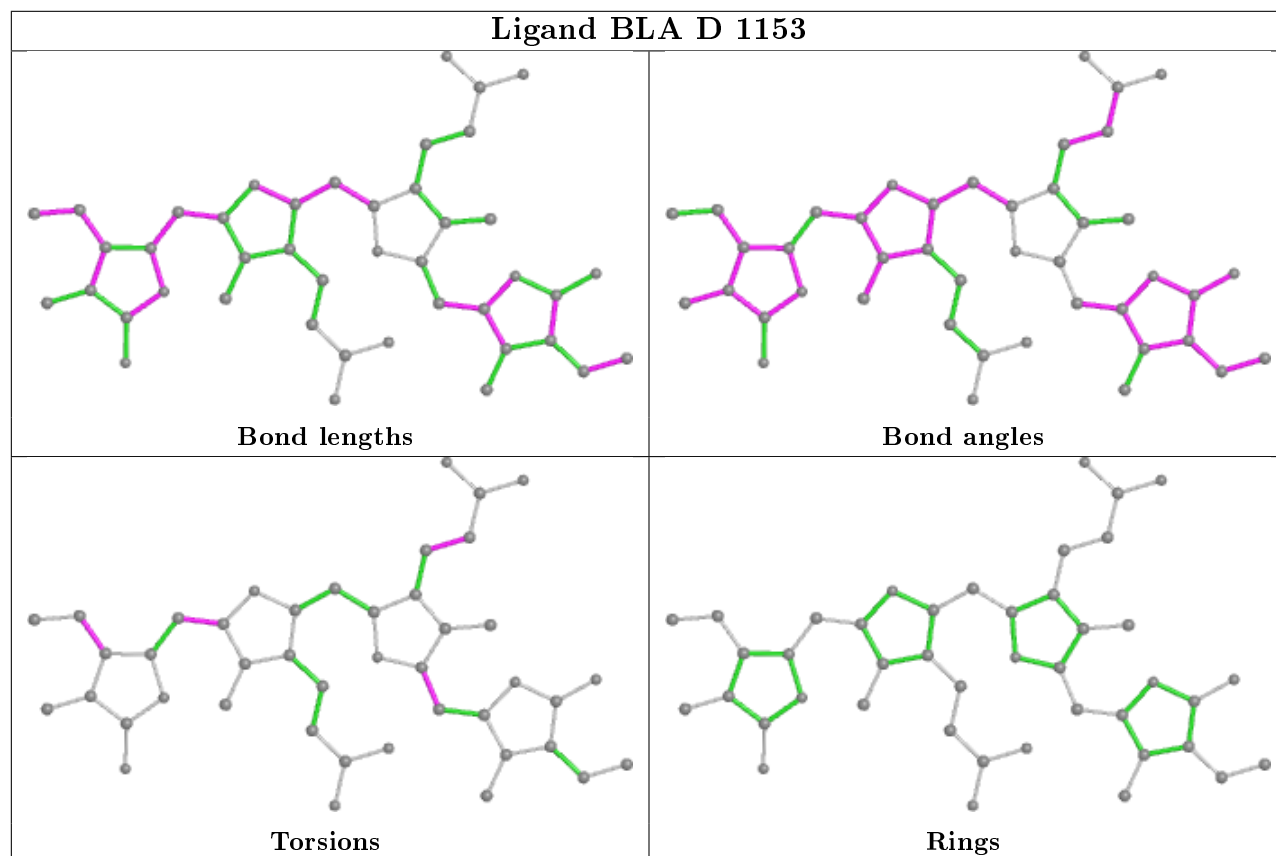
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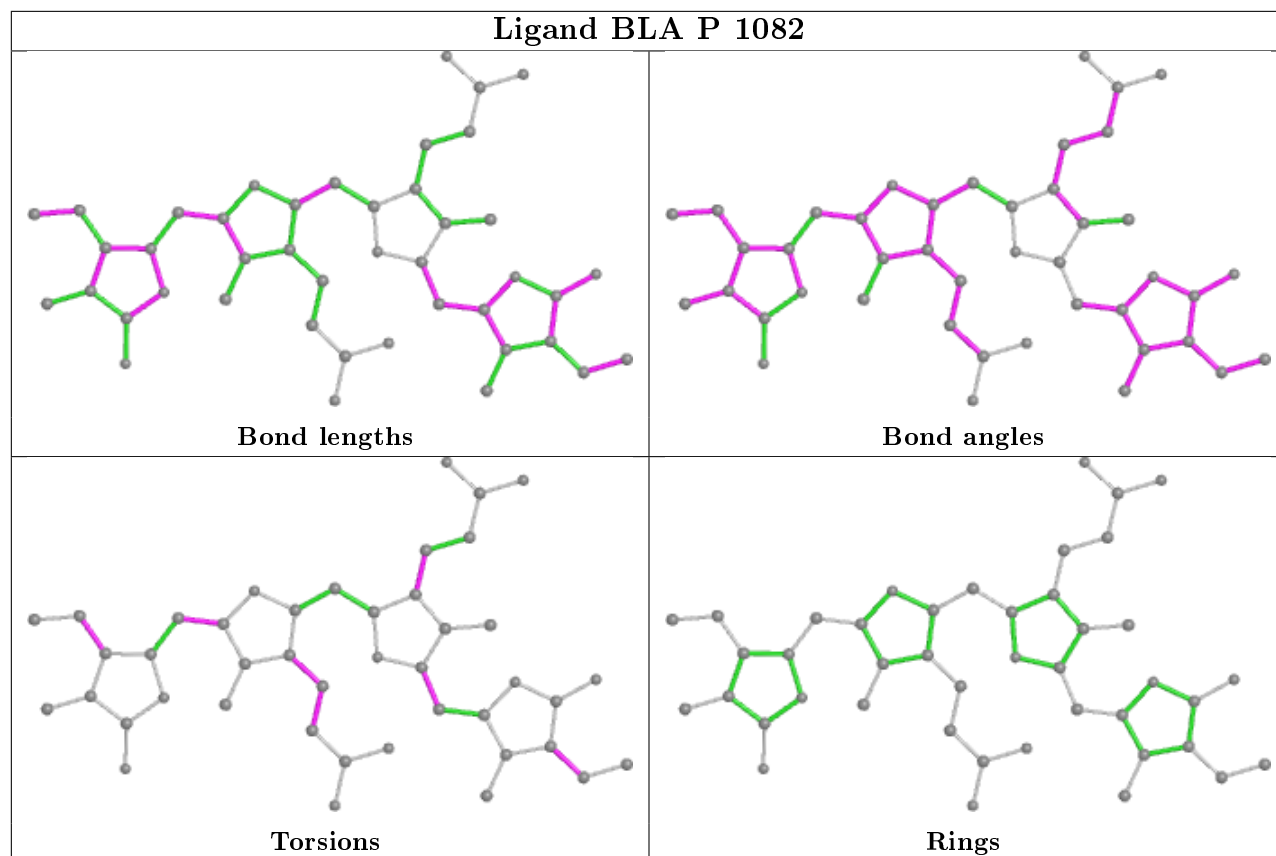
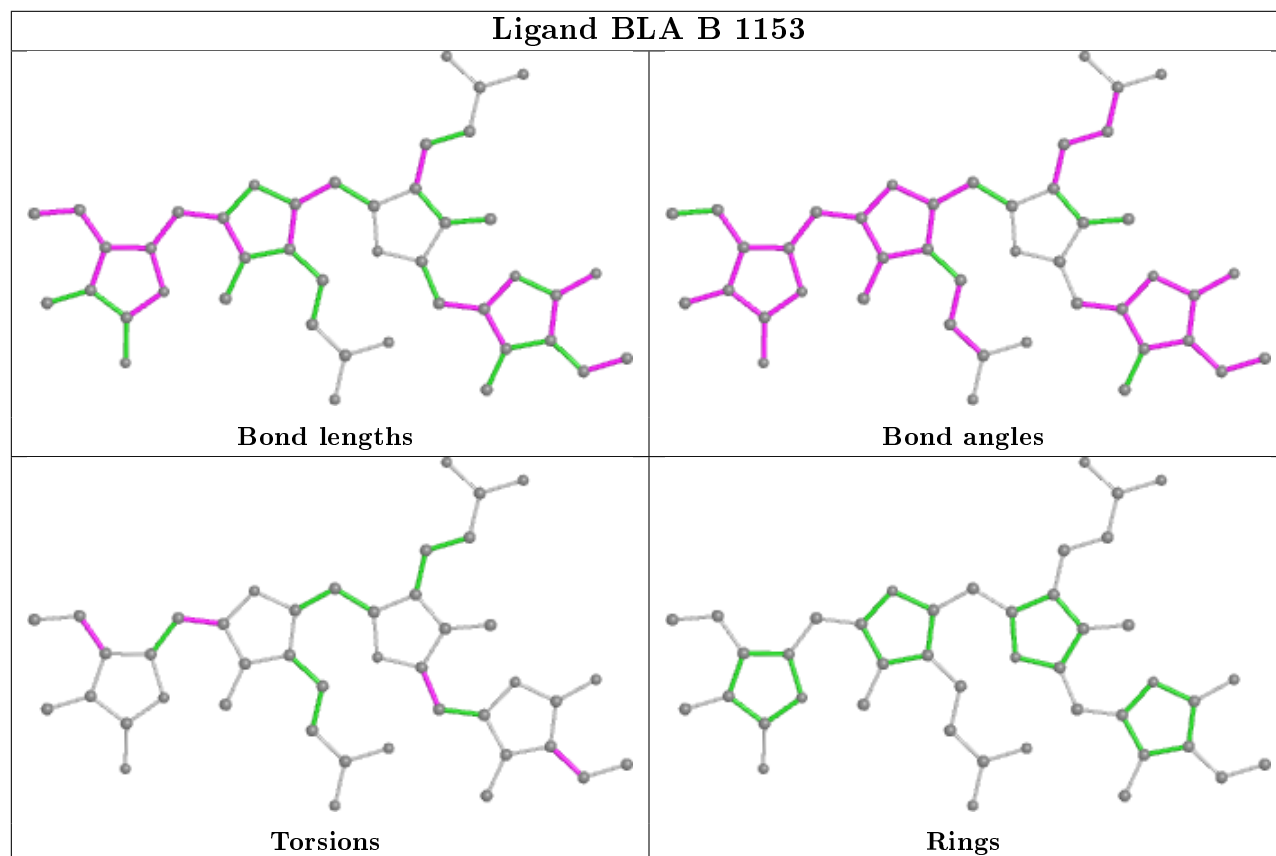
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1153	BLA	19	0
5	P	1082	BLA	13	0
5	B	1153	BLA	14	0
4	O	1084	CYC	18	0
4	M	1084	CYC	22	0
4	C	1084	CYC	15	0
4	A	1084	CYC	15	0
5	D	1082	BLA	12	0
5	L	1153	BLA	25	0
5	L	1082	BLA	15	0
4	W	1084	CYC	14	0
4	U	1084	CYC	15	0
4	K	1084	CYC	21	0
5	F	1153	BLA	15	0
4	R	1082	CYC	13	0
4	E	1084	CYC	12	0
5	B	1082	BLA	12	0
5	H	1153	BLA	18	0
5	I	1084	BLA	17	0
5	J	1082	BLA	19	0
4	Q	1084	CYC	16	0
5	N	1153	BLA	19	0
5	T	1082	BLA	10	0
5	V	1082	BLA	14	0
5	V	1153	BLA	15	0
5	F	1082	BLA	11	0
5	J	1153	BLA	18	0
5	X	1153	BLA	20	0
5	P	1153	BLA	16	0
5	X	1082	BLA	14	0
4	G	1084	CYC	12	0
5	T	1153	BLA	17	0
5	R	1153	BLA	15	0
5	H	1082	BLA	16	0

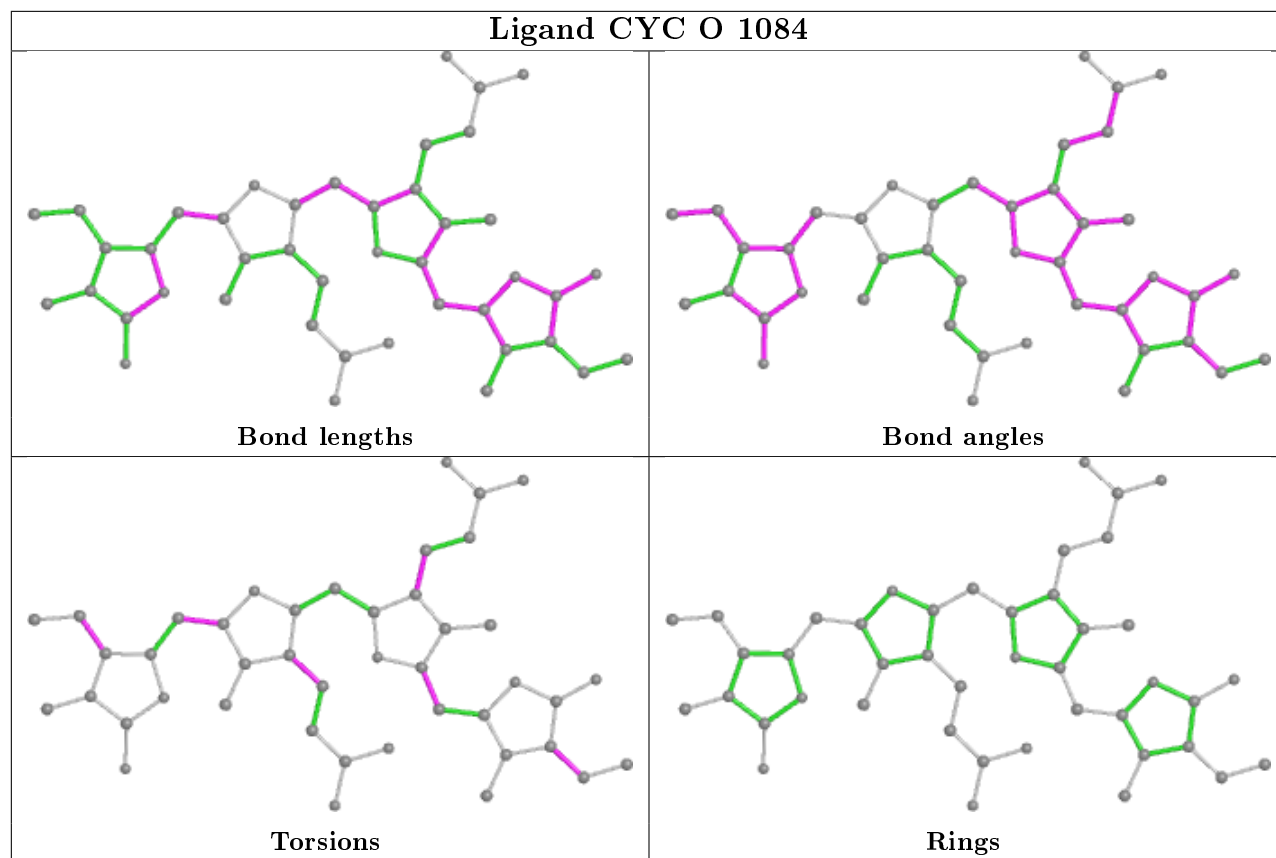
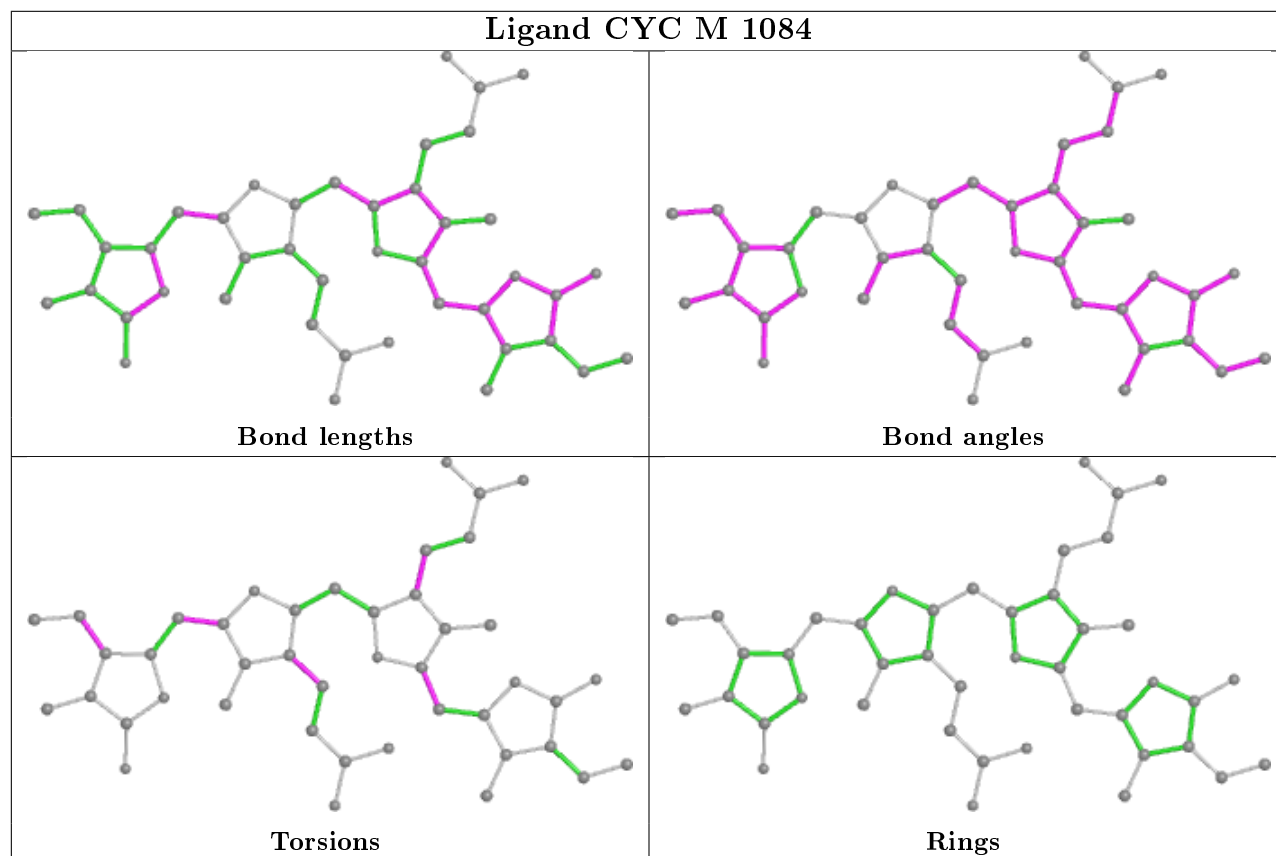
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

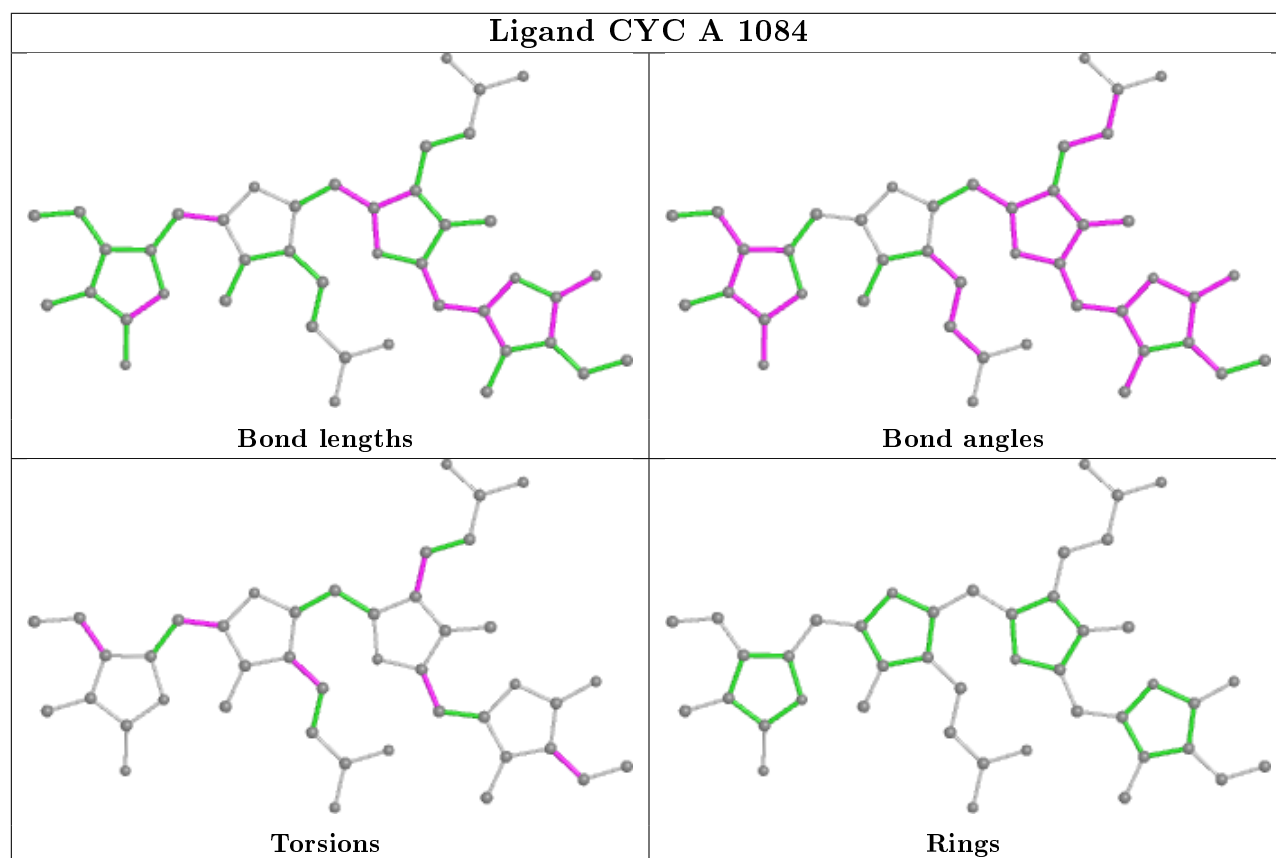
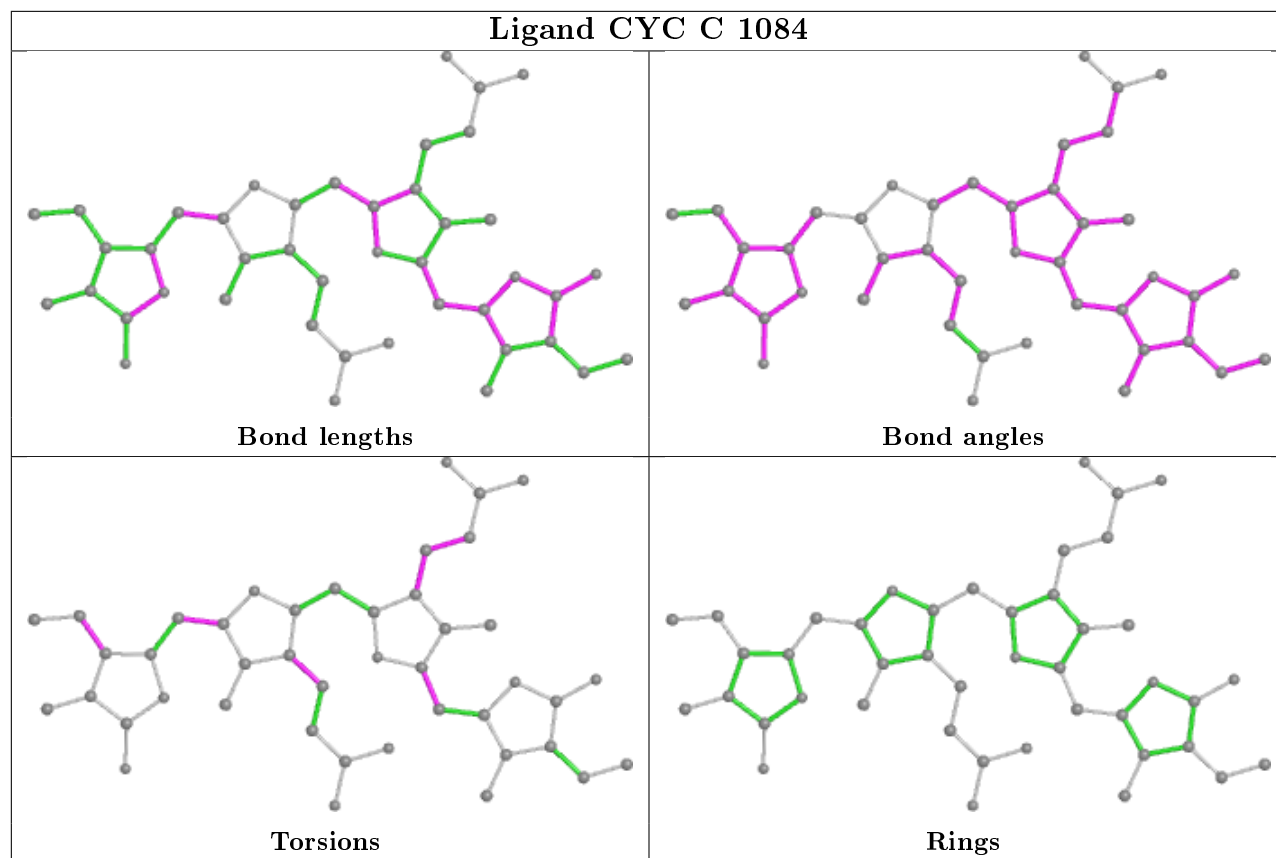
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



