



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 22, 2020 – 10:22 am GMT

PDB ID : 6Y3D
Title : X-ray structure of thermophilic C-phycocyanin from Galdiera phlegrea
Authors : Ferraro, G.; Lucignano, R.; Marseglia, A.; Merlino, A.
Deposited on : 2020-02-18
Resolution : 1.80 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	:	2.16
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)	:	2.16

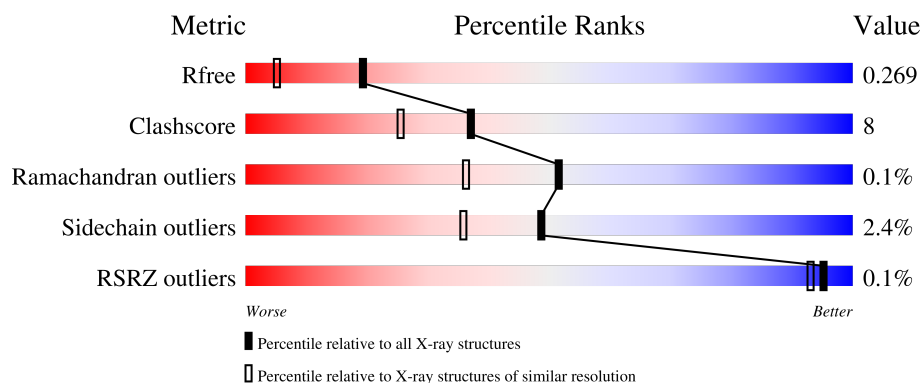
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AAA	162	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>90% 9% .</div>
1	CCC	162	<div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> </div> <div>91% 9%</div>
1	EEE	162	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>92% 7% .</div>
1	GGG	162	<div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> <div>91% 9% .</div>
1	III	162	<div> <div style="width: 90%;"></div> <div style="width: 10%;"></div> </div> <div>90% 10%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	KKK	162	<div><div>%</div><div><div></div></div><div>91%9%</div></div>
2	BBB	172	<div><div></div><div>94%6%</div></div>
2	DDD	172	<div><div></div><div>94%6%</div></div>
2	FFF	172	<div><div></div><div>88%12%</div></div>
2	HHH	172	<div><div></div><div>90%10%</div></div>
2	JJJ	172	<div><div></div><div>90%9%</div></div>
2	LLL	172	<div><div>%</div><div><div></div></div><div>87%13%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16970 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	AAA	162	Total	C	N	O	S	0	0	0
			1208	754	208	238	8			
1	CCC	162	Total	C	N	O	S	0	2	0
			1220	760	210	242	8			
1	EEE	162	Total	C	N	O	S	0	0	0
			1208	754	208	238	8			
1	GGG	162	Total	C	N	O	S	0	5	0
			1240	770	214	248	8			
1	III	162	Total	C	N	O	S	0	2	0
			1220	760	210	242	8			
1	KKK	162	Total	C	N	O	S	0	1	0
			1217	759	209	241	8			

- Molecule 2 is a protein called C-phycocyanin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	172	Total	C	N	O	S	0	1	0
			1277	790	224	255	8			
2	DDD	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
2	FFF	172	Total	C	N	O	S	0	1	0
			1279	792	224	254	9			
2	HHH	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
2	JJJ	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
2	LLL	172	Total	C	N	O	S	0	2	0
			1285	796	225	256	8			

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

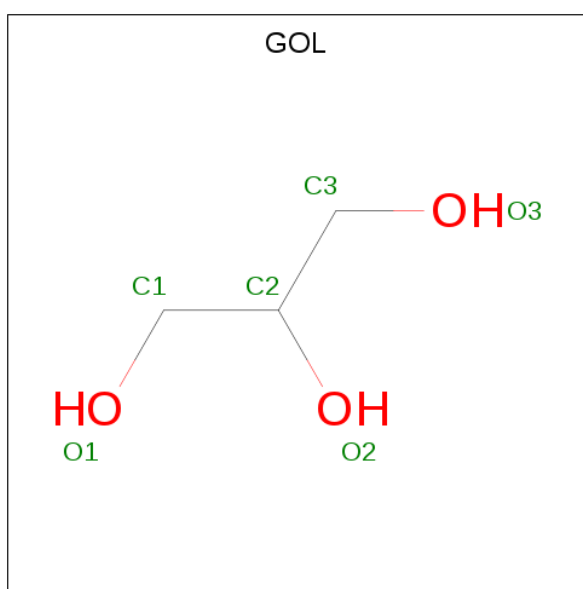


Continued on next page...