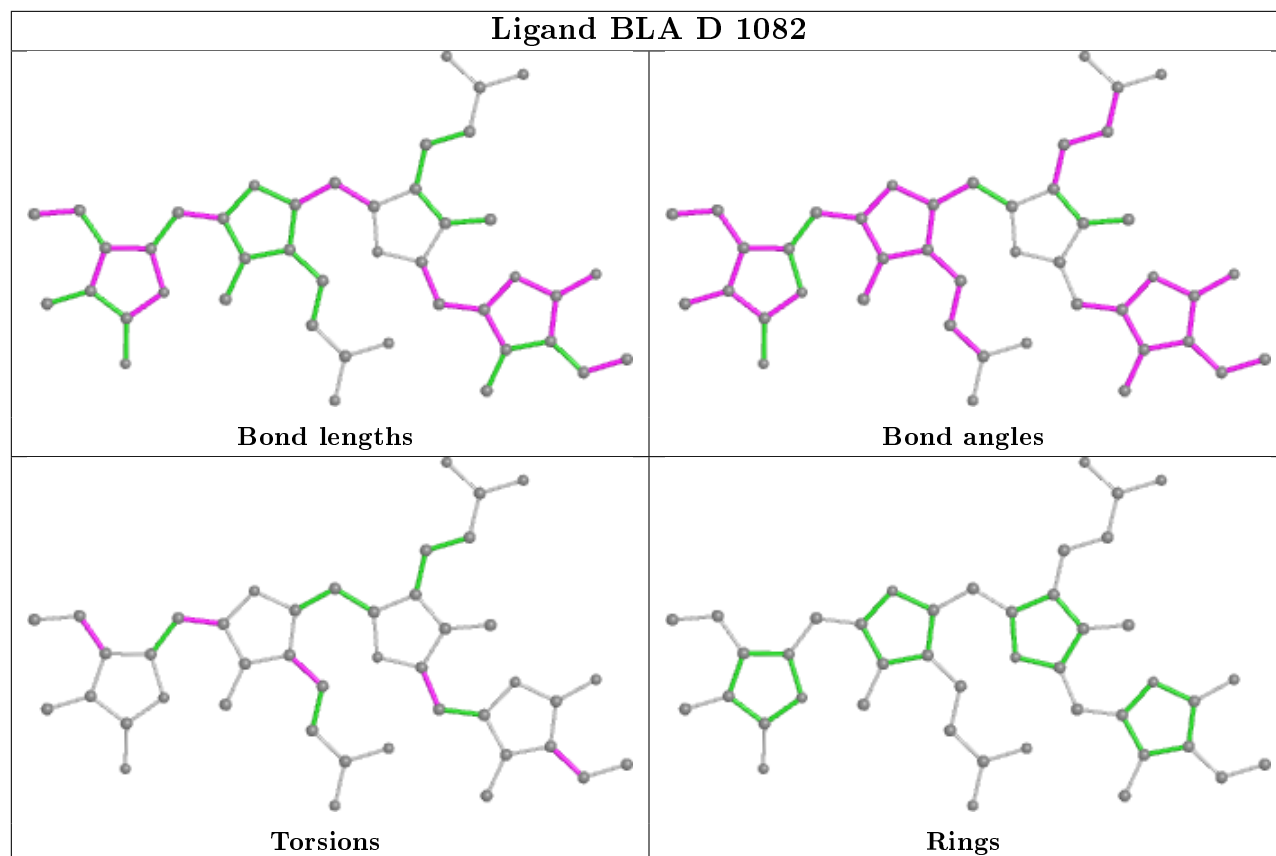
Ligand BLA N 1082**Ligand BLA D 1153**

Ligand BLA P 1082**Ligand BLA B 1153**

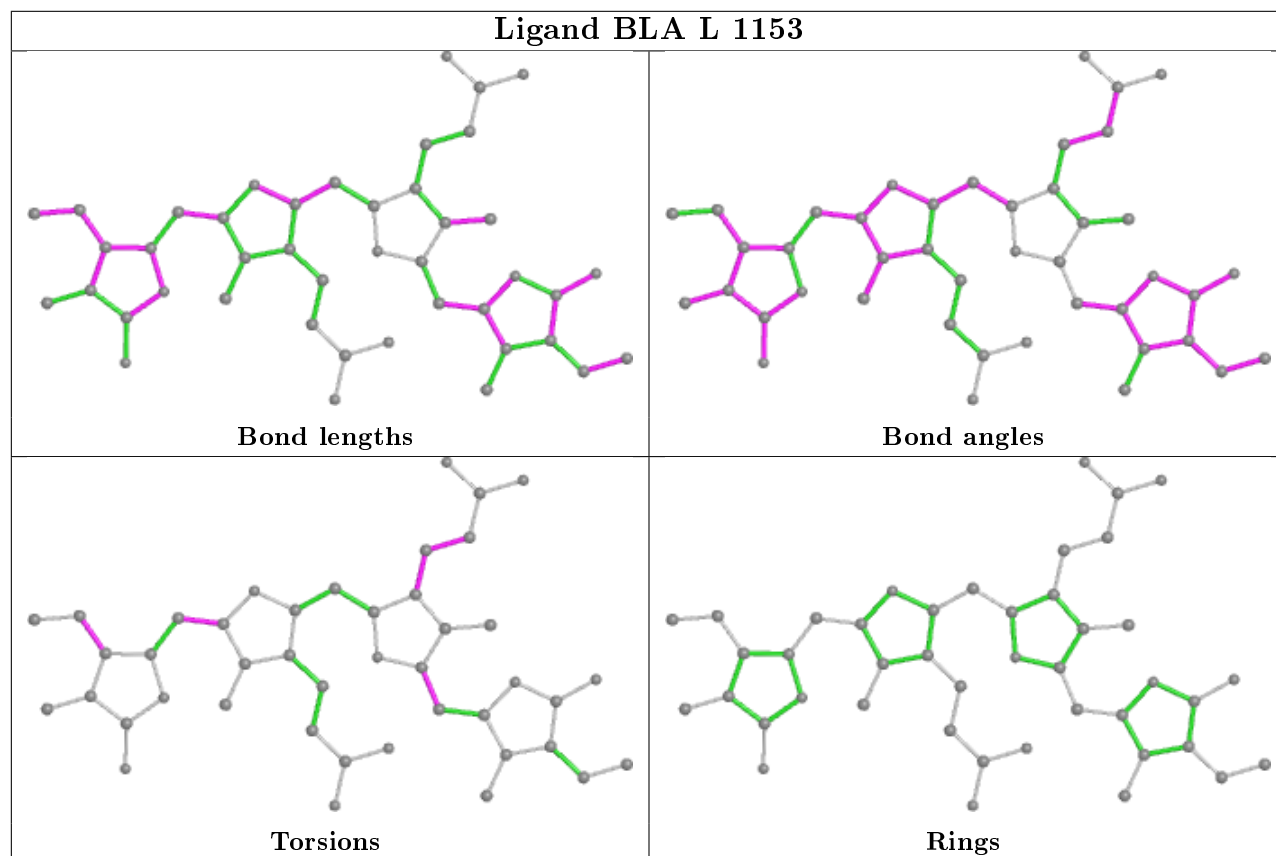
Ligand CYC O 1084**Ligand CYC M 1084**

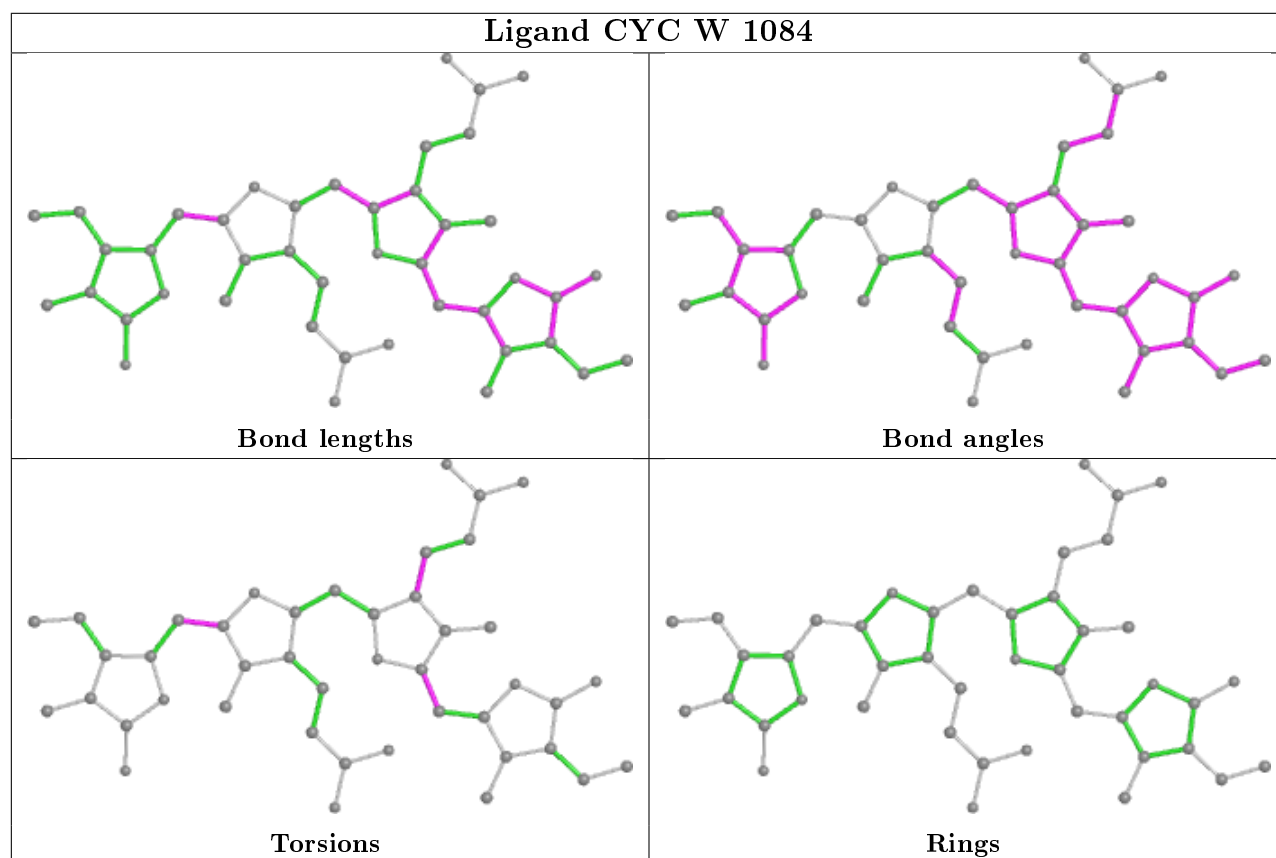
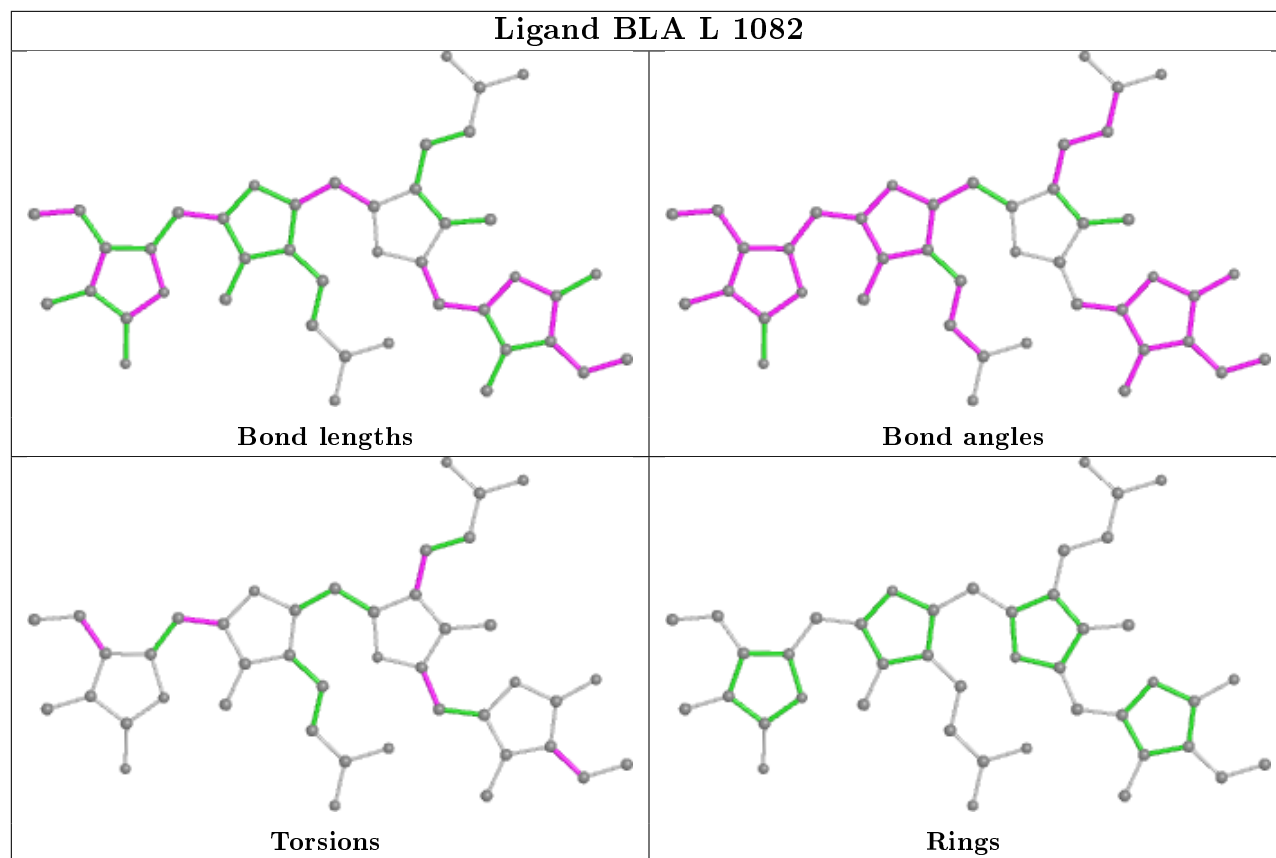


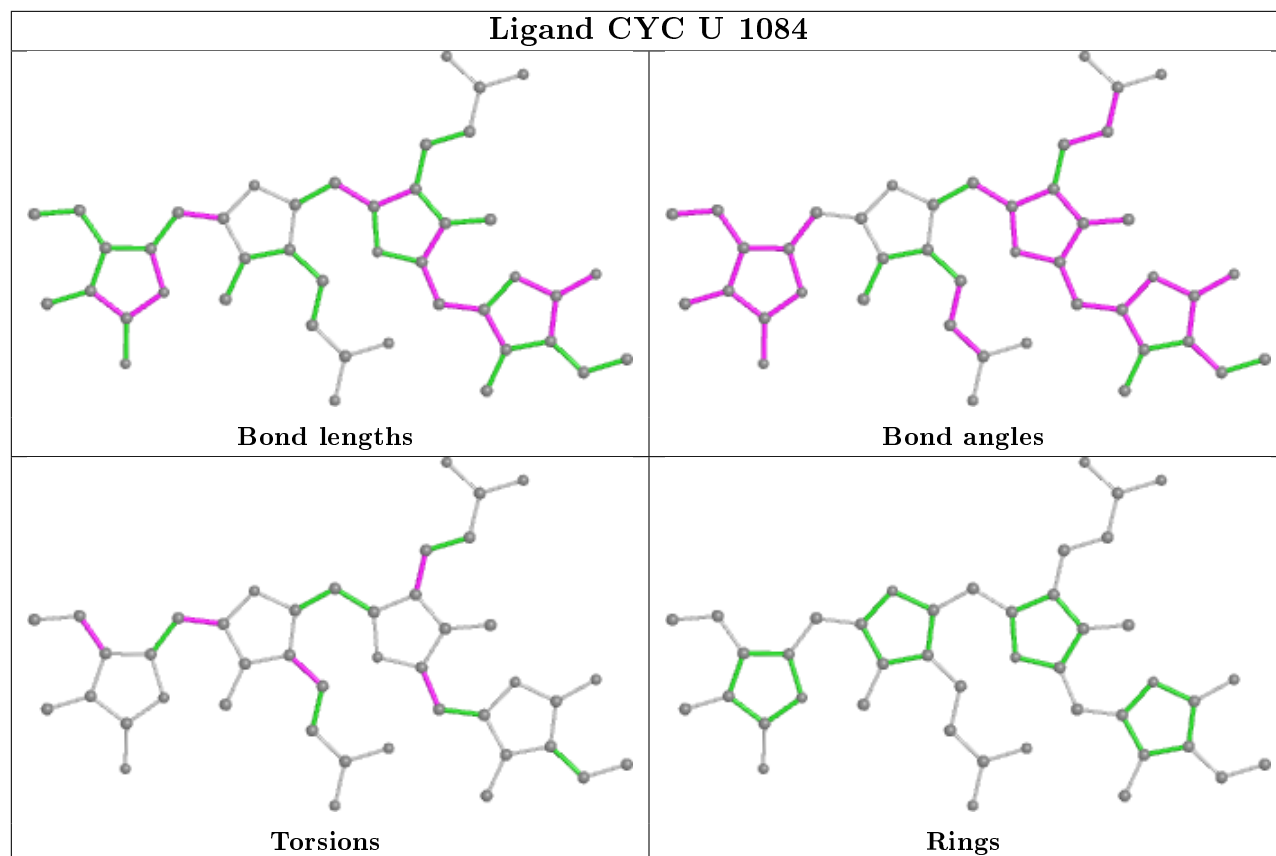
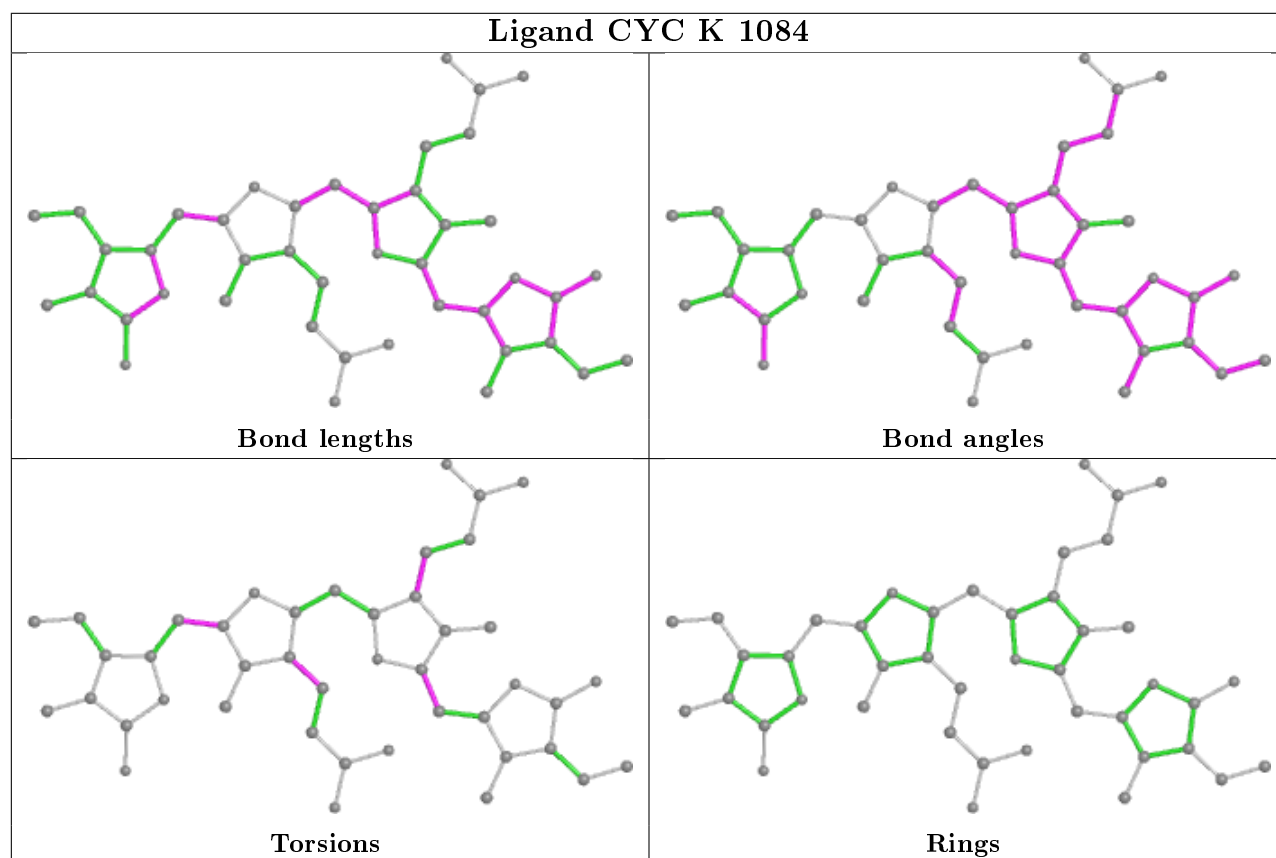
Ligand BLA D 1082