Continued from previous page...

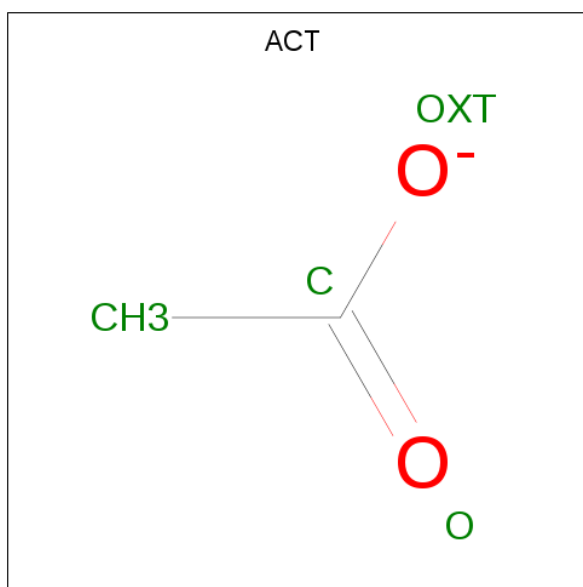
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	EEE	1	Total	C	O	0	0
			4	2	2		
5	LLL	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	106	Total	O	0	1
			106	106		
6	BBB	108	Total	O	0	0
			108	108		
6	CCC	111	Total	O	0	0
			111	111		
6	DDD	114	Total	O	0	0
			114	114		
6	EEE	102	Total	O	0	0
			102	102		
6	FFF	87	Total	O	0	0
			87	87		
6	GGG	121	Total	O	0	0
			121	121		
6	HHH	88	Total	O	0	0
			88	88		
6	III	109	Total	O	0	0
			109	109		
6	JJJ	84	Total	O	0	0
			84	84		

Continued on next page...

Continued from previous page...

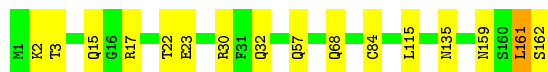
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	KKK	92	Total	O	0	0
			92	92		
6	LLL	93	Total	O	0	0
			93	93		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: C-phycoerythrin alpha chain

Chain AAA:  90% 9%



- Molecule 1: C-phycoerythrin alpha chain

Chain CCC:  91% 9%



- Molecule 1: C-phycoerythrin alpha chain

Chain EEE:  92% 7%



- Molecule 1: C-phycoerythrin alpha chain

Chain GGG:  91% 9%



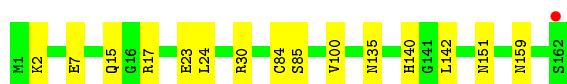
- Molecule 1: C-phycoerythrin alpha chain

Chain III:  90% 10%



- Molecule 1: C-phycoerythrin alpha chain

Chain KKK:  91% 9%



- Molecule 2: C-phycoerythrin beta chain

Chain BBB: 94% 6%



- Molecule 2: C-phycoerythrin beta chain

Chain DDD: 94% 6%



- Molecule 2: C-phycoerythrin beta chain

Chain FFF: 88% 12%



- Molecule 2: C-phycoerythrin beta chain

Chain HHH: 90% 10%



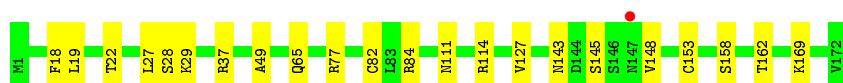
- Molecule 2: C-phycoerythrin beta chain