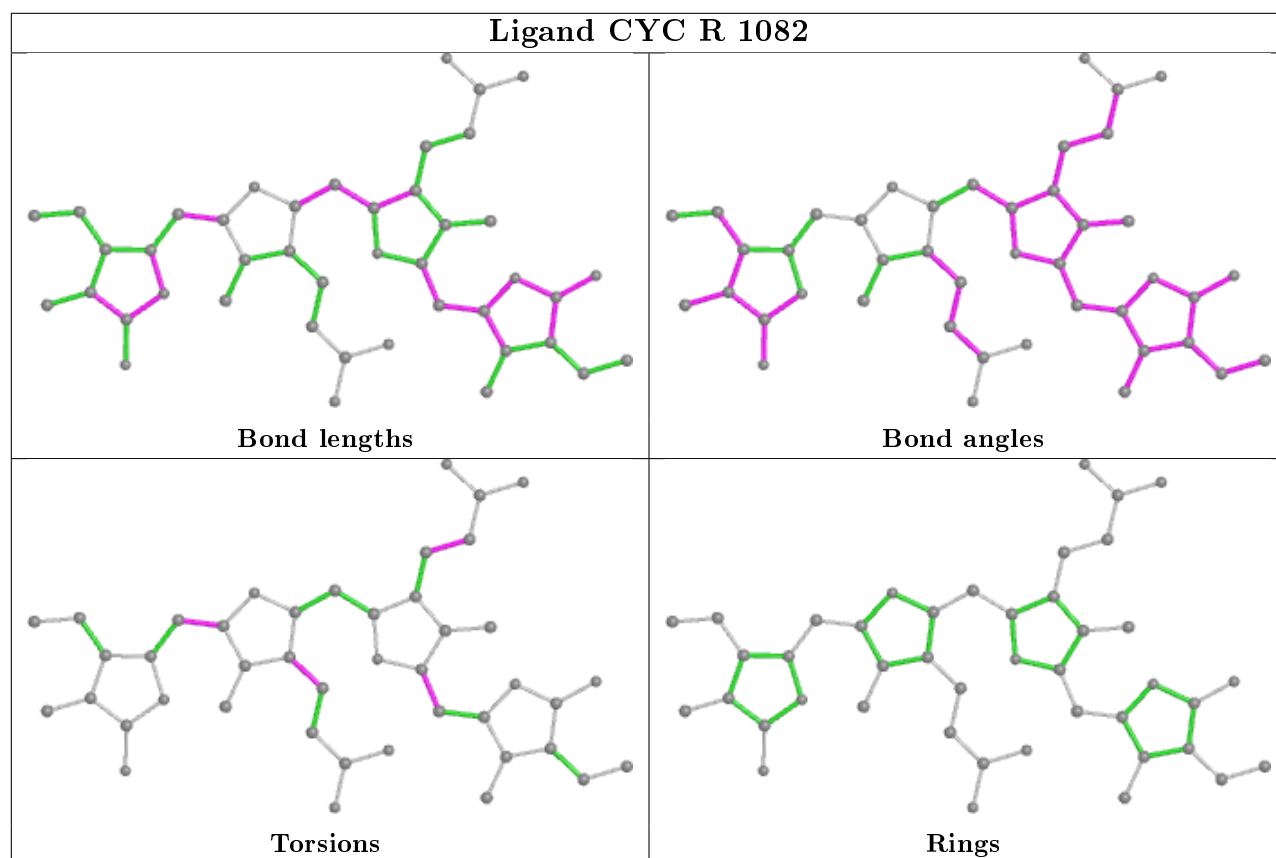
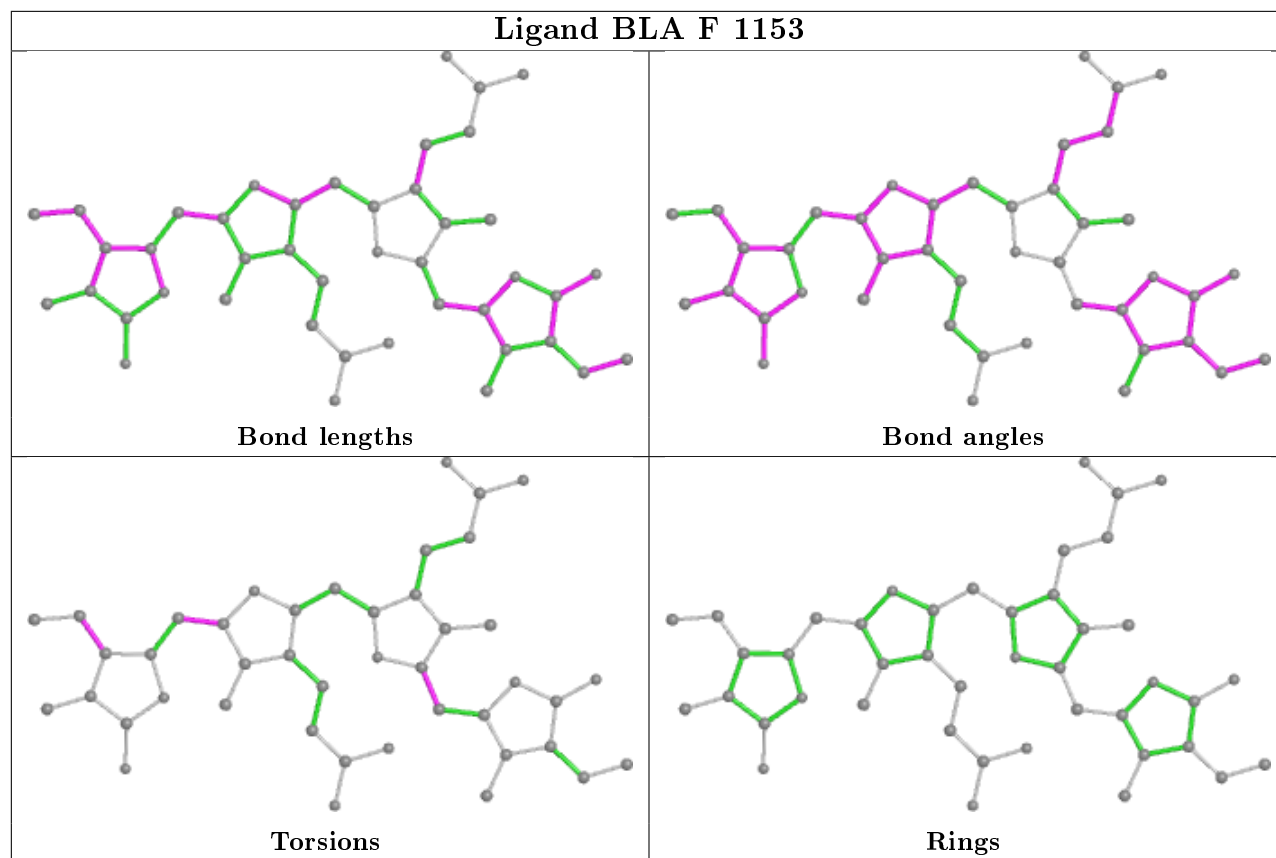


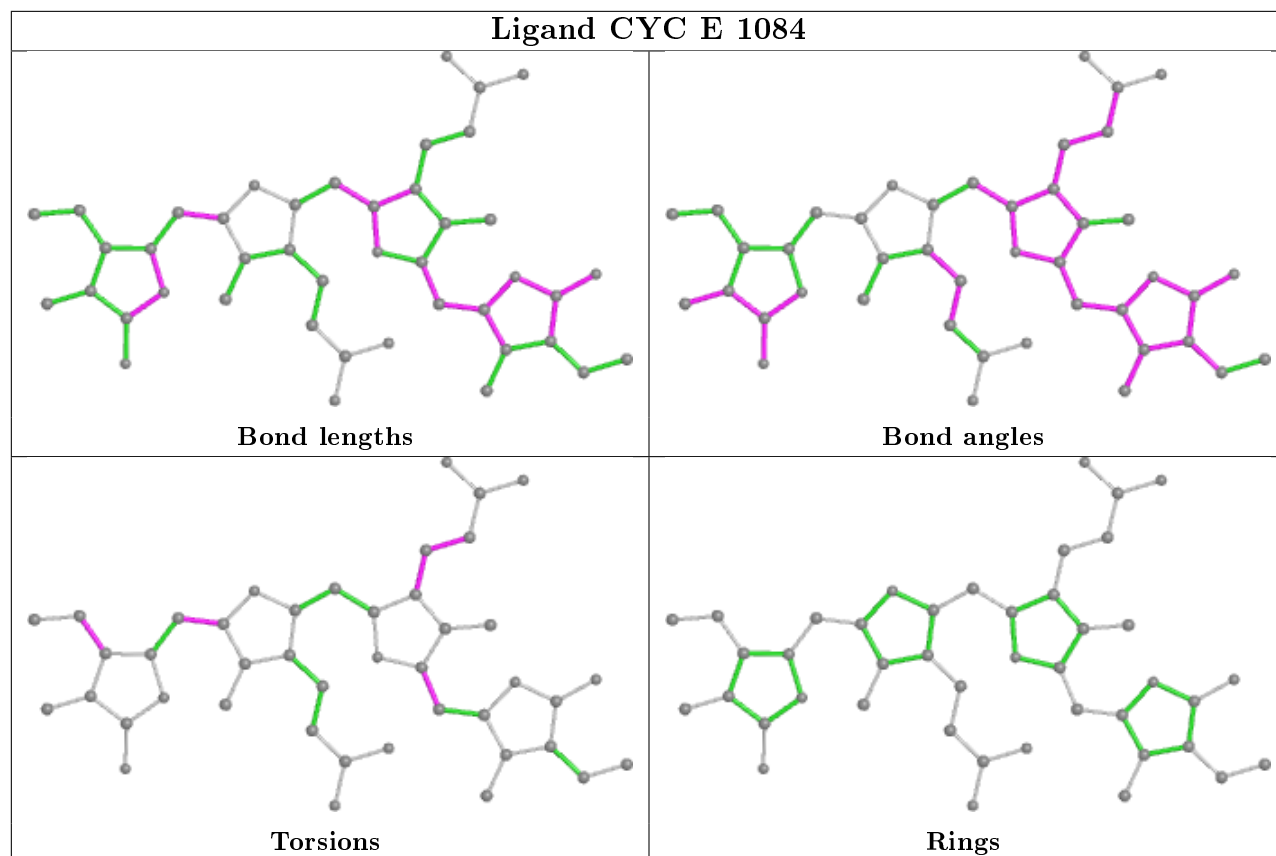
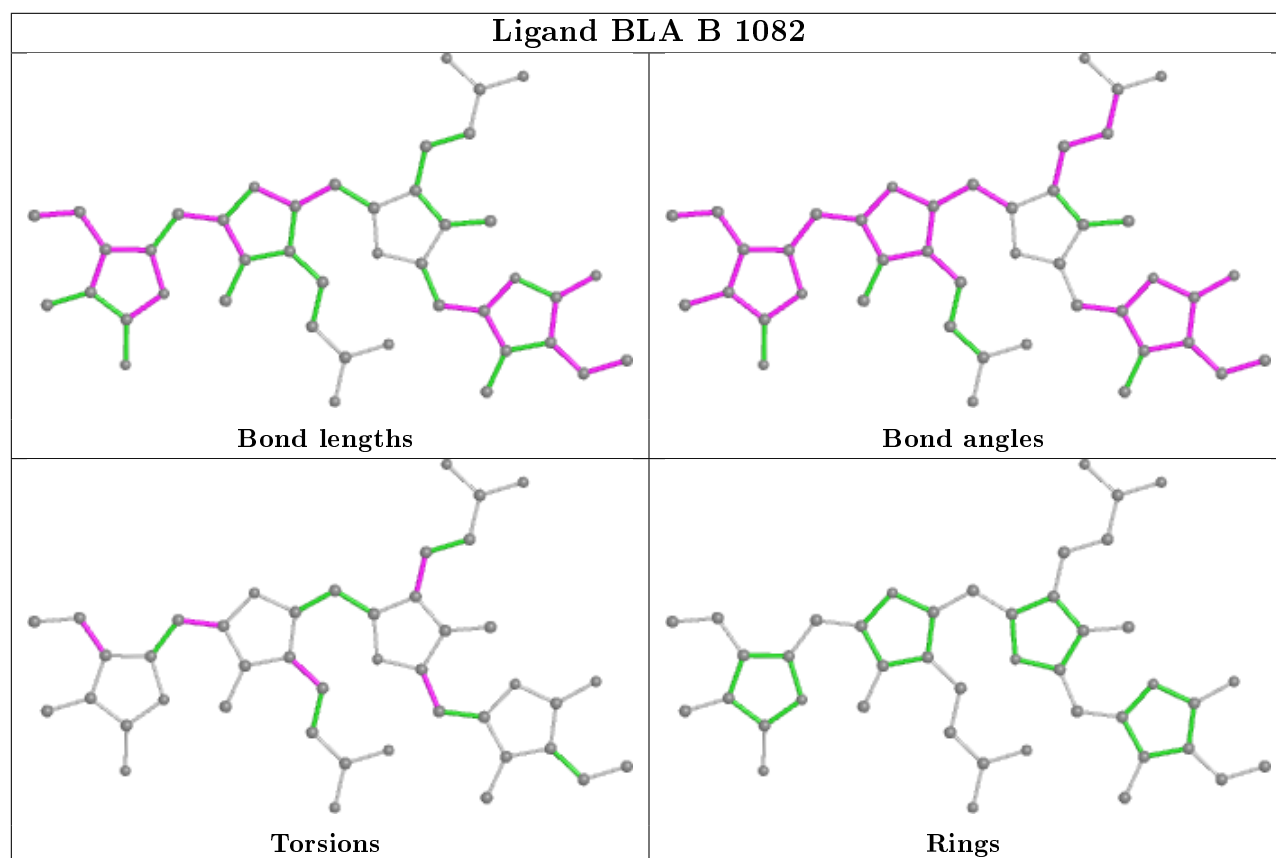
Ligand BLA L 1153



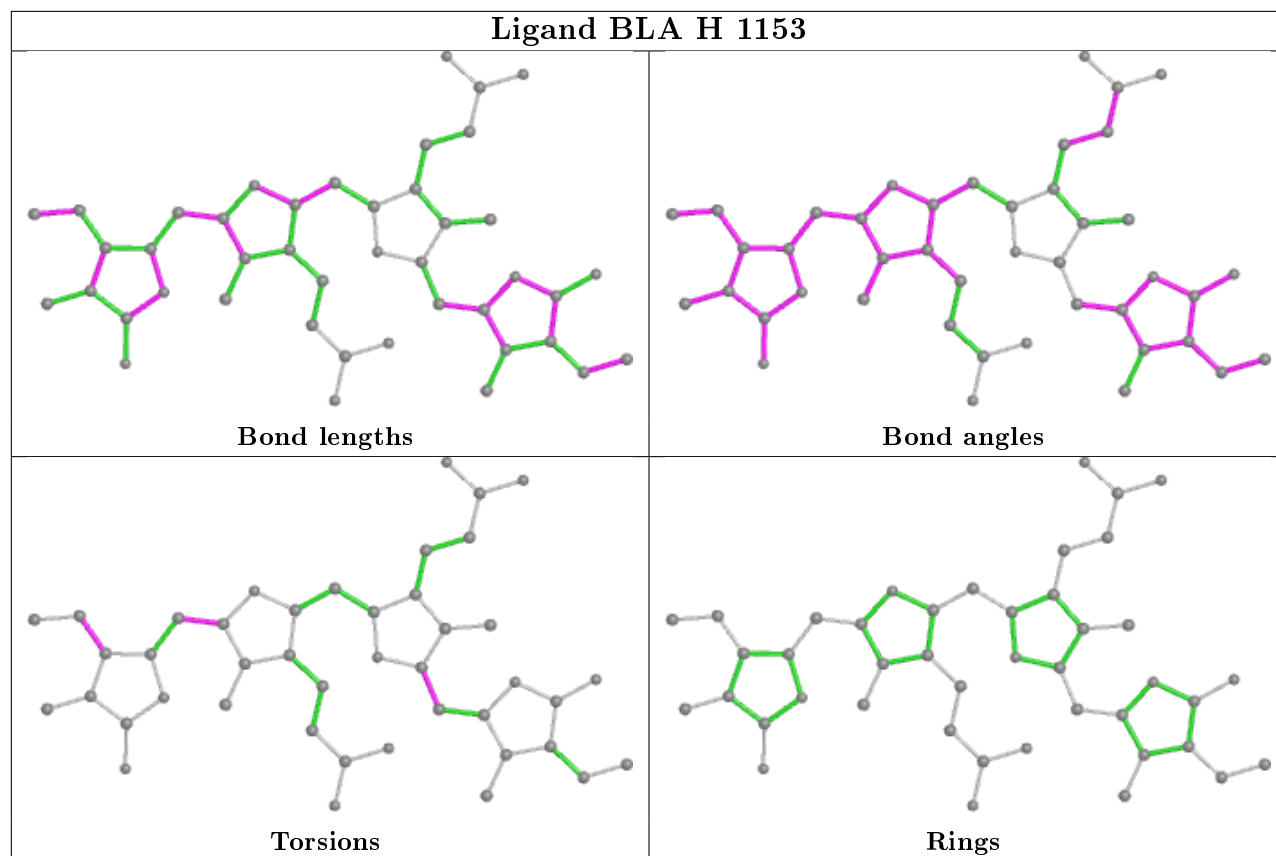


Ligand CYC U 1084**Ligand CYC K 1084**

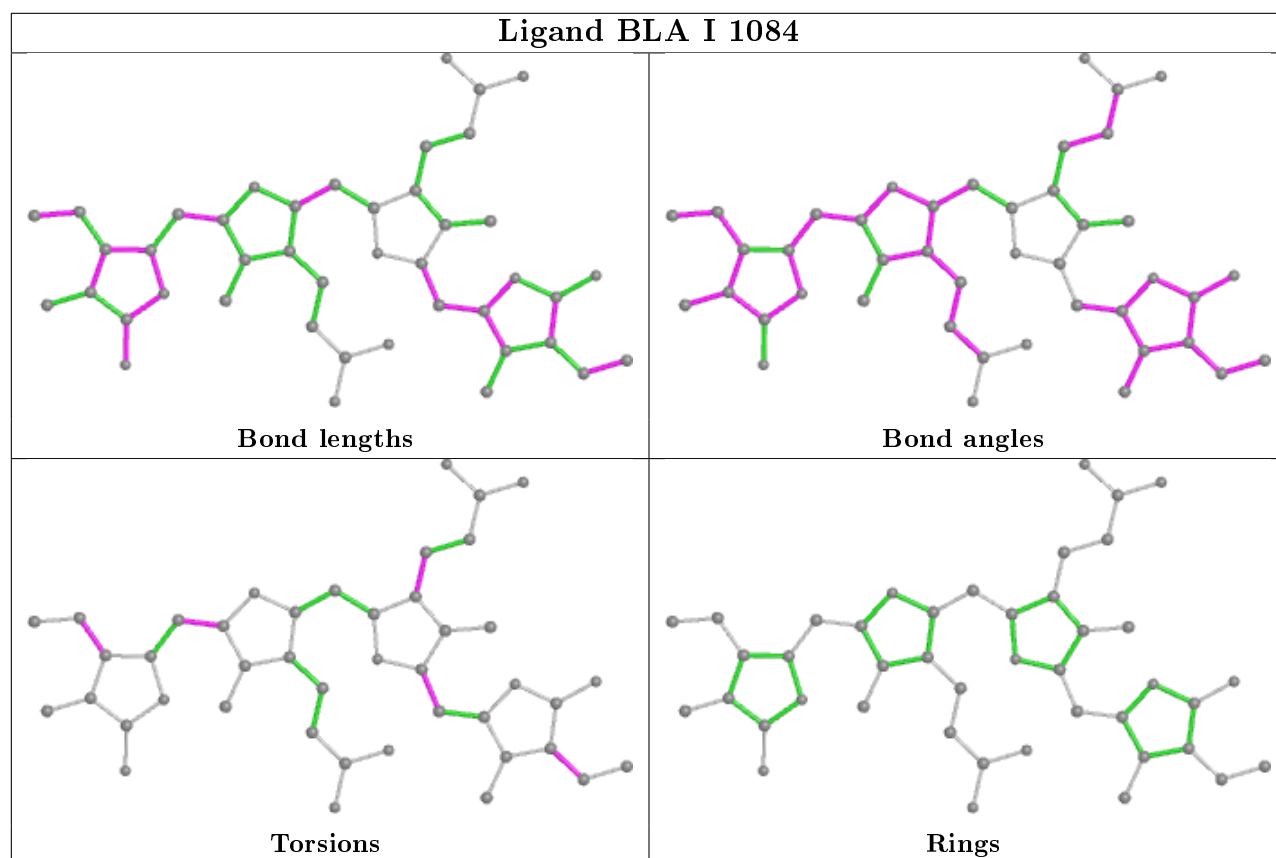


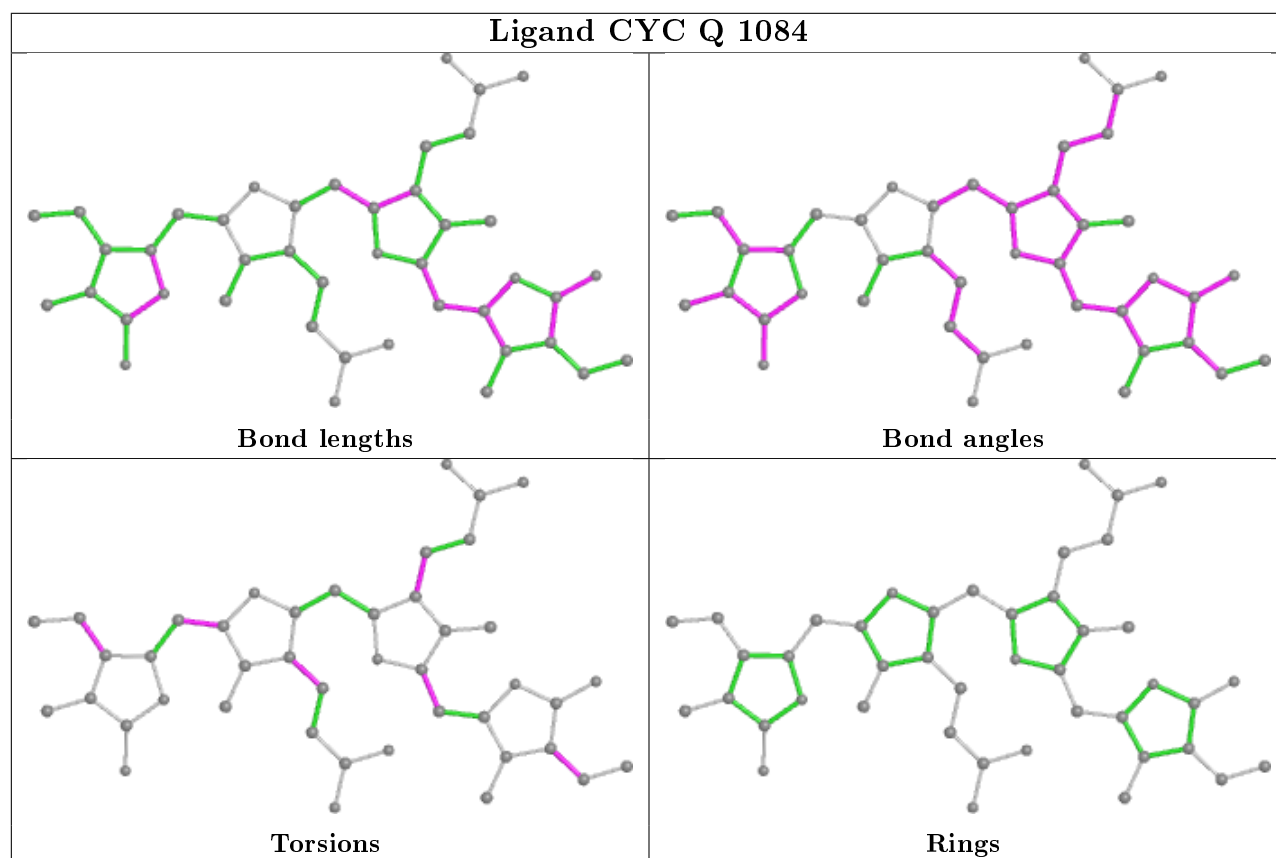
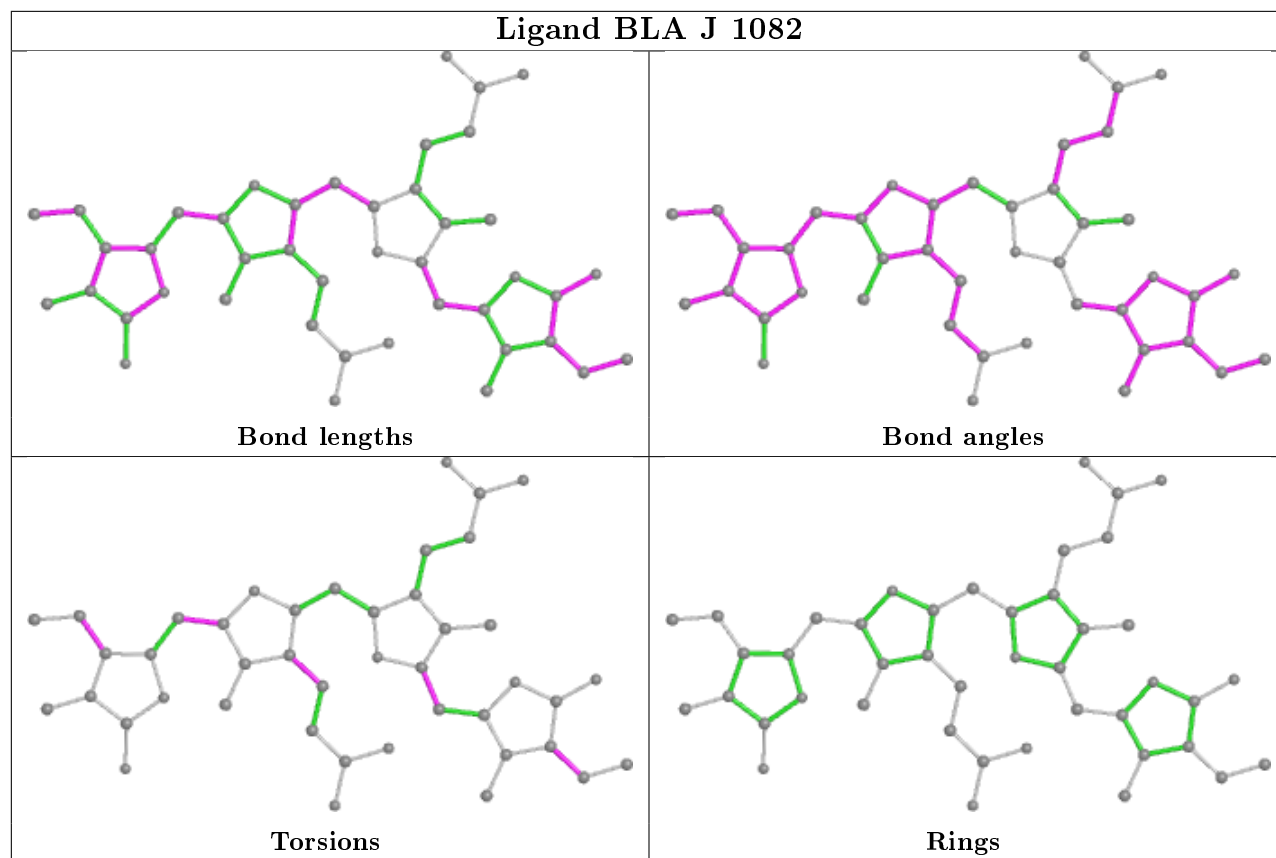
Ligand CYC E 1084**Ligand BLA B 1082**