Chain JJJ: 90% 9%



- Molecule 2: C-phycoerythrin beta chain

Chain LLL: 87% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	60.03Å 189.13Å 208.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.74 – 1.80 94.56 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (94.74-1.80) 98.7 (94.56-1.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.221 , 0.268 0.228 , 0.269	Depositor DCC
R_{free} test set	11109 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16970	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	AAA	0.77	0/1229	0.89	0/1665
1	CCC	0.76	0/1241	0.89	1/1681 (0.1%)
1	EEE	0.78	0/1229	0.87	0/1665
1	GGG	0.79	0/1261	0.88	0/1708
1	III	0.76	0/1241	0.85	0/1681
1	KKK	0.77	0/1238	0.86	0/1677
2	BBB	0.78	0/1279	0.90	1/1730 (0.1%)
2	DDD	0.76	0/1273	0.86	0/1722
2	FFF	0.75	0/1281	0.83	0/1732
2	HHH	0.75	0/1273	0.85	0/1722
2	JJJ	0.76	0/1273	0.85	0/1722
2	LLL	0.73	0/1287	0.82	0/1742
All	All	0.76	0/15105	0.86	2/20447 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	30	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	BBB	37	ARG	NE-CZ-NH1	5.91	123.25	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1208	0	1187	19	0
1	CCC	1220	0	1194	10	0
1	EEE	1208	0	1187	23	0
1	GGG	1240	0	1207	13	0
1	III	1220	0	1195	19	0
1	KKK	1217	0	1192	17	0
2	BBB	1277	0	1281	16	0
2	DDD	1271	0	1277	17	0
2	FFF	1279	0	1285	26	0
2	HHH	1271	0	1277	27	0
2	JJJ	1271	0	1277	24	0
2	LLL	1285	0	1291	25	0
3	AAA	43	0	38	7	0
3	BBB	86	0	76	14	0
3	CCC	43	0	37	2	0
3	DDD	86	0	76	19	0
3	EEE	43	0	38	11	0
3	FFF	86	0	76	23	0
3	GGG	43	0	37	3	0
3	HHH	86	0	76	18	0
3	III	43	0	38	7	0
3	JJJ	86	0	76	20	0
3	KKK	43	0	38	7	0
3	LLL	86	0	76	16	0
4	DDD	6	0	8	0	0
5	EEE	4	0	3	0	0
5	LLL	4	0	3	1	0
6	AAA	106	0	0	2	0
6	BBB	108	0	0	1	0
6	CCC	111	0	0	0	0
6	DDD	114	0	0	2	0
6	EEE	102	0	0	2	0
6	FFF	87	0	0	1	0
6	GGG	121	0	0	2	0
6	HHH	88	0	0	4	0
6	III	109	0	0	2	0
6	JJJ	84	0	0	2	0
6	KKK	92	0	0	1	0
6	LLL	93	0	0	2	0
All	All	16970	0	15546	243	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 243 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:EEE:84:CYS:SG	3:EEE:502:CYC:HAC2	1.22	1.75
2:BBB:82:CYS:SG	3:BBB:201:CYC:HAC2	1.23	1.74
1:KKK:84:CYS:SG	3:KKK:201:CYC:HAC2	1.23	1.73
2:DDD:82:CYS:SG	3:DDD:201:CYC:HAC2	1.17	1.72
2:LLL:153:CYS:SG	3:LLL:202:CYC:HAC1	1.30	1.72

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	AAA	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	CCC	162/162 (100%)	159 (98%)	3 (2%)	0	100	100
1	EEE	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	25	12
1	GGG	165/162 (102%)	162 (98%)	3 (2%)	0	100	100
1	III	162/162 (100%)	160 (99%)	2 (1%)	0	100	100
1	KKK	161/162 (99%)	157 (98%)	4 (2%)	0	100	100
2	BBB	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	DDD	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	FFF	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	HHH	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	JJJ	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	LLL	171/172 (99%)	168 (98%)	3 (2%)	0	100	100
All	All	1988/2004 (99%)	1947 (98%)	40 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EEE	105	GLY

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	AAA	123/123 (100%)	117 (95%)	6 (5%)	25	11
1	CCC	125/123 (102%)	124 (99%)	1 (1%)	81	78
1	EEE	123/123 (100%)	121 (98%)	2 (2%)	62	54
1	GGG	128/123 (104%)	125 (98%)	3 (2%)	50	37
1	III	125/123 (102%)	122 (98%)	3 (2%)	49	36
1	KKK	124/123 (101%)	121 (98%)	3 (2%)	49	36
2	BBB	131/130 (101%)	127 (97%)	4 (3%)	40	25
2	DDD	130/130 (100%)	129 (99%)	1 (1%)	81	78
2	FFF	131/130 (101%)	129 (98%)	2 (2%)	65	56
2	HHH	130/130 (100%)	128 (98%)	2 (2%)	65	56
2	JJJ	130/130 (100%)	125 (96%)	5 (4%)	33	18
2	LLL	132/130 (102%)	128 (97%)	4 (3%)	41	27
All	All	1532/1518 (101%)	1496 (98%)	36 (2%)	49	37

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GGG	22	THR
2	HHH	143	ASN
2	LLL	37	ARG
1	GGG	68	GLN
1	III	22	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	JJJ	72	2	7,8,9	0.62	0	6,9,11	0.42	0
2	MEN	DDD	72	2	7,8,9	0.66	0	6,9,11	0.52	0
2	MEN	FFF	72	2	7,8,9	0.57	0	6,9,11	1.05	0
2	MEN	BBB	72	2	7,8,9	0.66	0	6,9,11	0.47	0
2	MEN	LLL	72	2	7,8,9	0.97	0	6,9,11	0.79	0
2	MEN	HHH	72	2	7,8,9	0.71	0	6,9,11	1.29	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	JJJ	72	2	-	2/7/8/10	-
2	MEN	DDD	72	2	-	2/7/8/10	-
2	MEN	FFF	72	2	-	2/7/8/10	-
2	MEN	BBB	72	2	-	3/7/8/10	-
2	MEN	LLL	72	2	-	2/7/8/10	-
2	MEN	HHH	72	2	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	72	MEN	O-C-CA-CB
2	FFF	72	MEN	CA-CB-CG-OD1
2	BBB	72	MEN	CA-CB-CG-OD1
2	JJJ	72	MEN	CA-CB-CG-OD1
2	LLL	72	MEN	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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	BBB	202	-	36,46,46	1.37	1 (2%)	44,67,67	1.30	6 (13%)
3	CYC	JJJ	201	-	36,46,46	1.16	1 (2%)	44,67,67	1.26	6 (13%)
3	CYC	AAA	201	-	36,46,46	1.18	1 (2%)	44,67,67	1.00	2 (4%)
5	ACT	EEE	501	-	1,3,3	5.84	1 (100%)	0,3,3	0.00	-
3	CYC	DDD	201	-	36,46,46	1.35	1 (2%)	44,67,67	1.17	3 (6%)
3	CYC	JJJ	202	-	36,46,46	1.06	1 (2%)	44,67,67	1.11	2 (4%)
3	CYC	LLL	202	-	36,46,46	1.45	1 (2%)	44,67,67	1.27	5 (11%)
3	CYC	HHH	201	-	36,46,46	1.17	1 (2%)	44,67,67	1.24	4 (9%)
4	GOL	DDD	203	-	5,5,5	0.23	0	5,5,5	0.46	0
3	CYC	EEE	502	-	36,46,46	1.22	1 (2%)	44,67,67	1.16	2 (4%)
3	CYC	FFF	201	-	36,46,46	1.54	1 (2%)	44,67,67	1.14	3 (6%)
3	CYC	KKK	201	-	36,46,46	1.45	1 (2%)	44,67,67	1.06	4 (9%)
3	CYC	DDD	202	-	36,46,46	2.09	1 (2%)	44,67,67	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	FFF	202	-	36,46,46	1.07	1 (2%)	44,67,67	1.30	5 (11%)
3	CYC	GGG	201	-	36,46,46	1.07	3 (8%)	44,67,67	1.15	3 (6%)
3	CYC	HHH	202	-	36,46,46	1.37	1 (2%)	44,67,67	1.49	6 (13%)
3	CYC	CCC	201	1	36,46,46	1.38	1 (2%)	44,67,67	1.13	4 (9%)
3	CYC	BBB	201	-	36,46,46	1.00	1 (2%)	44,67,67	1.42	9 (20%)
3	CYC	III	201	-	36,46,46	1.45	2 (5%)	44,67,67	1.11	4 (9%)
5	ACT	LLL	203	-	1,3,3	4.62	1 (100%)	0,3,3	0.00	-
3	CYC	LLL	201	-	36,46,46	0.99	1 (2%)	44,67,67	1.14	4 (9%)