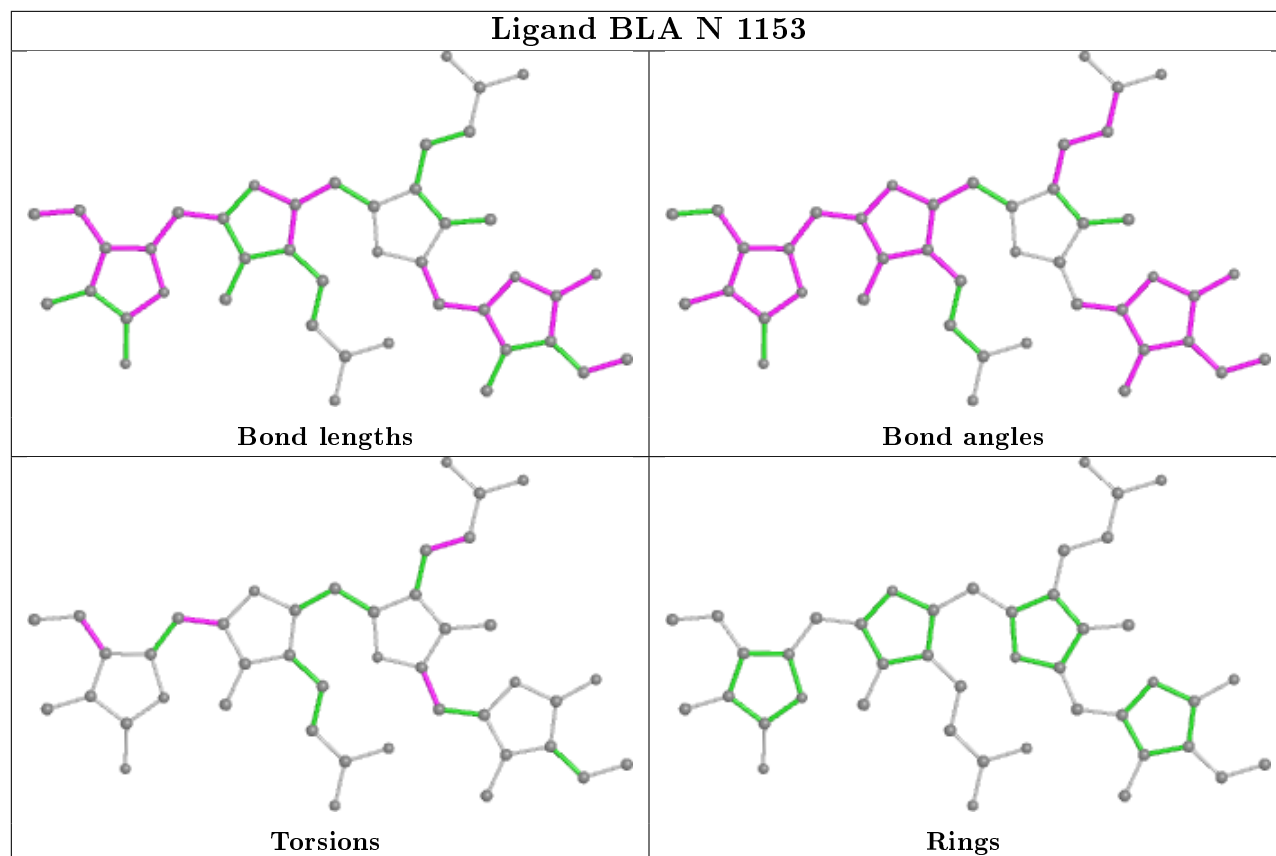
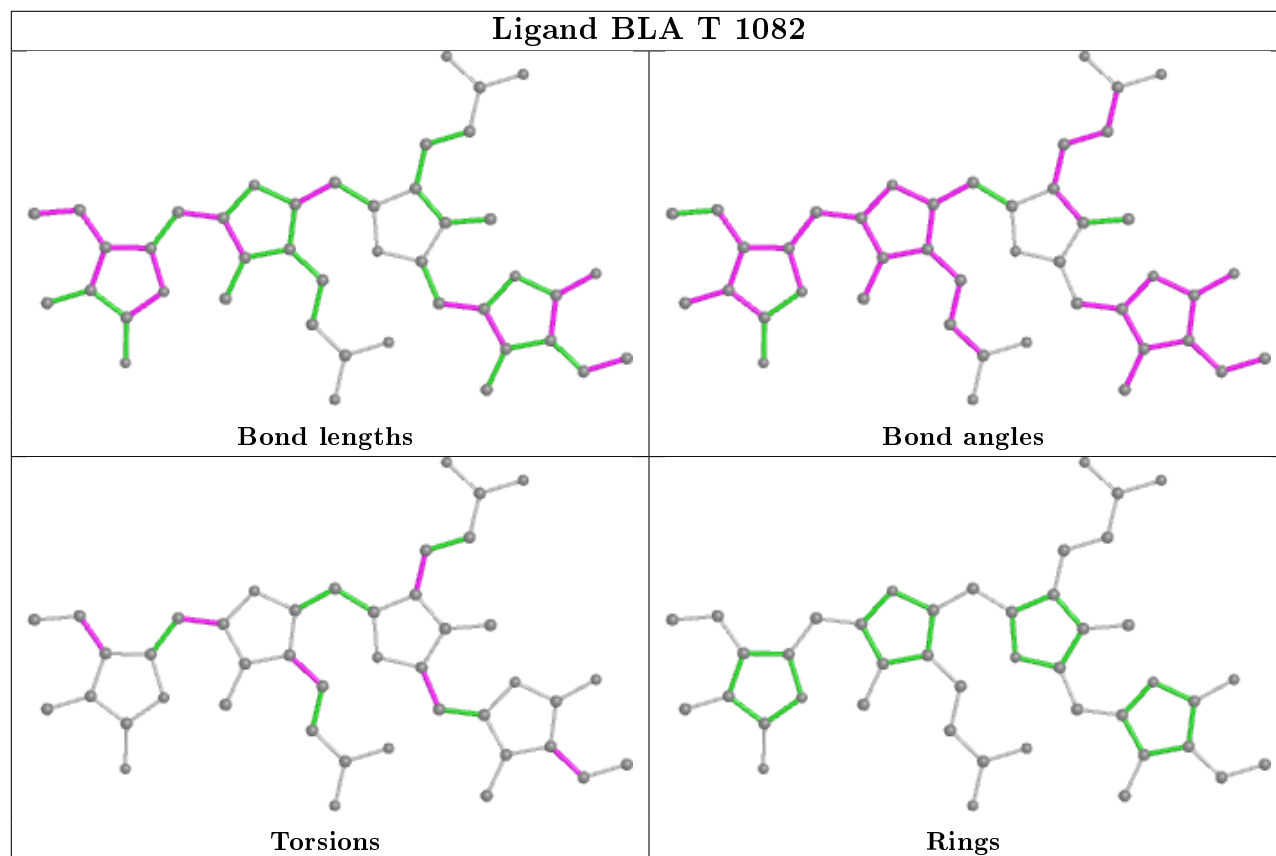
Ligand BLA H 1153



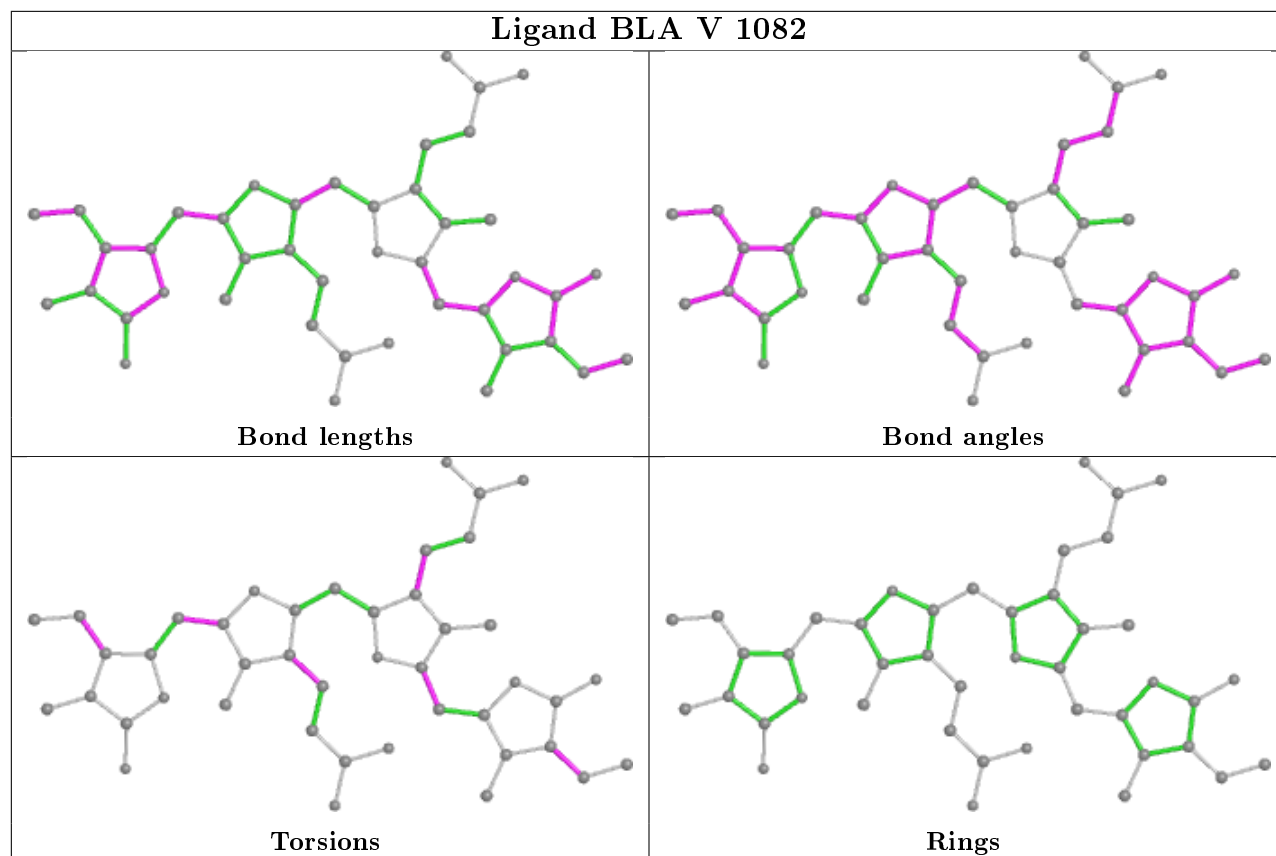
Ligand BLA I 1084



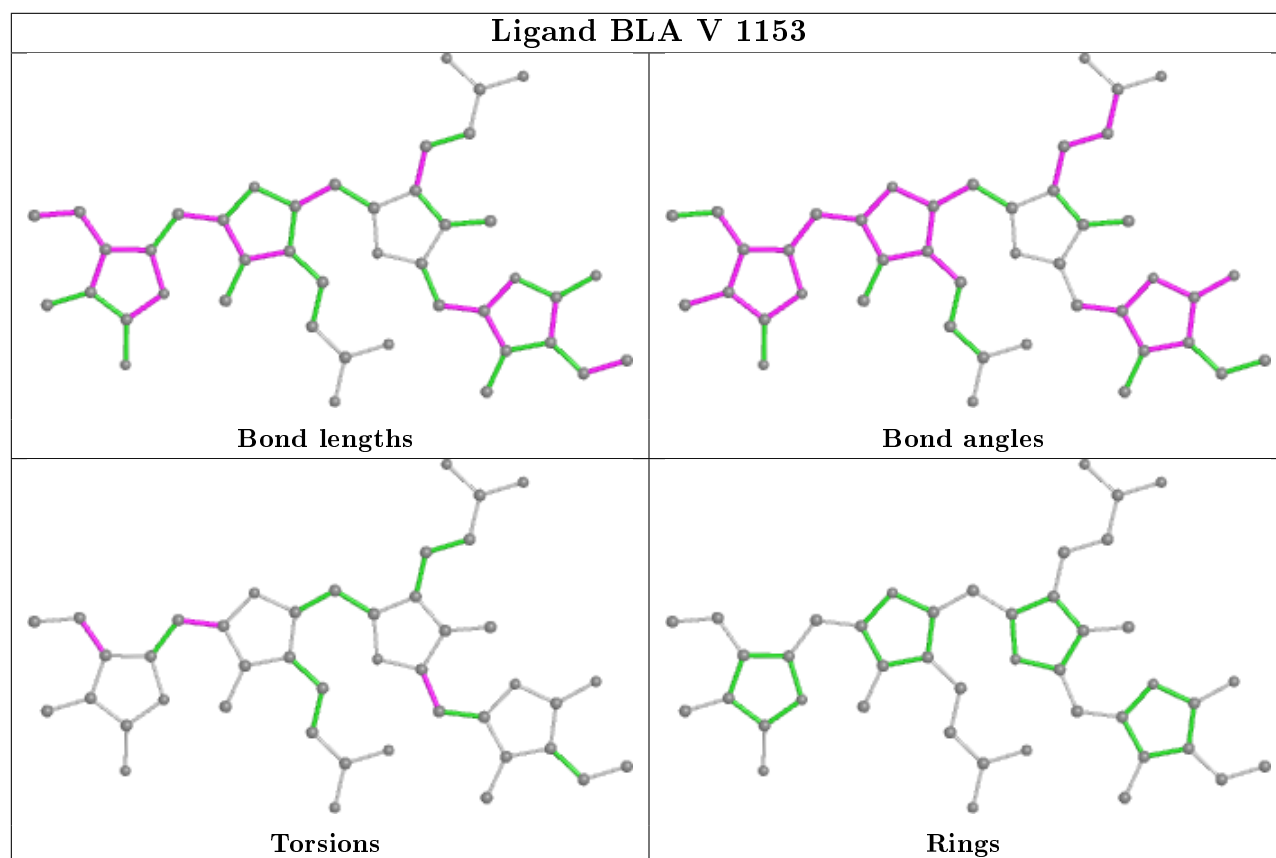


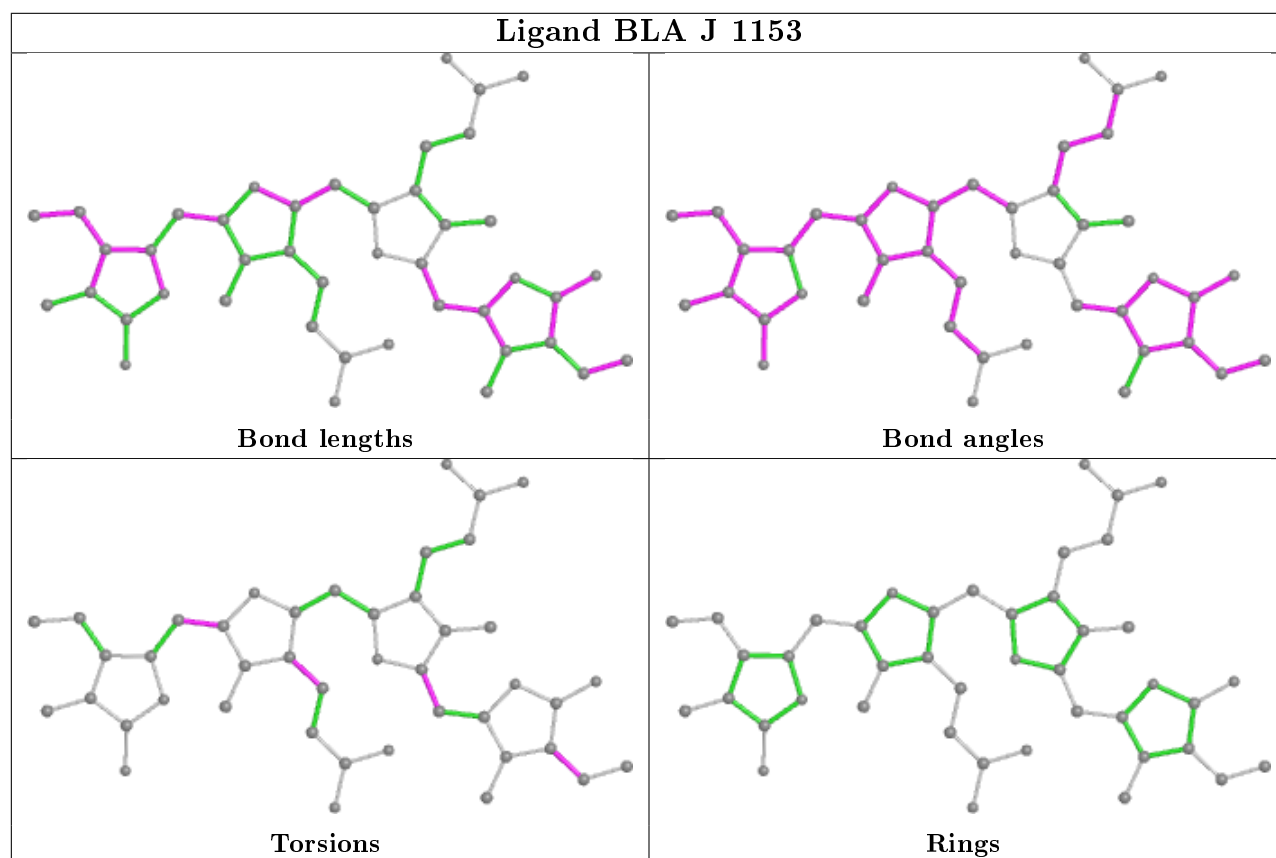
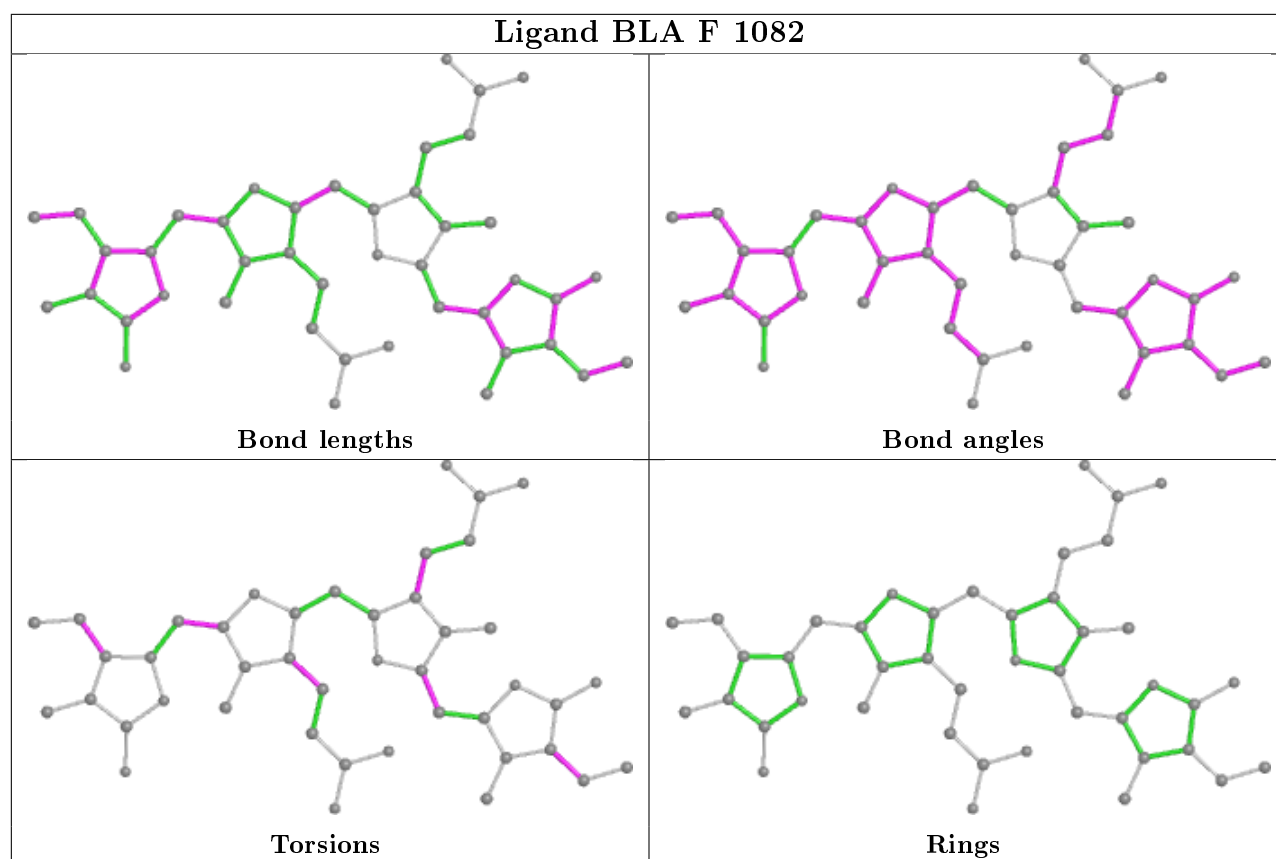
Ligand BLA N 1153**Ligand BLA T 1082**