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	BBB	202	-	-	11/21/74/74	0/4/4/4
3	CYC	JJJ	201	-	-	6/21/74/74	0/4/4/4
3	CYC	AAA	201	-	-	5/21/74/74	0/4/4/4
3	CYC	DDD	201	-	-	5/21/74/74	0/4/4/4
3	CYC	JJJ	202	-	-	7/21/74/74	0/4/4/4
3	CYC	LLL	202	-	-	7/21/74/74	0/4/4/4
3	CYC	HHH	201	-	-	5/21/74/74	0/4/4/4
4	GOL	DDD	203	-	-	1/4/4/4	-
3	CYC	EEE	502	-	-	5/21/74/74	0/4/4/4
3	CYC	FFF	201	-	-	7/21/74/74	0/4/4/4
3	CYC	KKK	201	-	-	5/21/74/74	0/4/4/4
3	CYC	DDD	202	-	-	6/21/74/74	0/4/4/4
3	CYC	FFF	202	-	-	9/21/74/74	0/4/4/4
3	CYC	GGG	201	-	-	4/21/74/74	0/4/4/4
3	CYC	HHH	202	-	-	10/21/74/74	0/4/4/4
3	CYC	CCC	201	1	-	7/21/74/74	0/4/4/4
3	CYC	BBB	201	-	-	6/21/74/74	0/4/4/4
3	CYC	III	201	-	-	5/21/74/74	0/4/4/4
3	CYC	LLL	201	-	-	5/21/74/74	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	202	CYC	CHA-C1A	11.93	1.45	1.35
3	FFF	201	CYC	CHA-C1A	8.31	1.42	1.35
3	KKK	201	CYC	CHA-C1A	8.04	1.41	1.35
3	LLL	202	CYC	CHA-C1A	7.92	1.41	1.35
3	III	201	CYC	CHA-C1A	7.54	1.41	1.35

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	201	CYC	CMB-C2B-C1B	5.28	130.76	124.17
3	EEE	502	CYC	CMB-C2B-C1B	4.55	129.85	124.17
3	JJJ	201	CYC	CMB-C2B-C1B	4.27	129.50	124.17
3	FFF	201	CYC	CMB-C2B-C1B	4.20	129.41	124.17
3	FFF	202	CYC	CMB-C2B-C1B	4.17	129.37	124.17

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	202	CYC	ND-C4D-CHA-C1A
3	BBB	202	CYC	C3D-C4D-CHA-C1A
3	BBB	202	CYC	NA-C4A-CHB-C1B
3	BBB	202	CYC	C3A-C4A-CHB-C1B
3	BBB	202	CYC	C2B-C3B-CAB-CBB

There are no ring outliers.

19 monomers are involved in 148 short contacts:

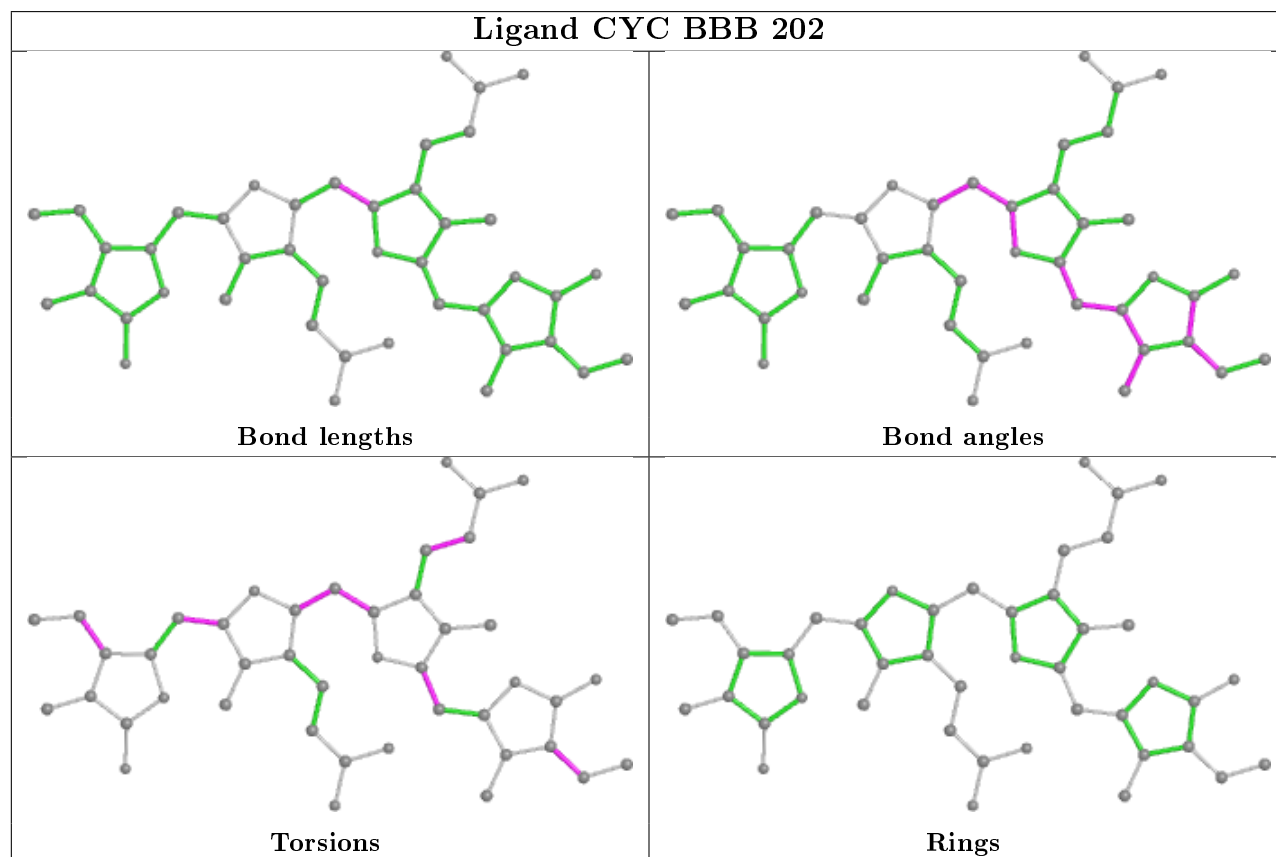
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	202	CYC	7	0
3	JJJ	201	CYC	11	0
3	AAA	201	CYC	7	0
3	DDD	201	CYC	10	0
3	JJJ	202	CYC	9	0
3	LLL	202	CYC	8	0
3	HHH	201	CYC	9	0
3	EEE	502	CYC	11	0
3	FFF	201	CYC	13	0
3	KKK	201	CYC	7	0
3	DDD	202	CYC	9	0
3	FFF	202	CYC	10	0
3	GGG	201	CYC	3	0

Continued on next page...

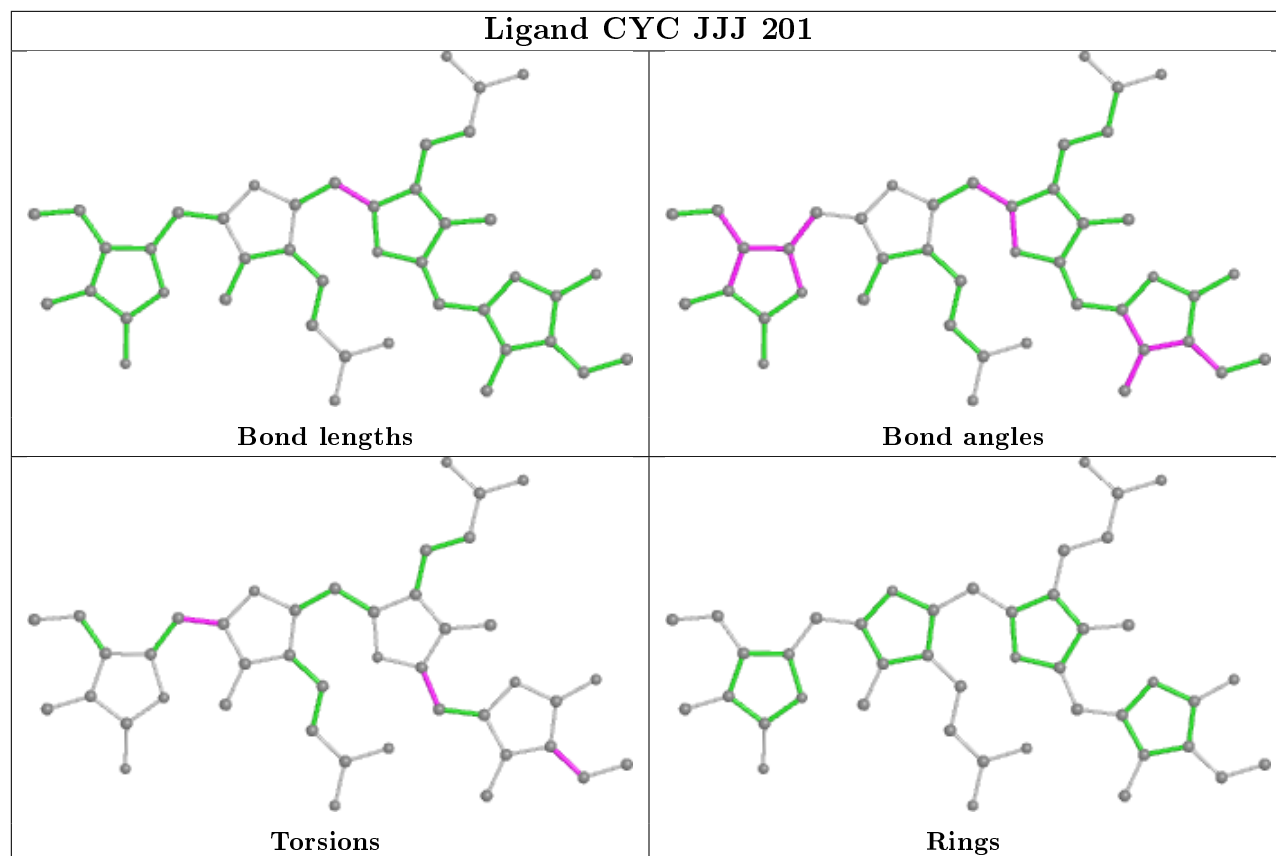
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	HHH	202	CYC	9	0
3	CCC	201	CYC	2	0
3	BBB	201	CYC	7	0
3	III	201	CYC	7	0
5	LLL	203	ACT	1	0
3	LLL	201	CYC	8	0