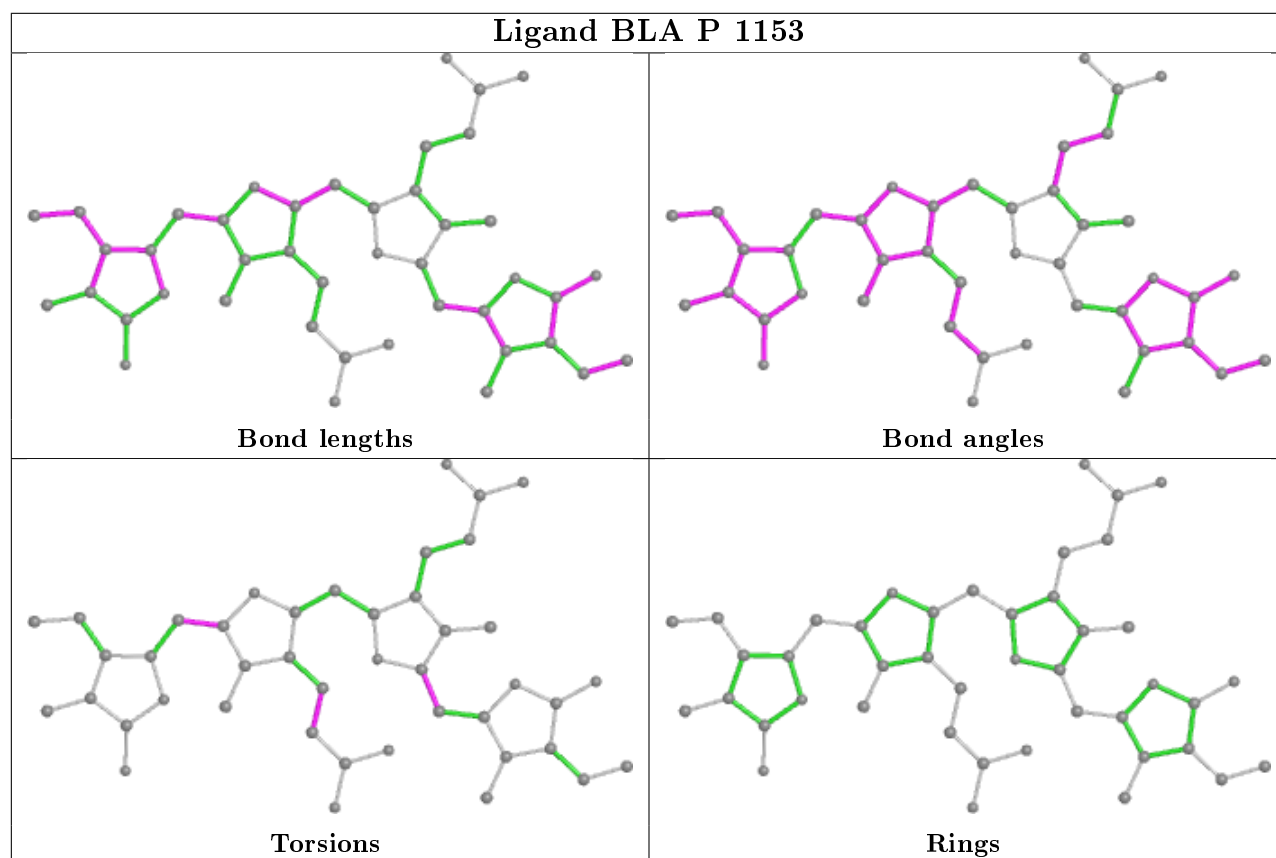
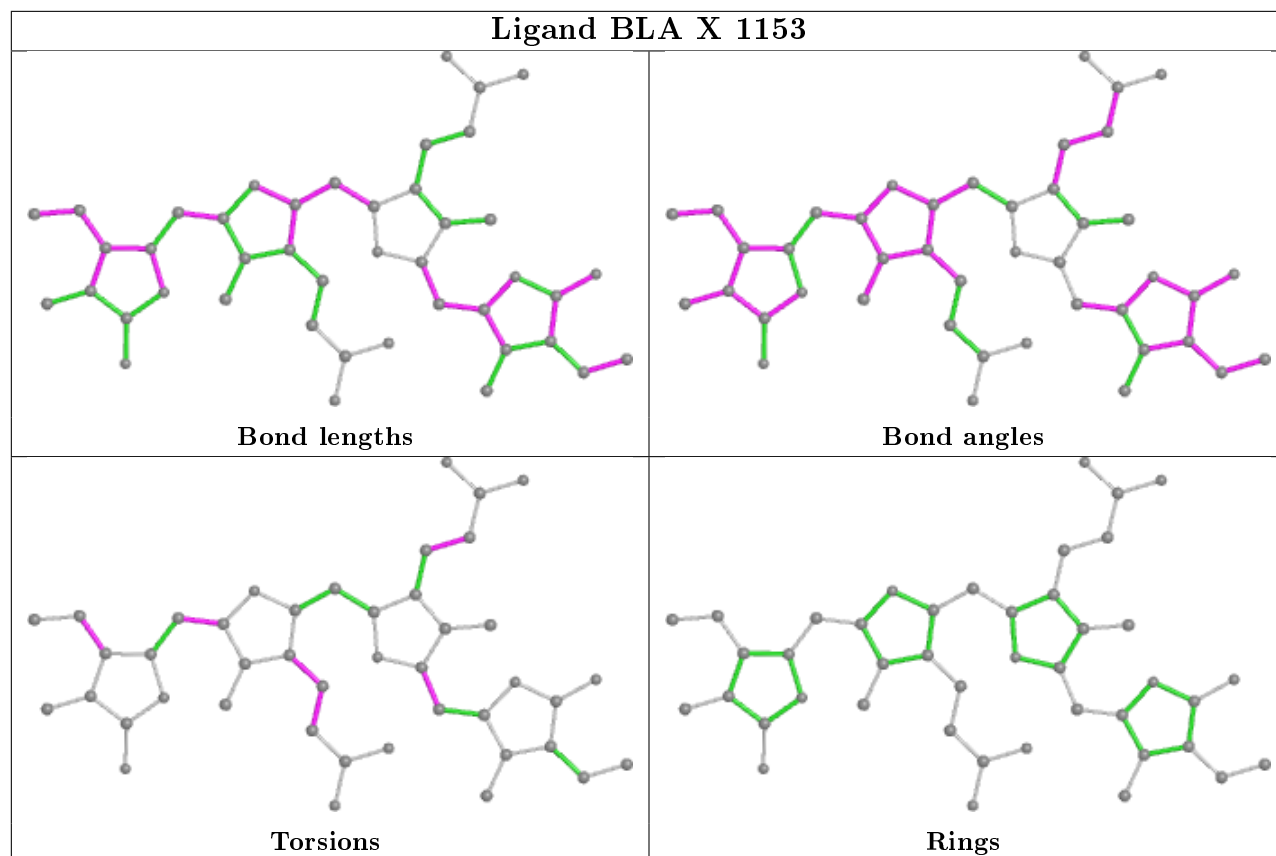
Ligand BLA V 1082



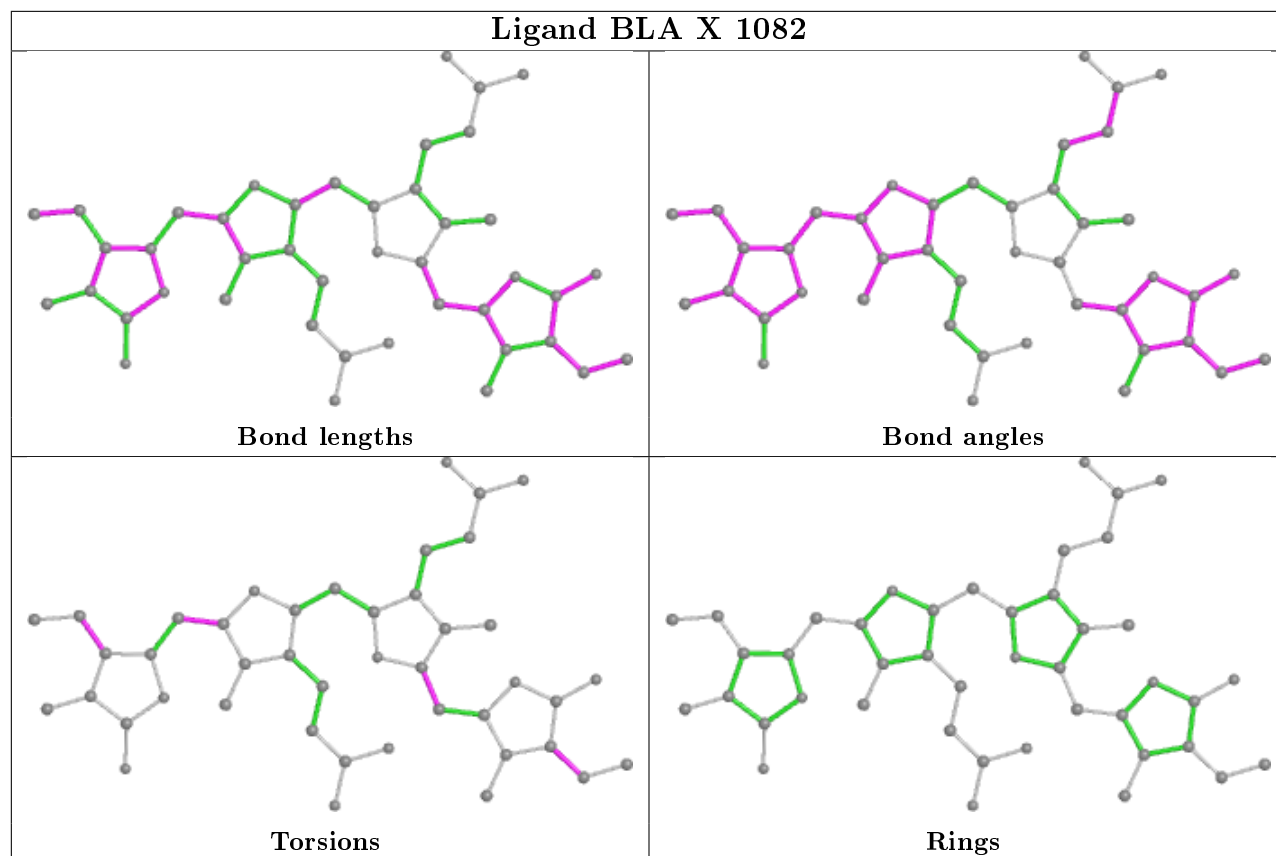
Ligand BLA V 1153



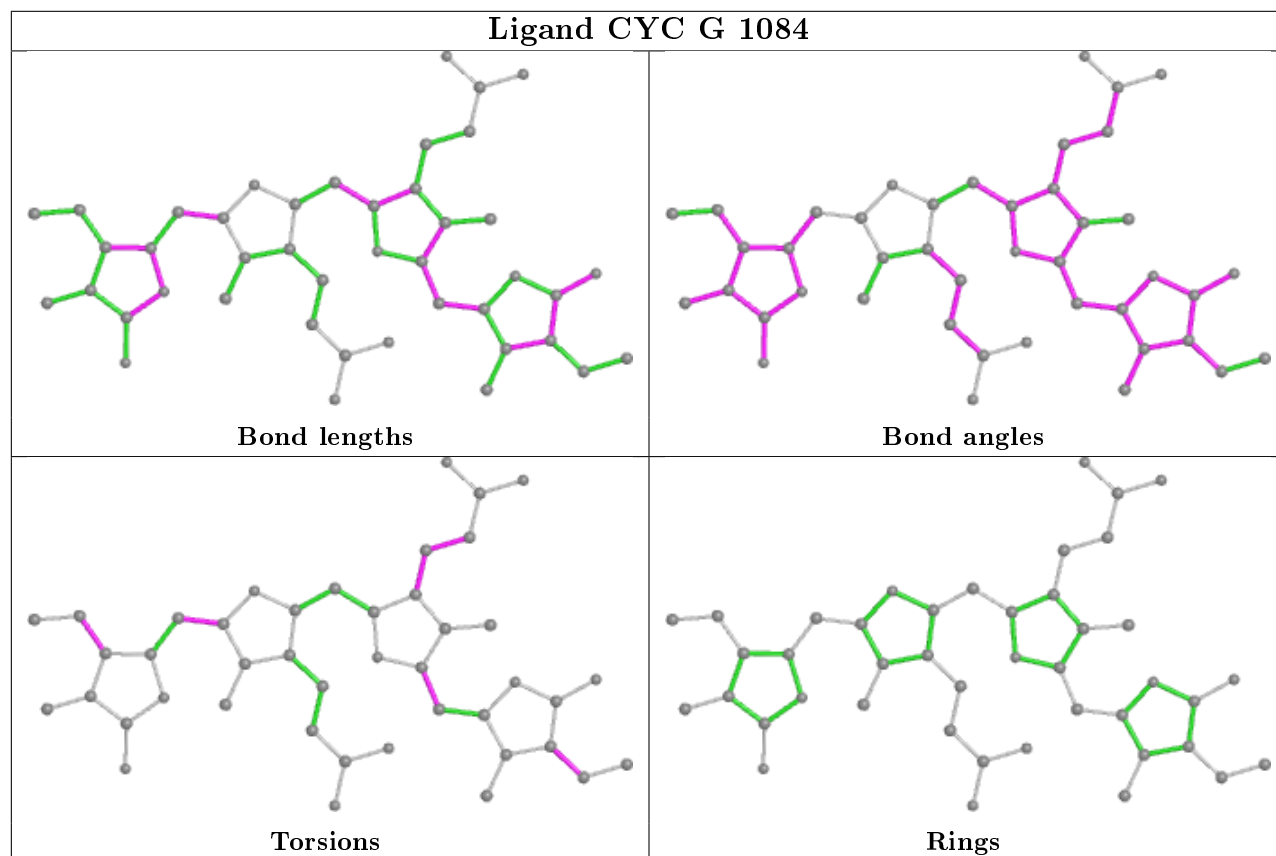


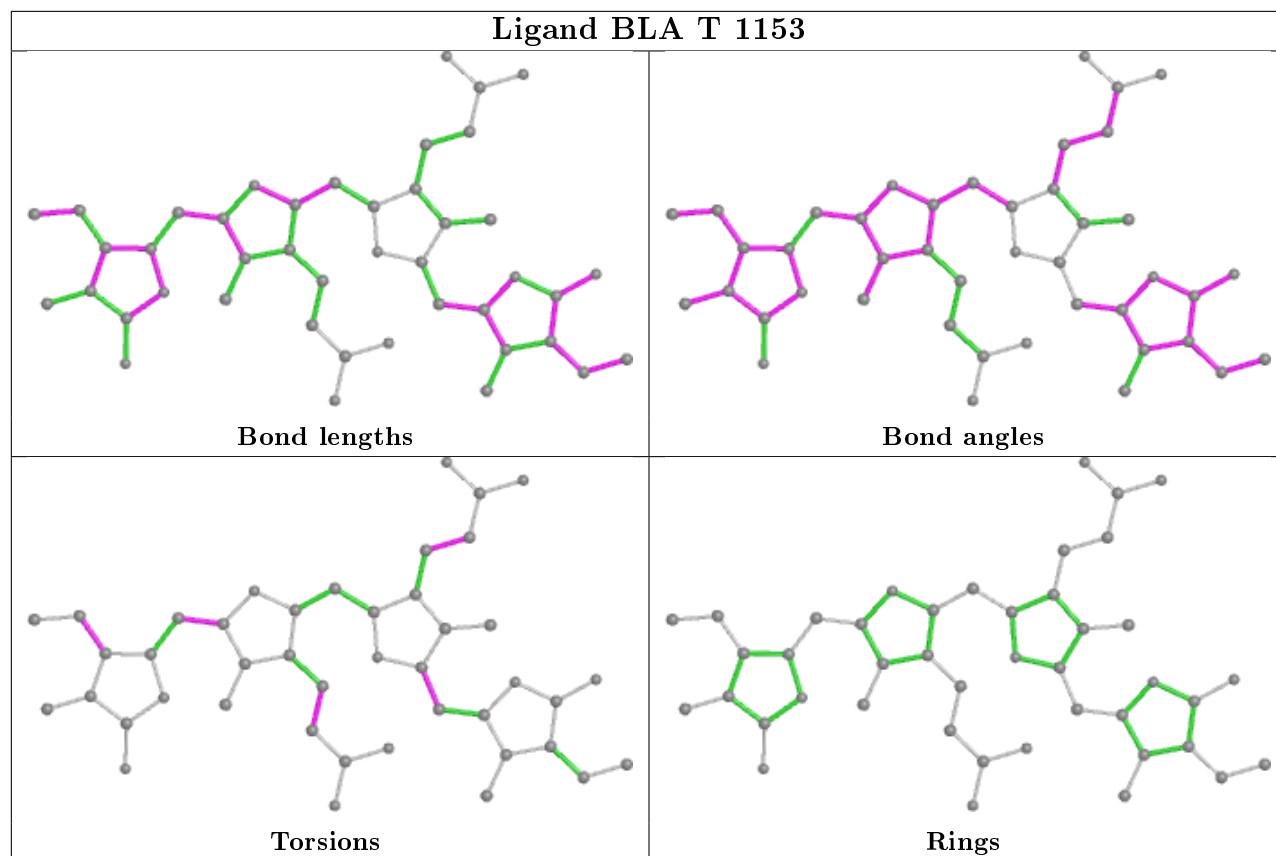
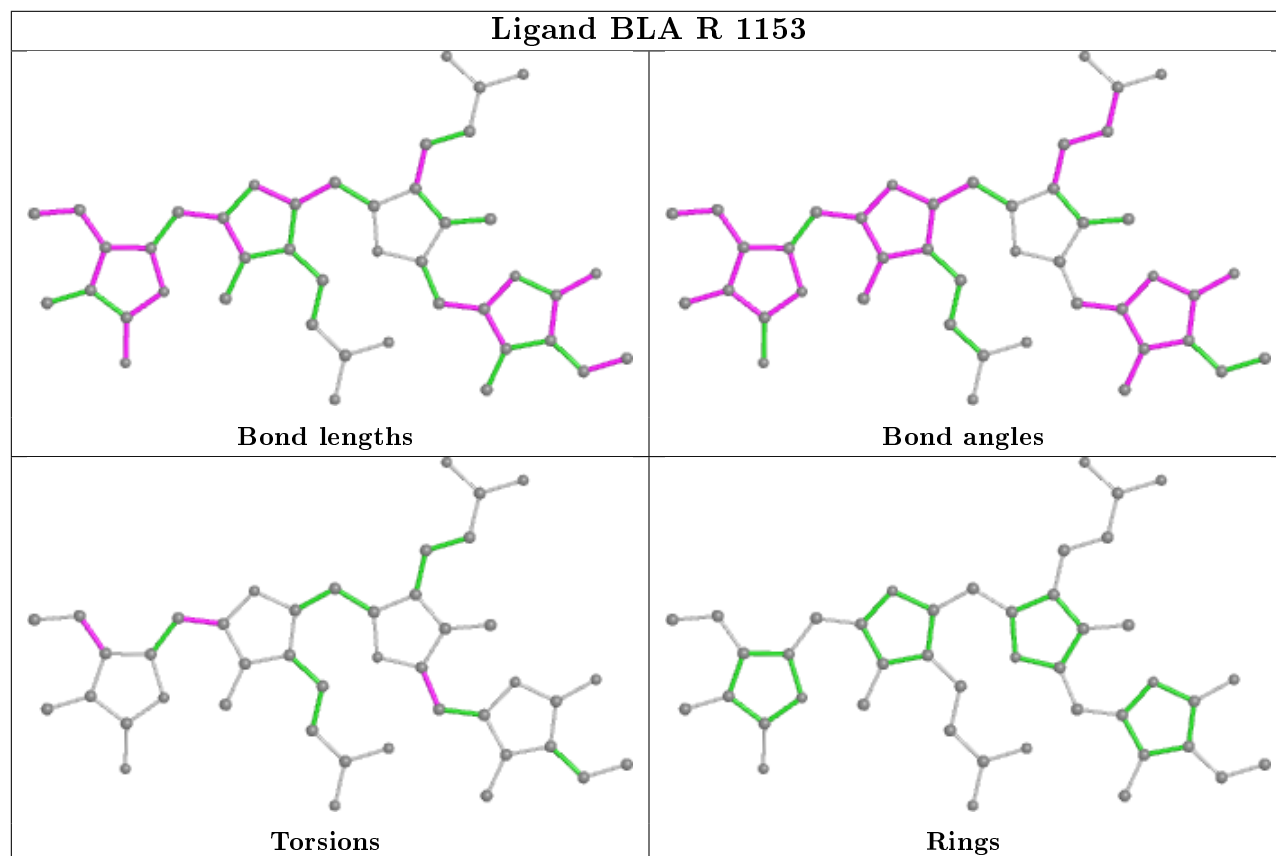


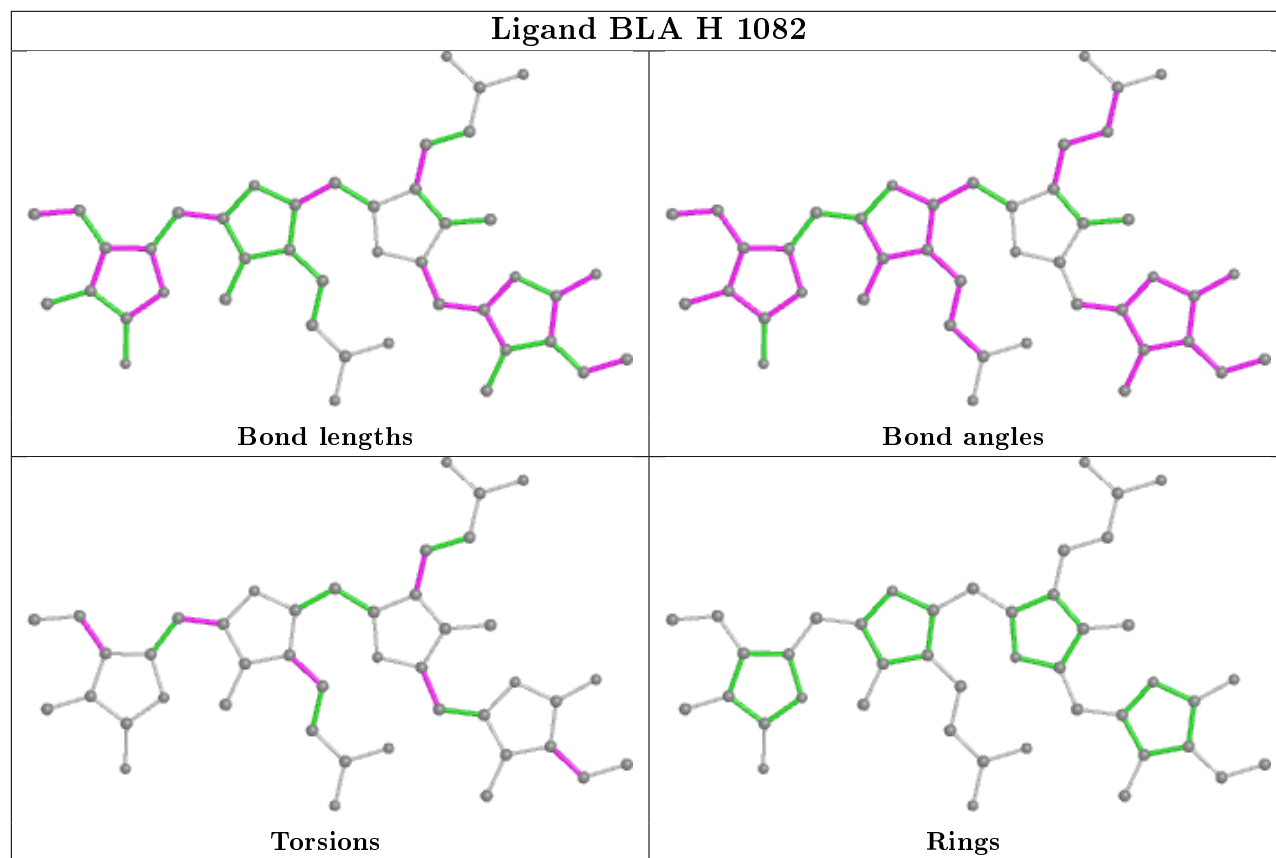
Ligand BLA X 1082



Ligand CYC G 1084



Ligand BLA T 1153**Ligand BLA R 1153**



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/162 (100%)	-0.70	0 100 100	16, 24, 32, 42	0
1	C	162/162 (100%)	-0.79	0 100 100	16, 24, 32, 42	0
1	E	162/162 (100%)	-0.74	0 100 100	16, 23, 32, 42	0
1	G	162/162 (100%)	-0.78	0 100 100	16, 24, 32, 42	0
1	I	162/162 (100%)	-0.77	0 100 100	16, 24, 32, 42	0
1	K	162/162 (100%)	-0.71	0 100 100	16, 24, 32, 42	0
1	M	162/162 (100%)	-0.68	0 100 100	16, 24, 32, 42	0
1	O	162/162 (100%)	-0.73	0 100 100	16, 24, 32, 42	0
1	Q	162/162 (100%)	-0.72	0 100 100	16, 24, 32, 42	0
1	S	162/162 (100%)	-0.71	0 100 100	16, 24, 32, 42	0
1	U	162/162 (100%)	-0.78	0 100 100	16, 24, 32, 42	0
1	W	162/162 (100%)	-0.80	0 100 100	16, 24, 32, 42	0
2	B	172/172 (100%)	-0.70	0 100 100	15, 24, 35, 41	0
2	D	172/172 (100%)	-0.77	0 100 100	15, 24, 35, 41	0
2	F	172/172 (100%)	-0.78	0 100 100	15, 24, 35, 41	0
2	H	172/172 (100%)	-0.64	0 100 100	15, 24, 35, 41	0
2	J	172/172 (100%)	-0.65	0 100 100	15, 24, 35, 41	0
2	L	172/172 (100%)	-0.70	0 100 100	15, 24, 35, 41	0
2	N	172/172 (100%)	-0.72	0 100 100	15, 24, 35, 41	0
2	P	172/172 (100%)	-0.63	0 100 100	15, 24, 35, 41	0
2	R	172/172 (100%)	-0.68	0 100 100	15, 24, 35, 41	0
2	T	172/172 (100%)	-0.67	0 100 100	15, 24, 35, 41	0
2	V	172/172 (100%)	-0.69	0 100 100	15, 24, 35, 41	0
3	X	172/172 (100%)	-0.72	0 100 100	15, 24, 35, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4008/4008 (100%)	-0.72	0 100 100	15, 24, 35, 42	0

There are no RSRZ outliers to report.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BLA	P	1082	43/43	0.85	0.30	45,52,54,57	0
5	BLA	J	1082	43/43	0.86	0.28	38,45,49,50	0
4	CYC	R	1082	43/43	0.87	0.32	31,38,42,50	0
5	BLA	D	1082	43/43	0.87	0.26	32,41,43,44	0
5	BLA	X	1082	43/43	0.87	0.32	36,45,49,52	0
5	BLA	L	1082	43/43	0.88	0.29	23,30,36,41	0
5	BLA	V	1082	43/43	0.88	0.29	33,39,47,54	0
5	BLA	J	1153	43/43	0.88	0.26	34,51,51,54	0
5	BLA	B	1082	43/43	0.88	0.31	25,32,39,41	0
5	BLA	H	1153	43/43	0.89	0.22	24,33,35,37	0
5	BLA	L	1153	43/43	0.89	0.23	17,31,31,33	0
5	BLA	X	1153	43/43	0.89	0.24	34,45,45,46	0
5	BLA	P	1153	43/43	0.89	0.24	29,43,44,45	0
5	BLA	T	1082	43/43	0.89	0.29	30,38,43,47	0
5	BLA	B	1153	43/43	0.90	0.25	19,26,27,29	0
5	BLA	N	1153	43/43	0.90	0.24	16,31,31,32	0
5	BLA	V	1153	43/43	0.90	0.23	18,31,32,32	0
5	BLA	F	1082	43/43	0.90	0.29	35,40,46,51	0
5	BLA	T	1153	43/43	0.90	0.24	19,42,43,43	0

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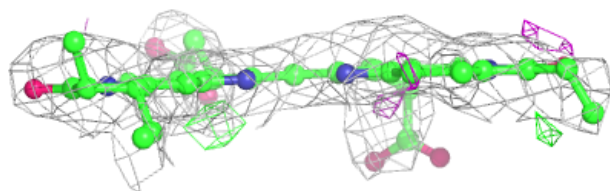
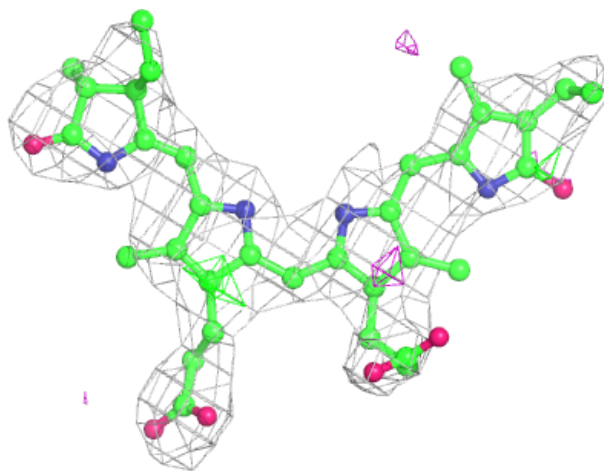
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BLA	R	1153	43/43	0.90	0.22	18,31,32,32	0
5	BLA	H	1082	43/43	0.90	0.26	23,32,38,44	0
4	CYC	M	1084	43/43	0.91	0.21	36,42,44,48	0
5	BLA	D	1153	43/43	0.91	0.22	26,34,35,38	0
5	BLA	N	1082	43/43	0.92	0.28	28,31,36,39	0
4	CYC	G	1084	43/43	0.92	0.20	21,27,31,33	0
4	CYC	S	1084	43/43	0.92	0.20	13,23,24,28	0
4	CYC	W	1084	43/43	0.92	0.19	26,33,33,34	0
5	BLA	F	1153	43/43	0.92	0.23	18,34,34,35	0
4	CYC	U	1084	43/43	0.93	0.19	27,29,30,31	0
4	CYC	O	1084	43/43	0.93	0.18	13,23,24,25	0
5	BLA	I	1084	43/43	0.93	0.20	16,23,24,29	0
4	CYC	A	1084	43/43	0.93	0.18	15,21,21,26	0
4	CYC	Q	1084	43/43	0.93	0.20	14,22,24,25	0
4	CYC	E	1084	43/43	0.93	0.21	12,21,22,23	0
4	CYC	K	1084	43/43	0.94	0.19	10,22,22,23	0
4	CYC	C	1084	43/43	0.94	0.20	23,29,29,31	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.

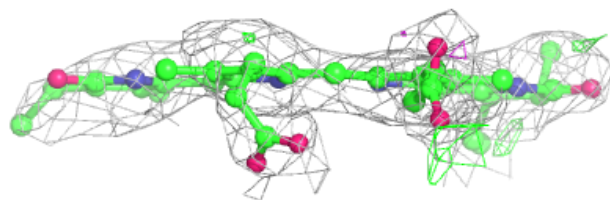
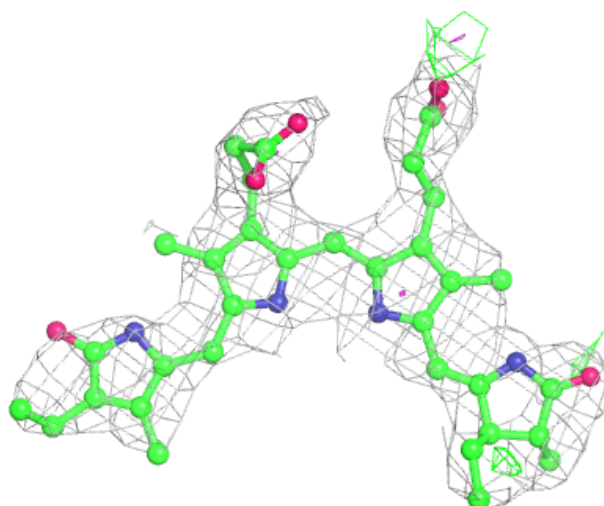
Electron density around BLA P 1082:

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



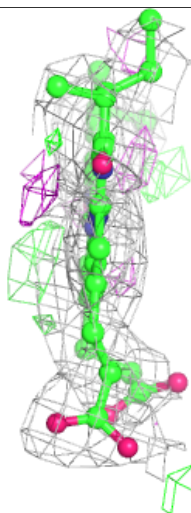
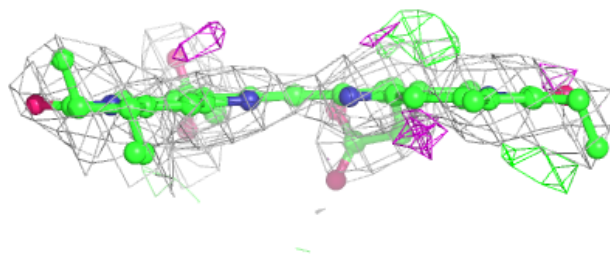
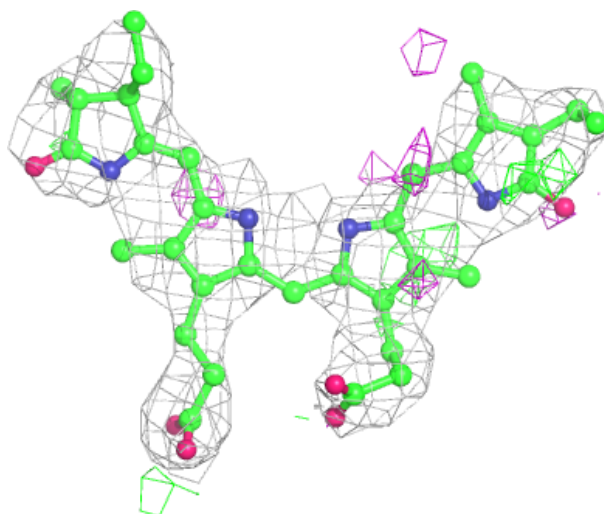
Electron density around BLA J 1082:

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



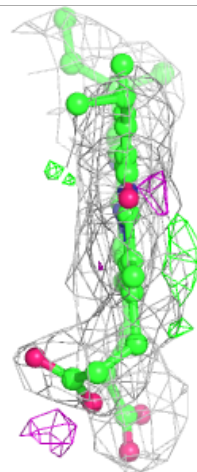
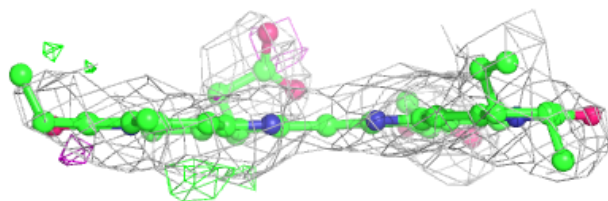
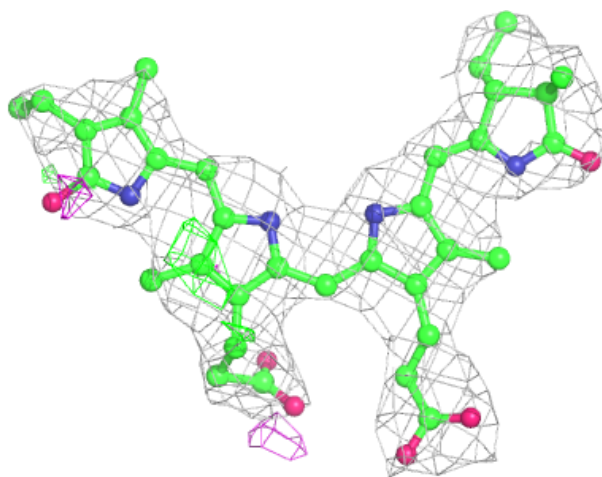
Electron density around CYC R 1082:

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



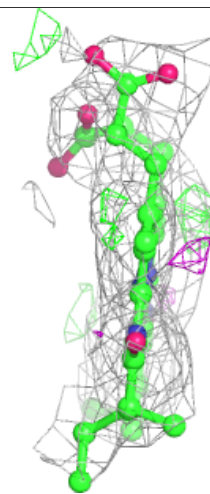
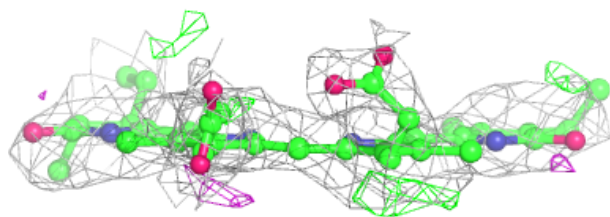
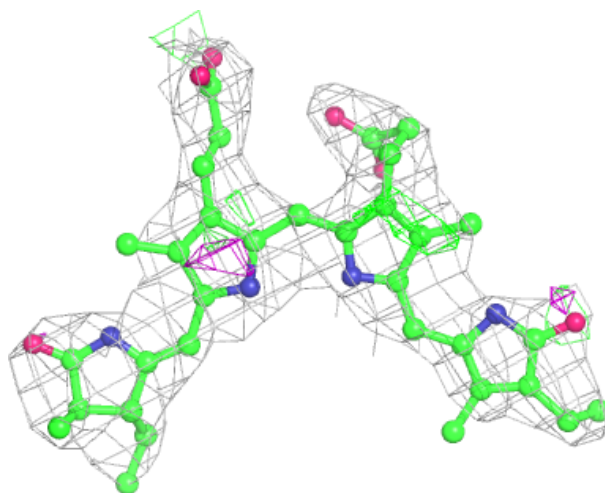
Electron density around BLA D 1082:

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



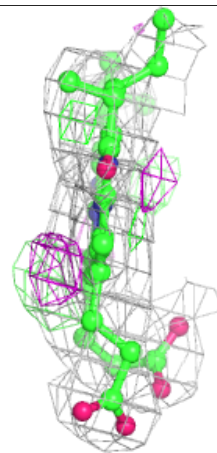
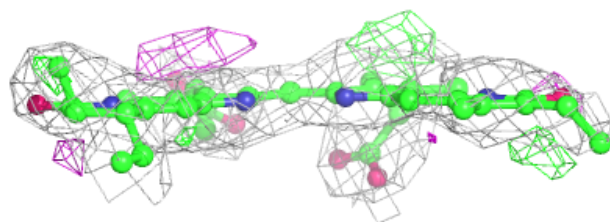
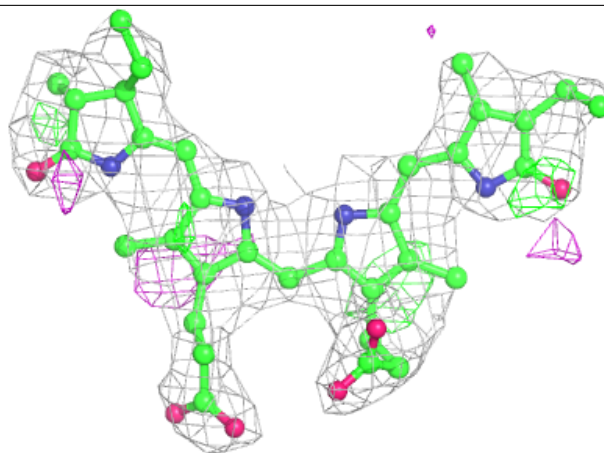
Electron density around BLA X 1082:

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



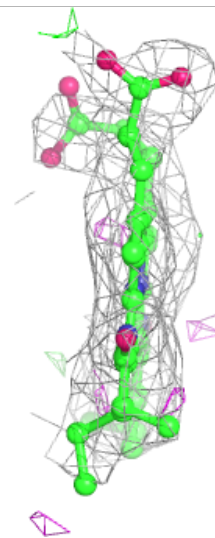
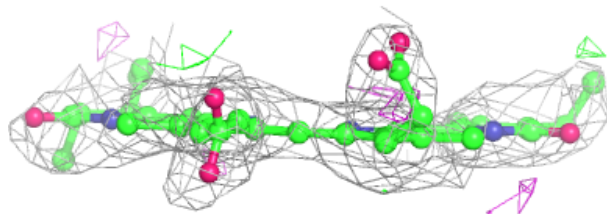
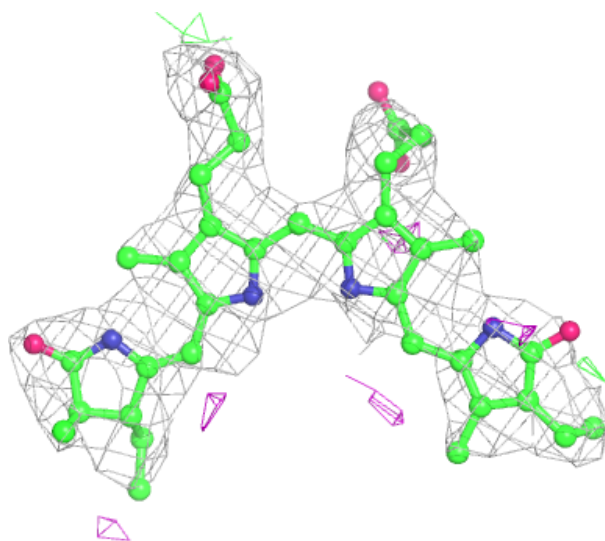
Electron density around BLA L 1082:

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



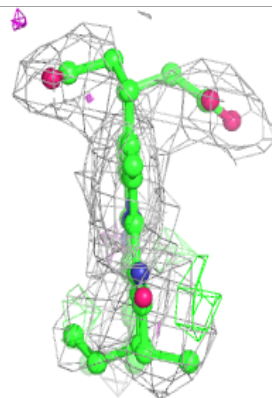
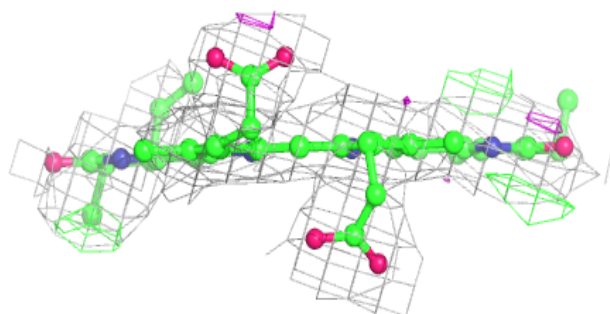
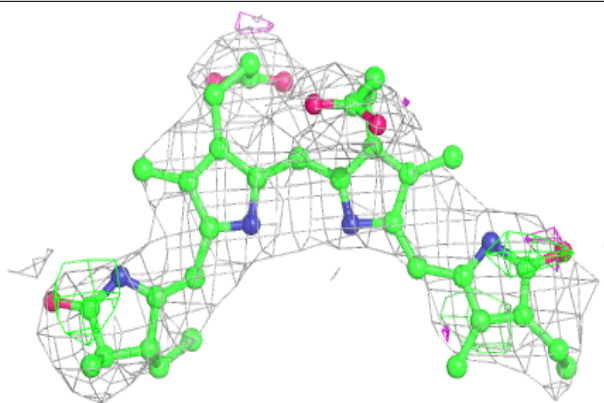
Electron density around BLA V 1082:

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



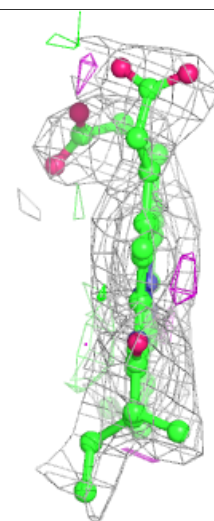
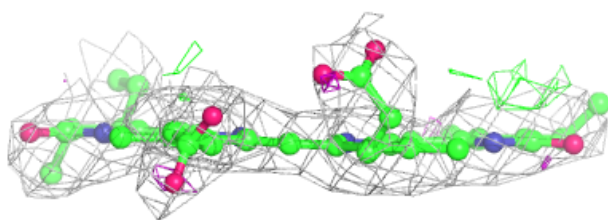
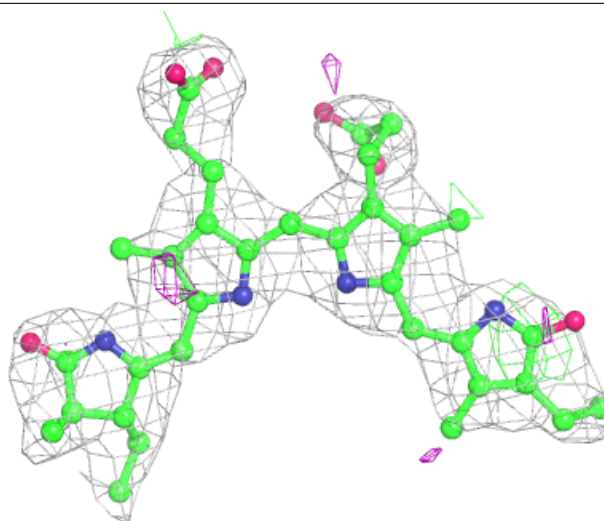
Electron density around BLA J 1153:

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



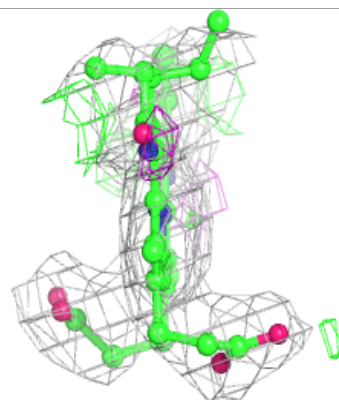
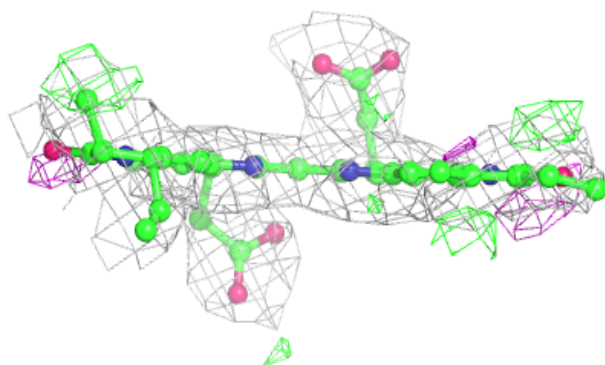
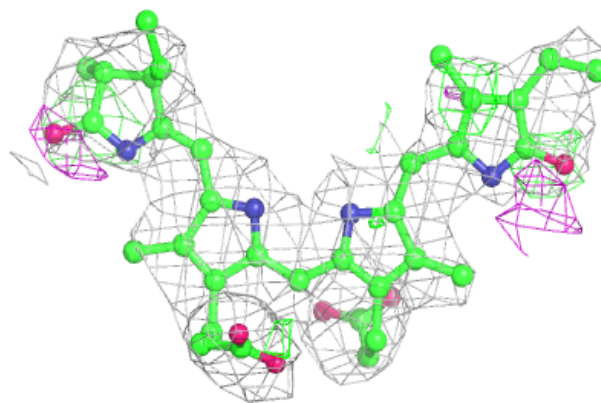
Electron density around BLA B 1082:

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

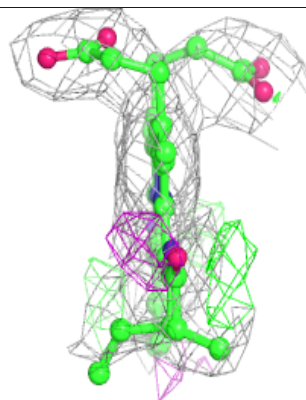
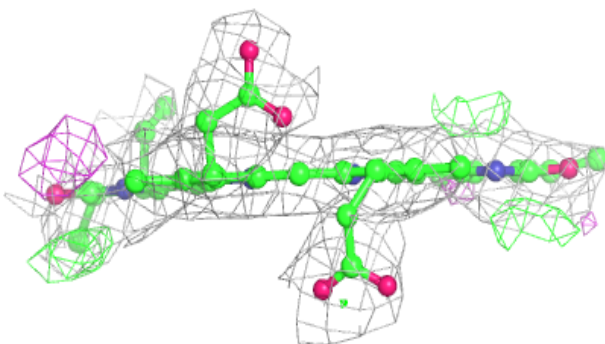
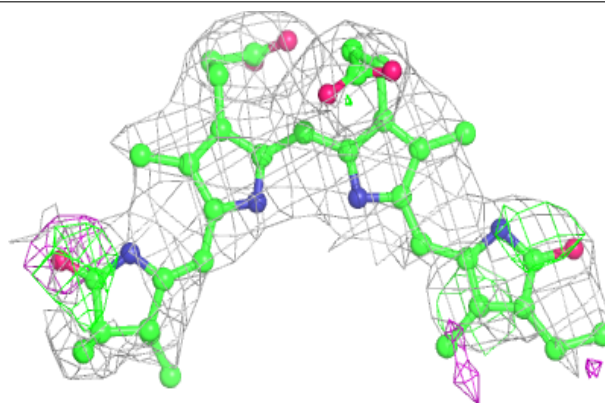