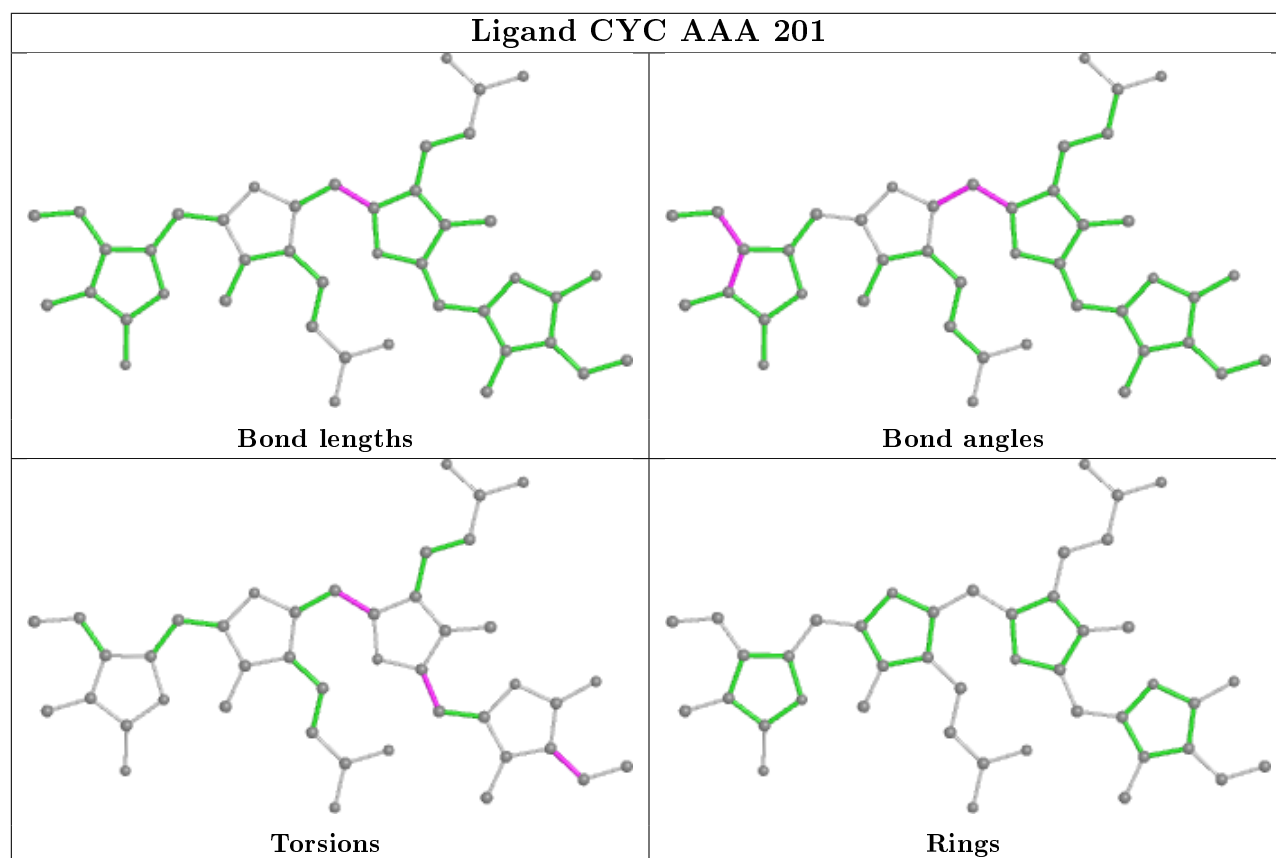
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