Electron density around BLA H 1153:

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

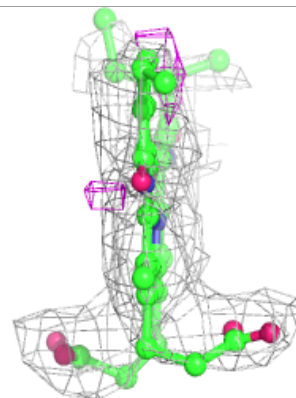
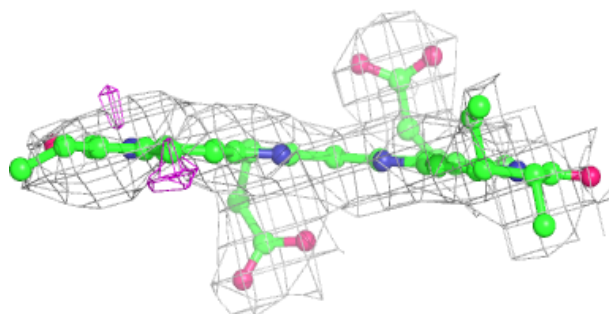
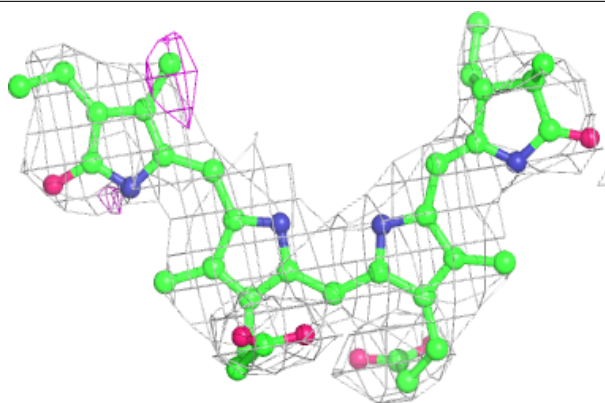
**Electron density around BLA L 1153:**

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

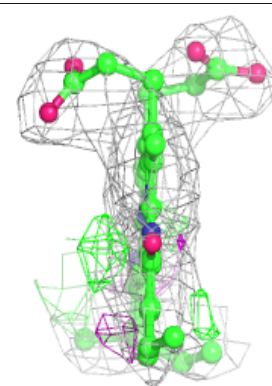
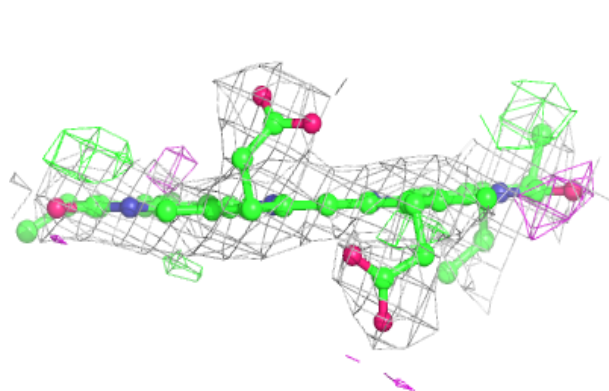
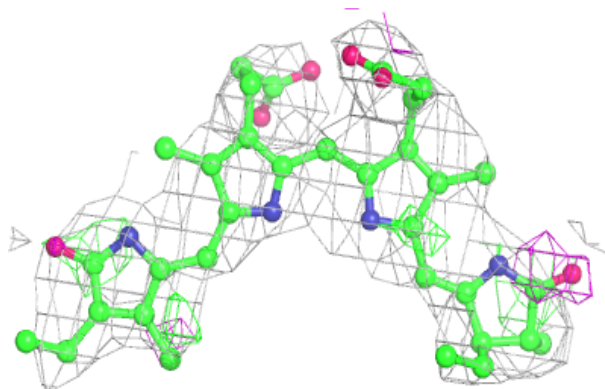


Electron density around BLA X 1153:

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

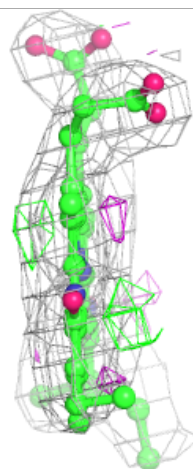
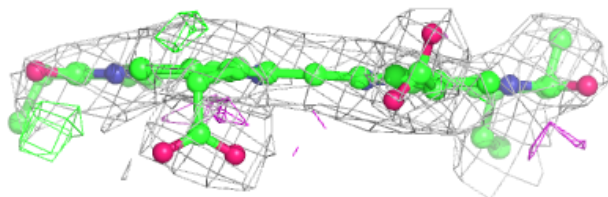
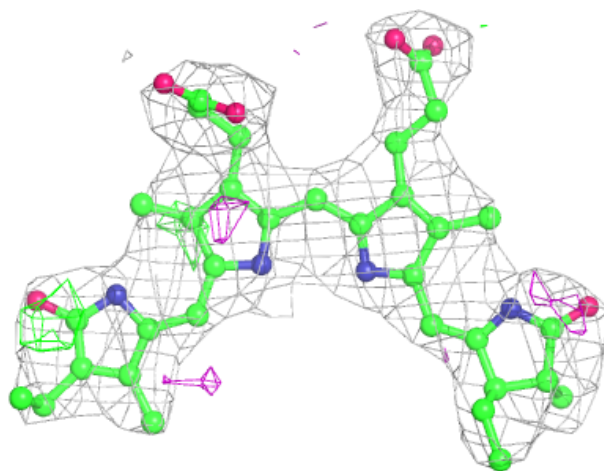
**Electron density around BLA P 1153:**

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



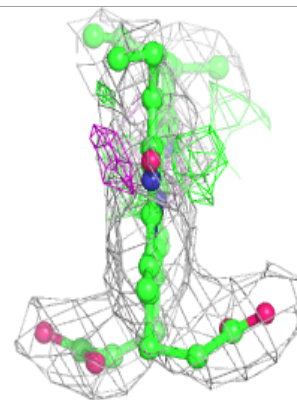
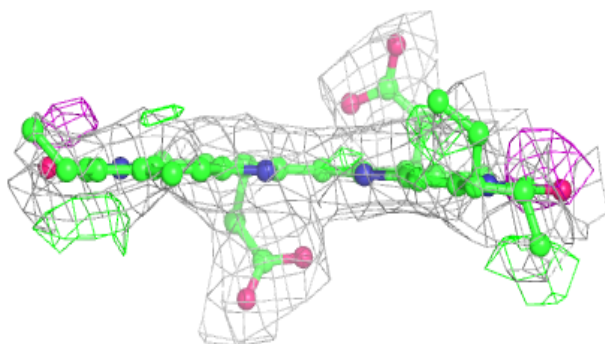
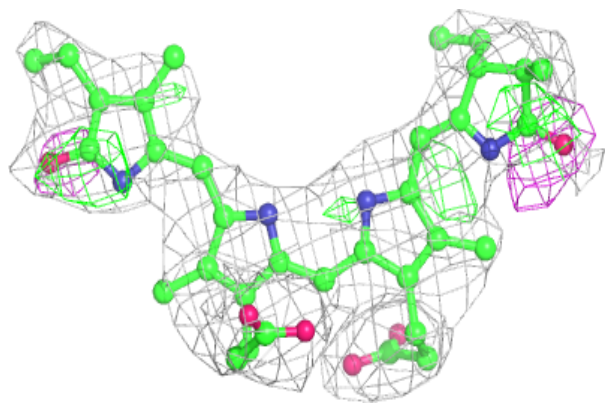
Electron density around BLA T 1082:

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

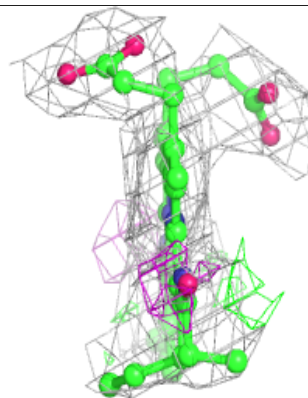
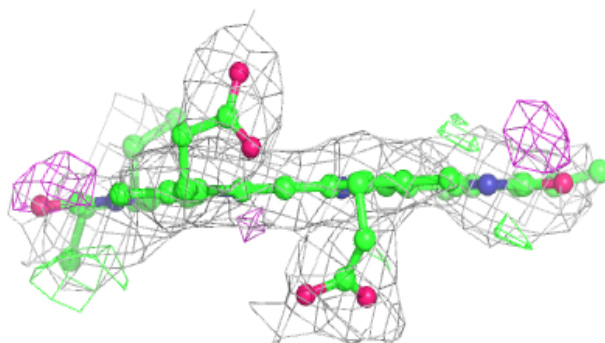
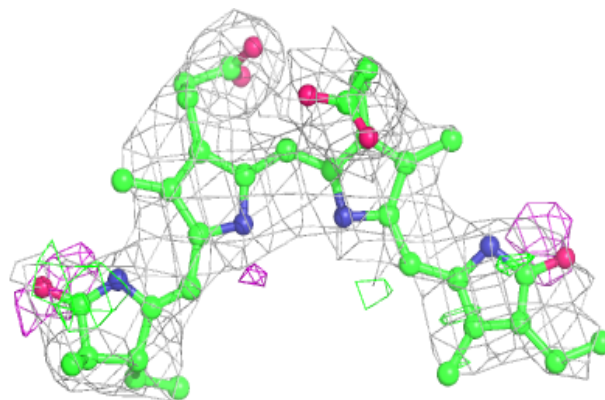


Electron density around BLA B 1153:

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

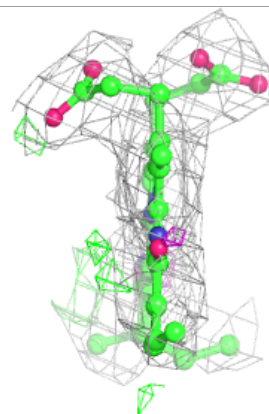
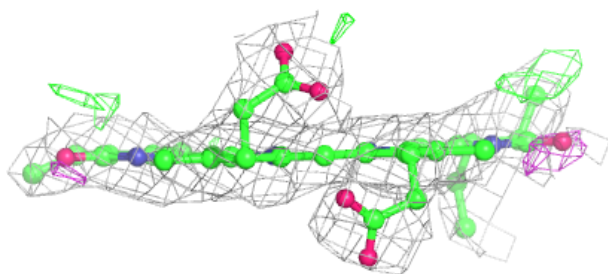
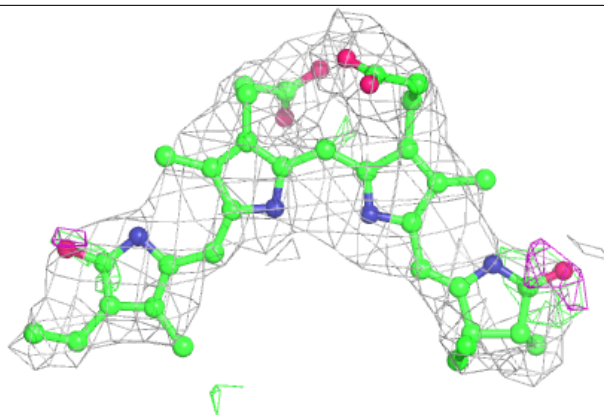
**Electron density around BLA N 1153:**

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



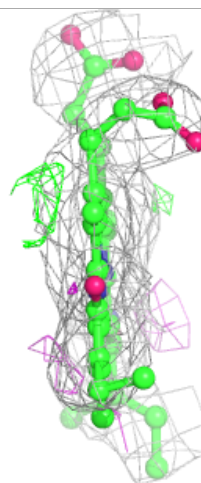
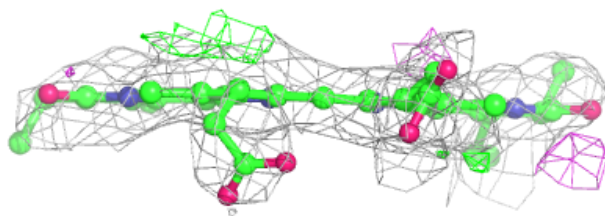
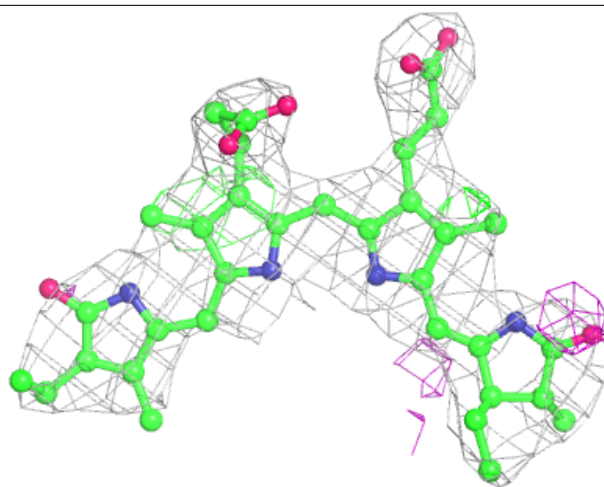
Electron density around BLA V 1153:

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



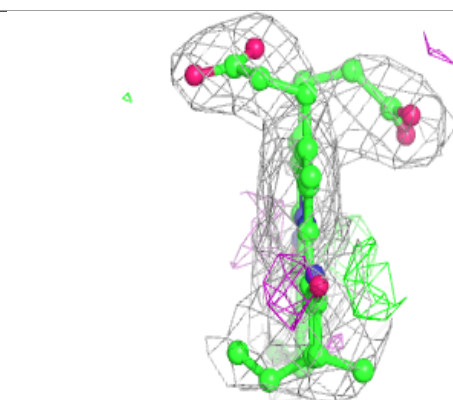
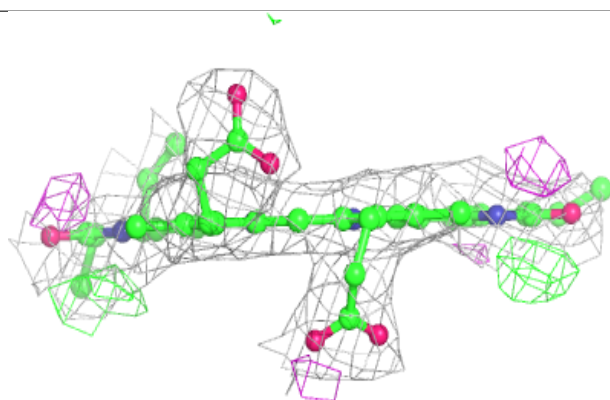
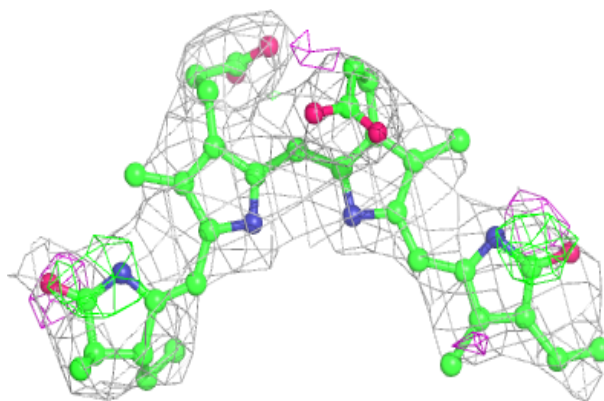
Electron density around BLA F 1082:

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

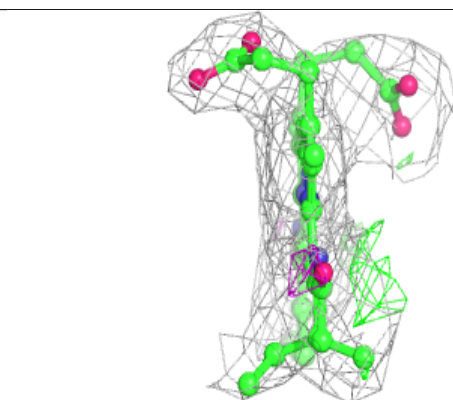
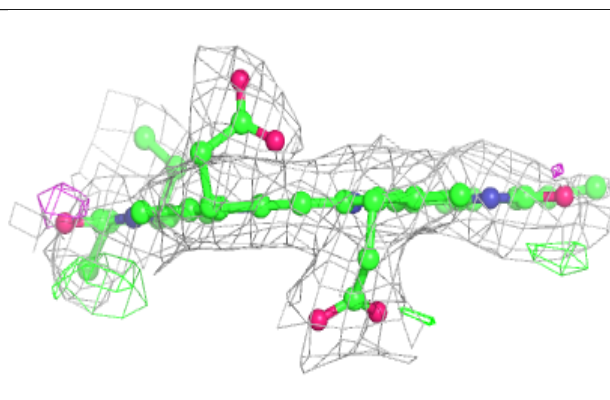
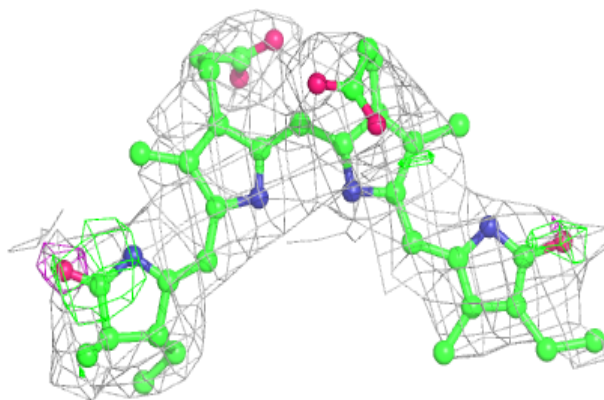


Electron density around BLA T 1153:

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

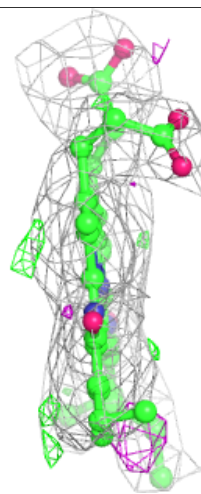
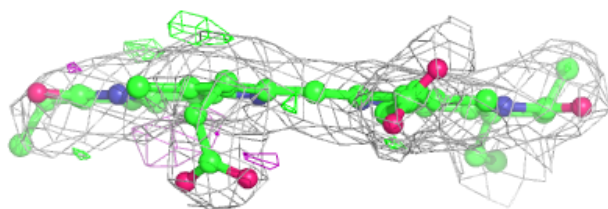
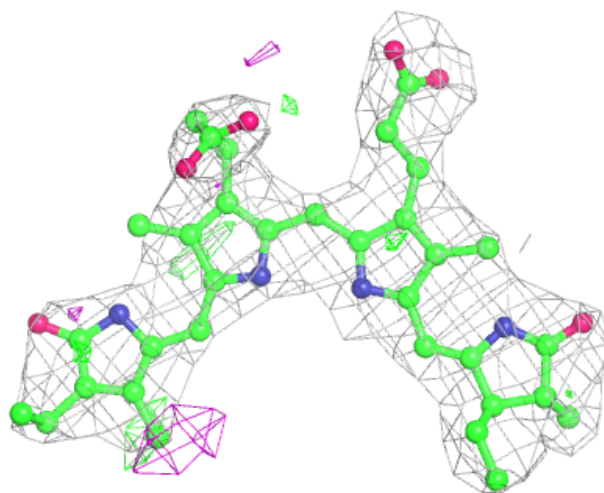
**Electron density around BLA R 1153:**

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



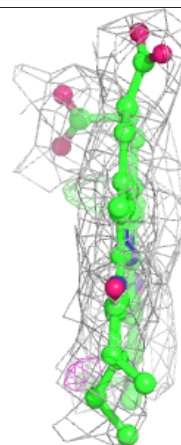
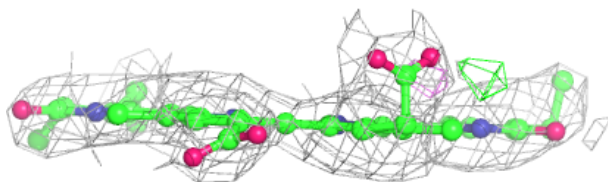
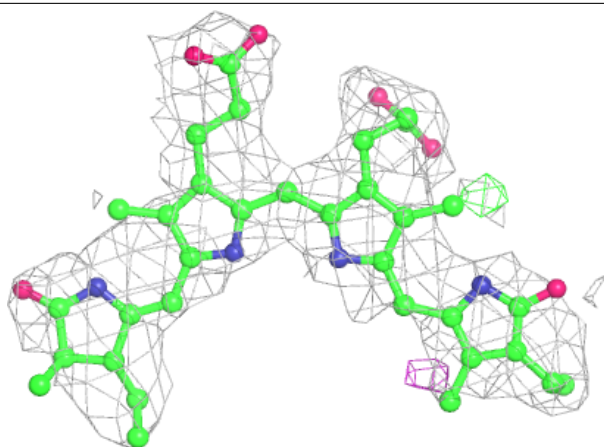
Electron density around BLA H 1082:

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

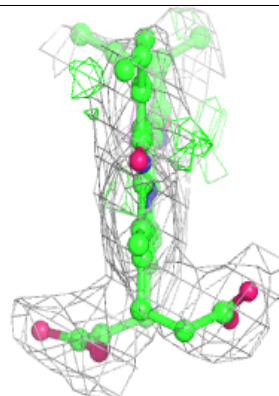
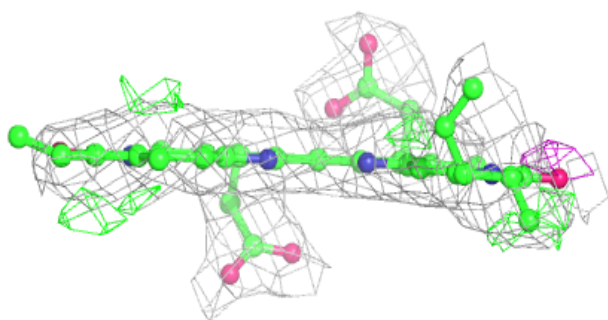
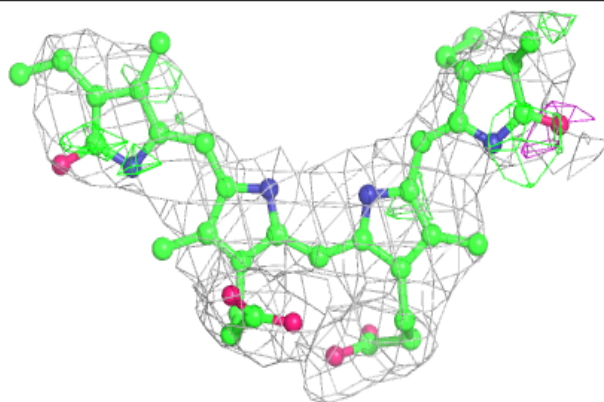


Electron density around CYC M 1084:

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

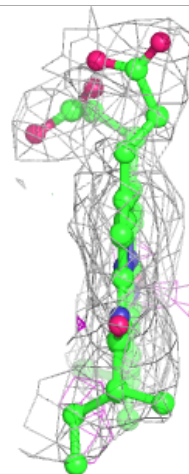
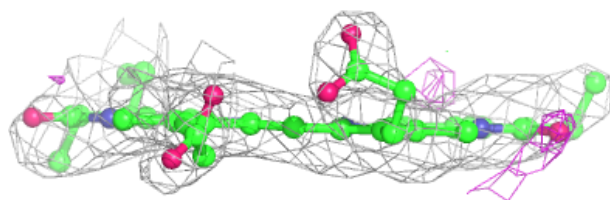
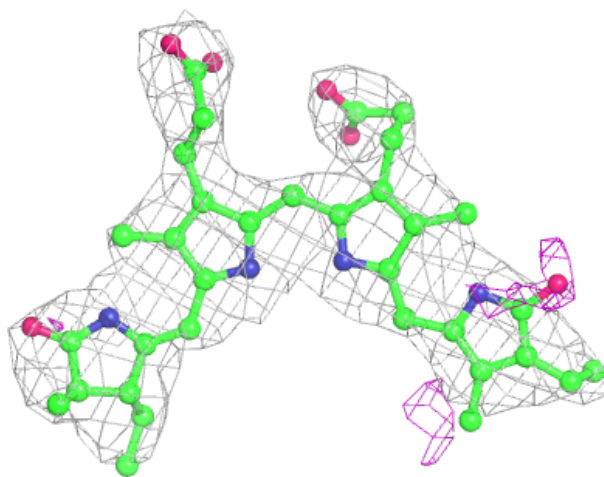
**Electron density around BLA D 1153:**

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



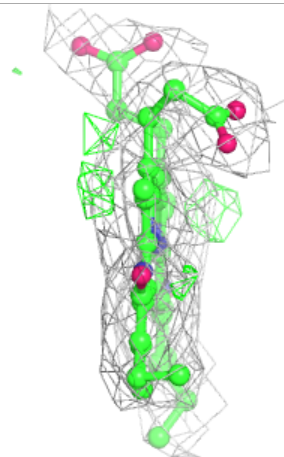
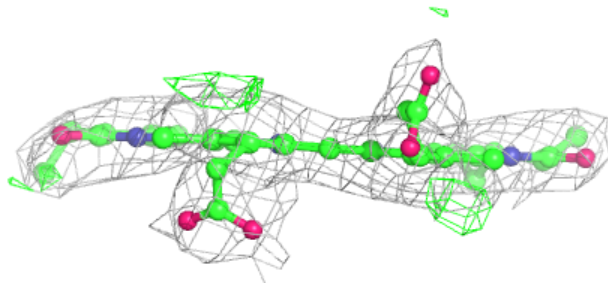
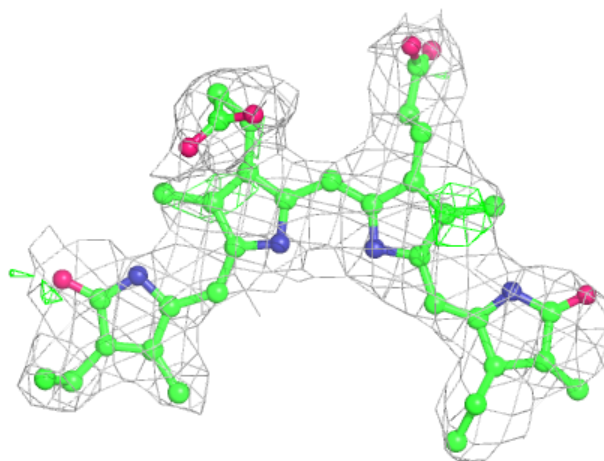
Electron density around BLA N 1082:

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



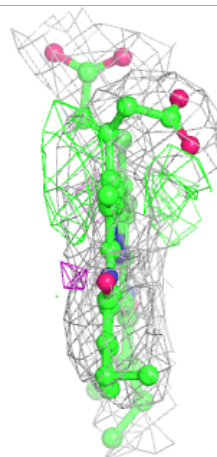
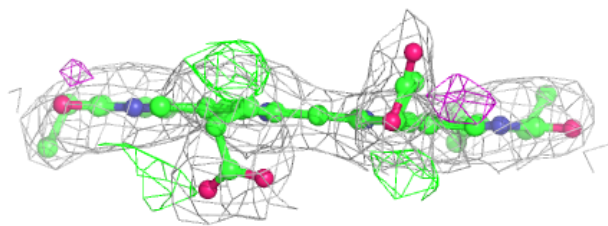
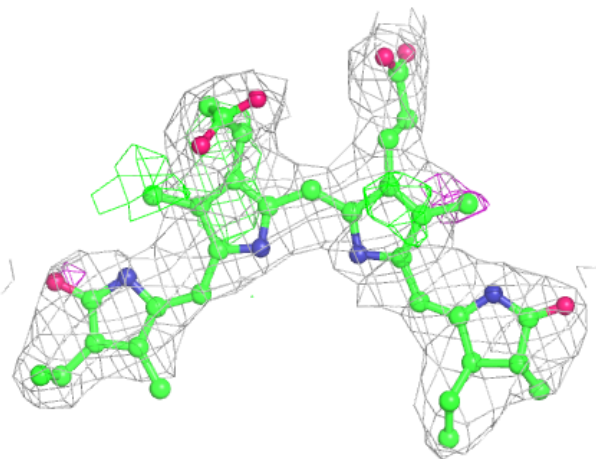
Electron density around CYC G 1084:

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



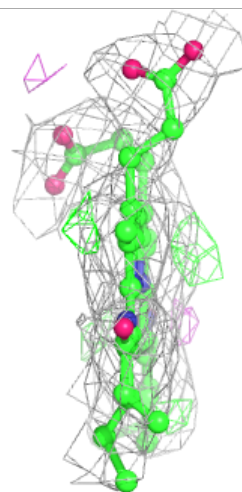
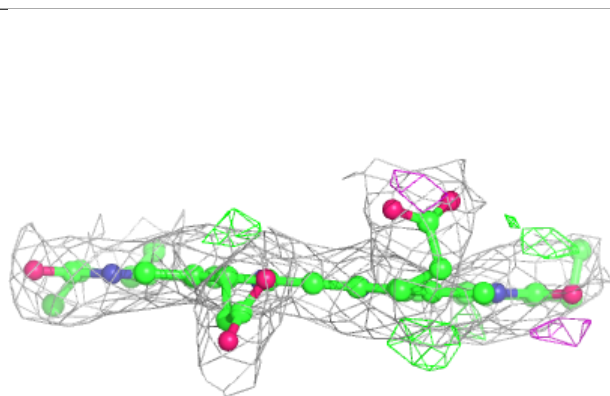
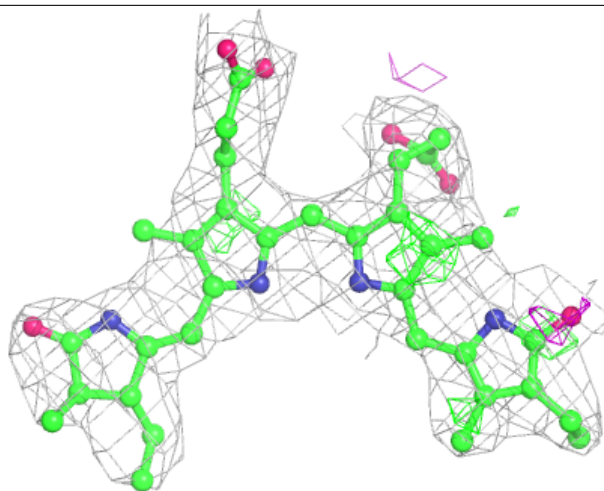
Electron density around CYC S 1084:

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



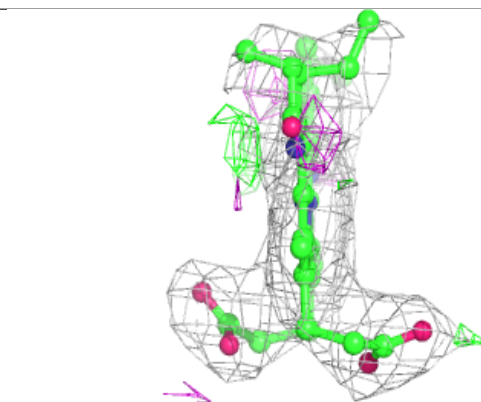
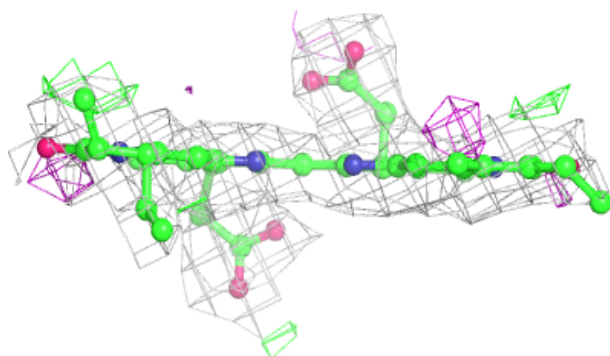
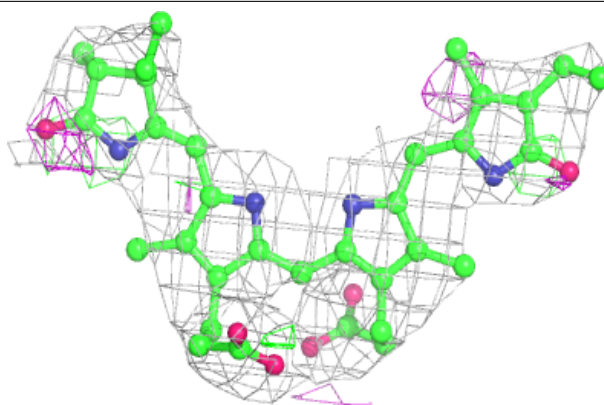
Electron density around CYC W 1084:

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

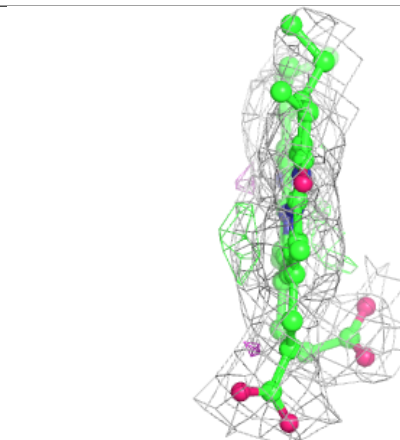
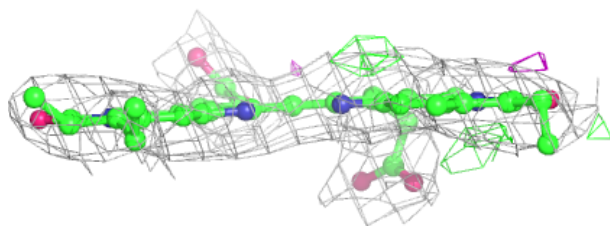
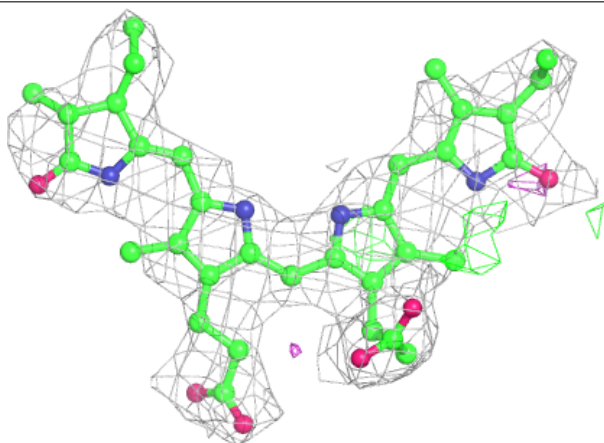


Electron density around BLA F 1153:

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

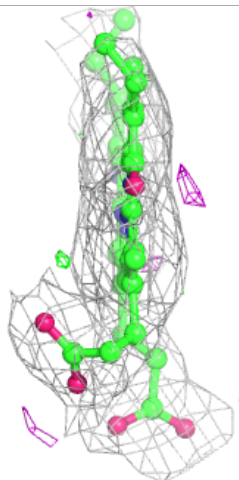
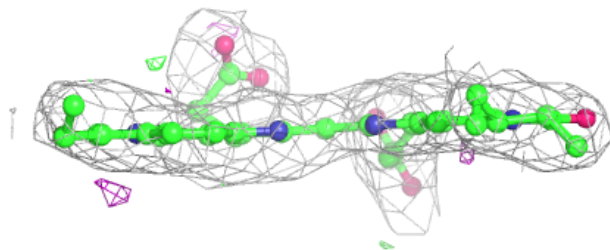
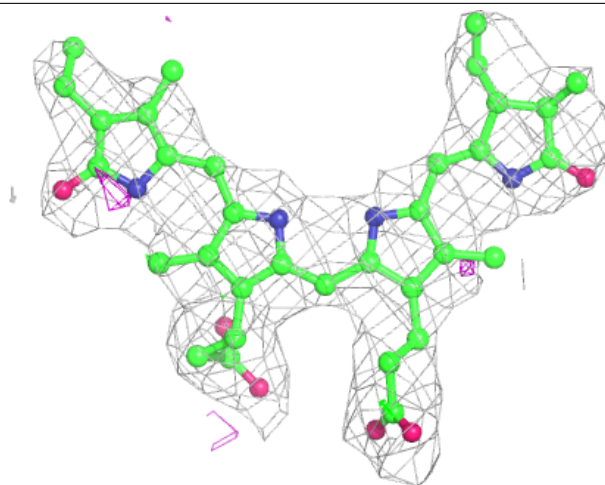
**Electron density around CYC U 1084:**

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



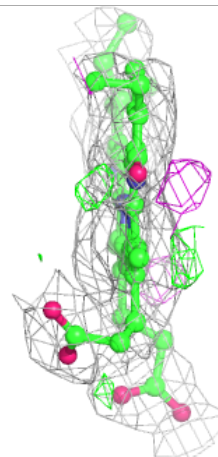
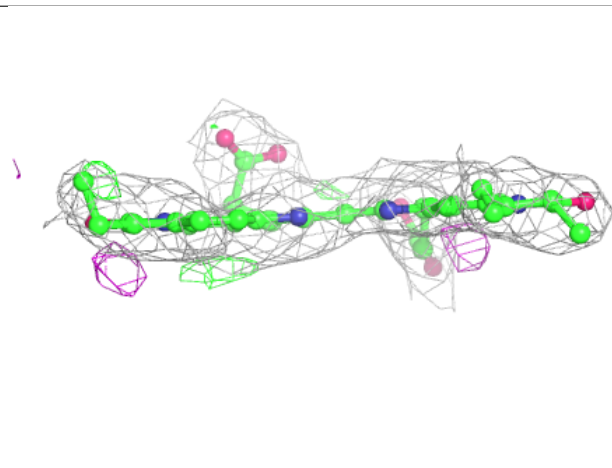
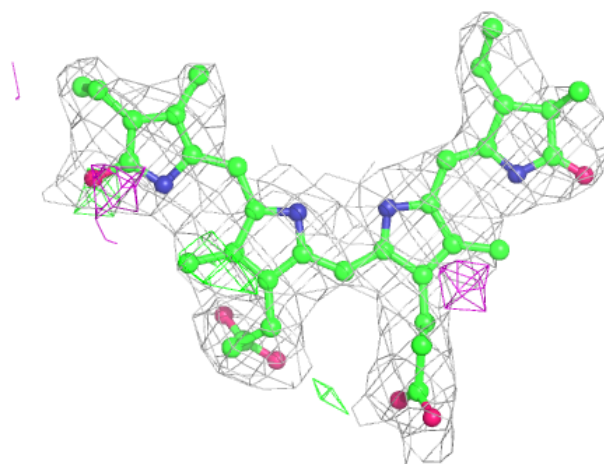
Electron density around CYC O 1084:

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



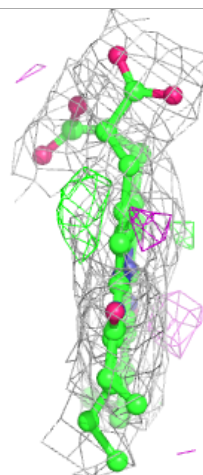
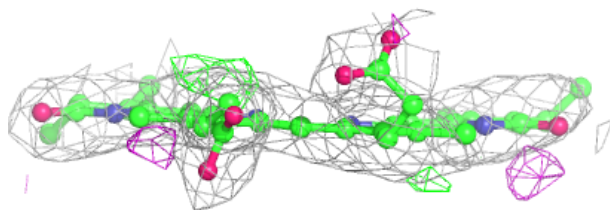
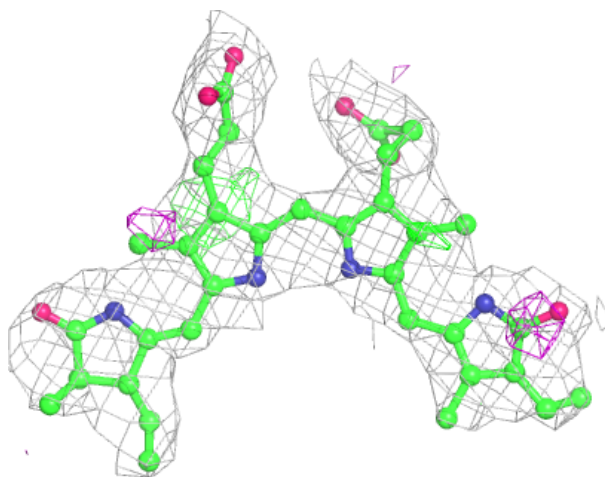
Electron density around BLA I 1084:

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



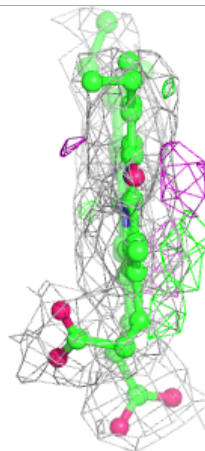
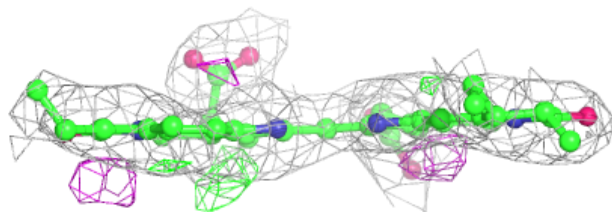
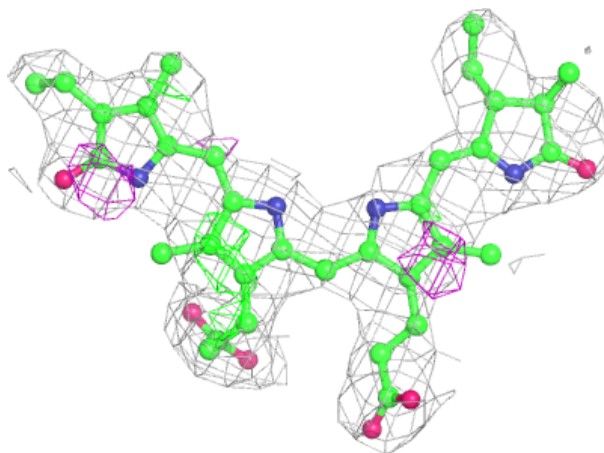
Electron density around CYC A 1084:

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



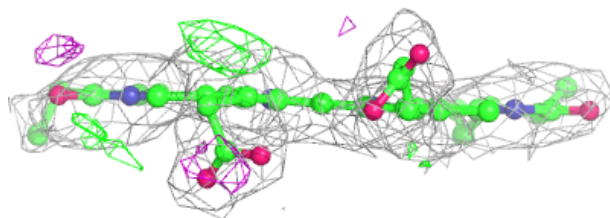
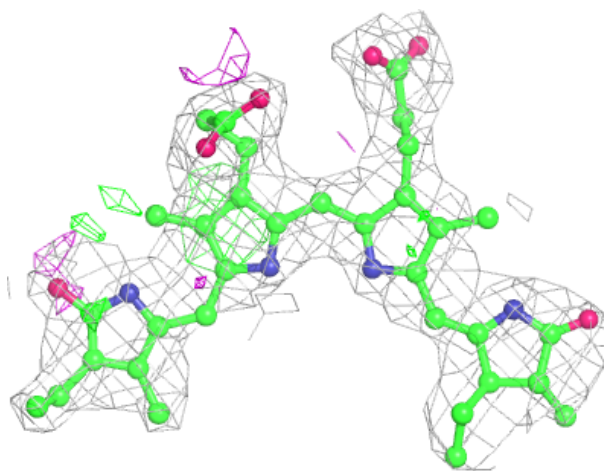
Electron density around CYC Q 1084:

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



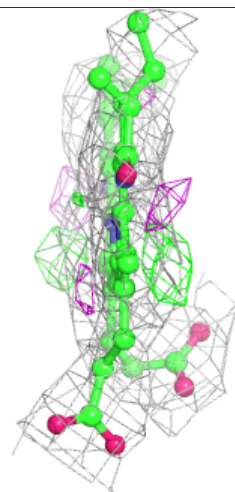
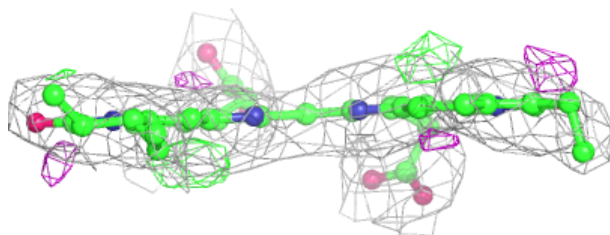
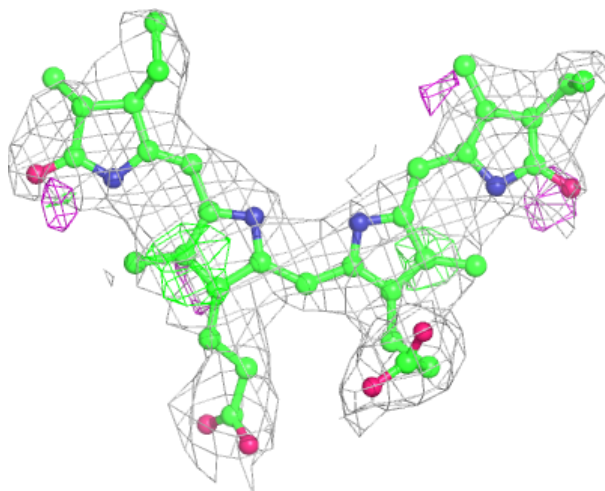
Electron density around CYC E 1084:

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



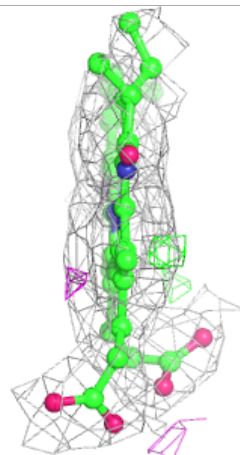
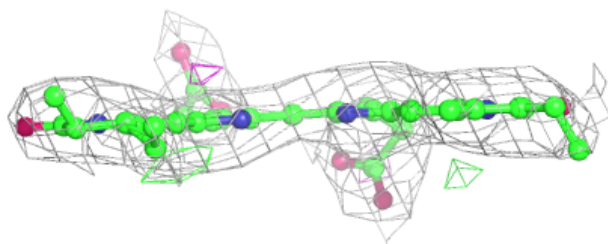
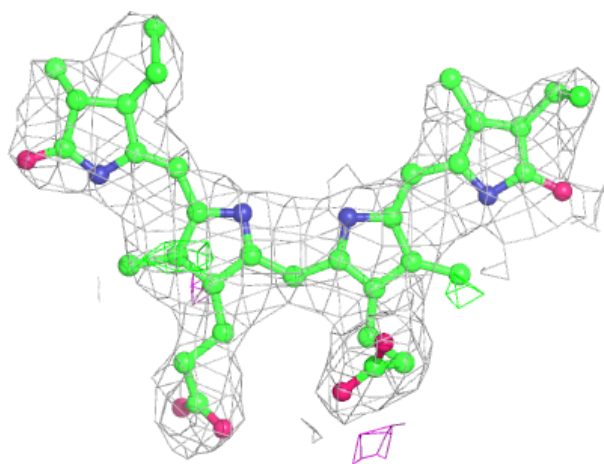
Electron density around CYC K 1084:

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



Electron density around CYC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.