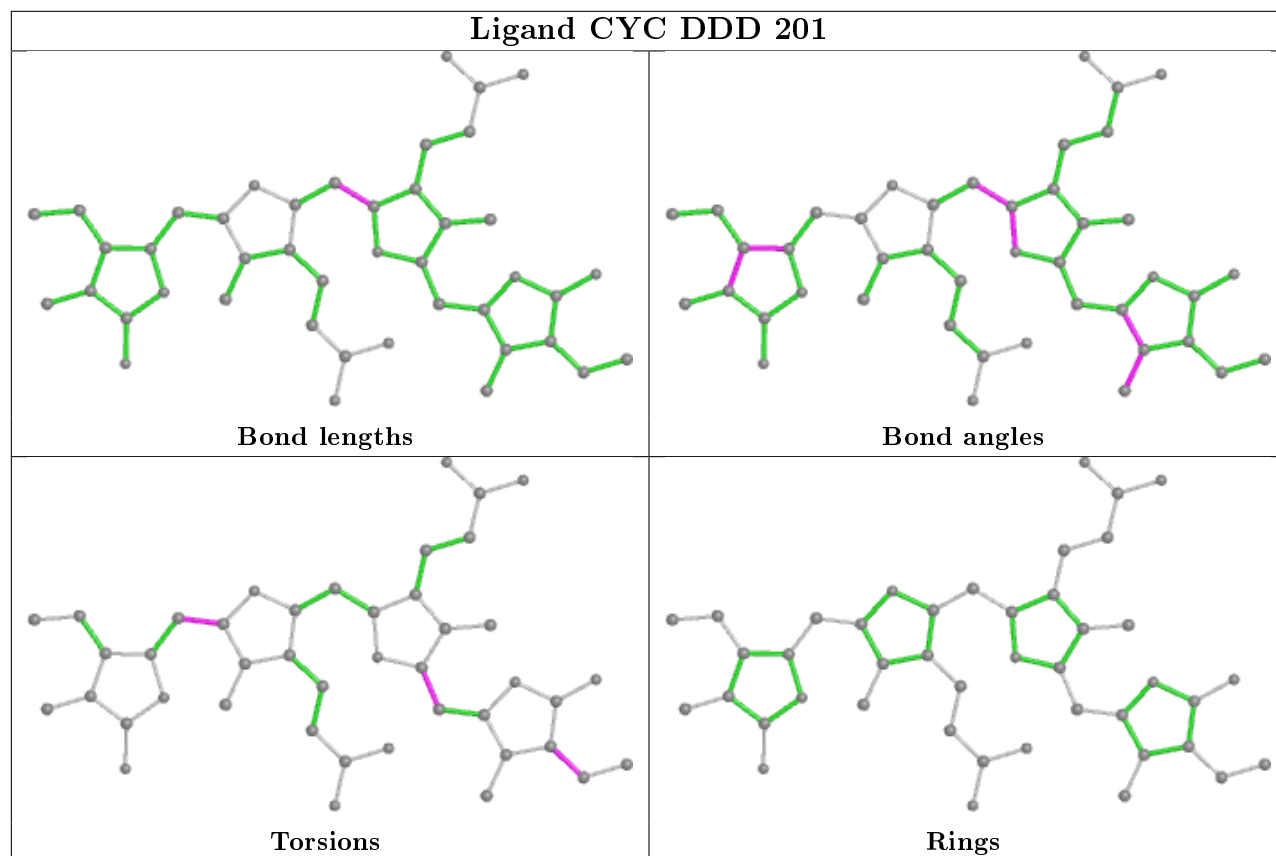
Ligand CYC JJJ 201



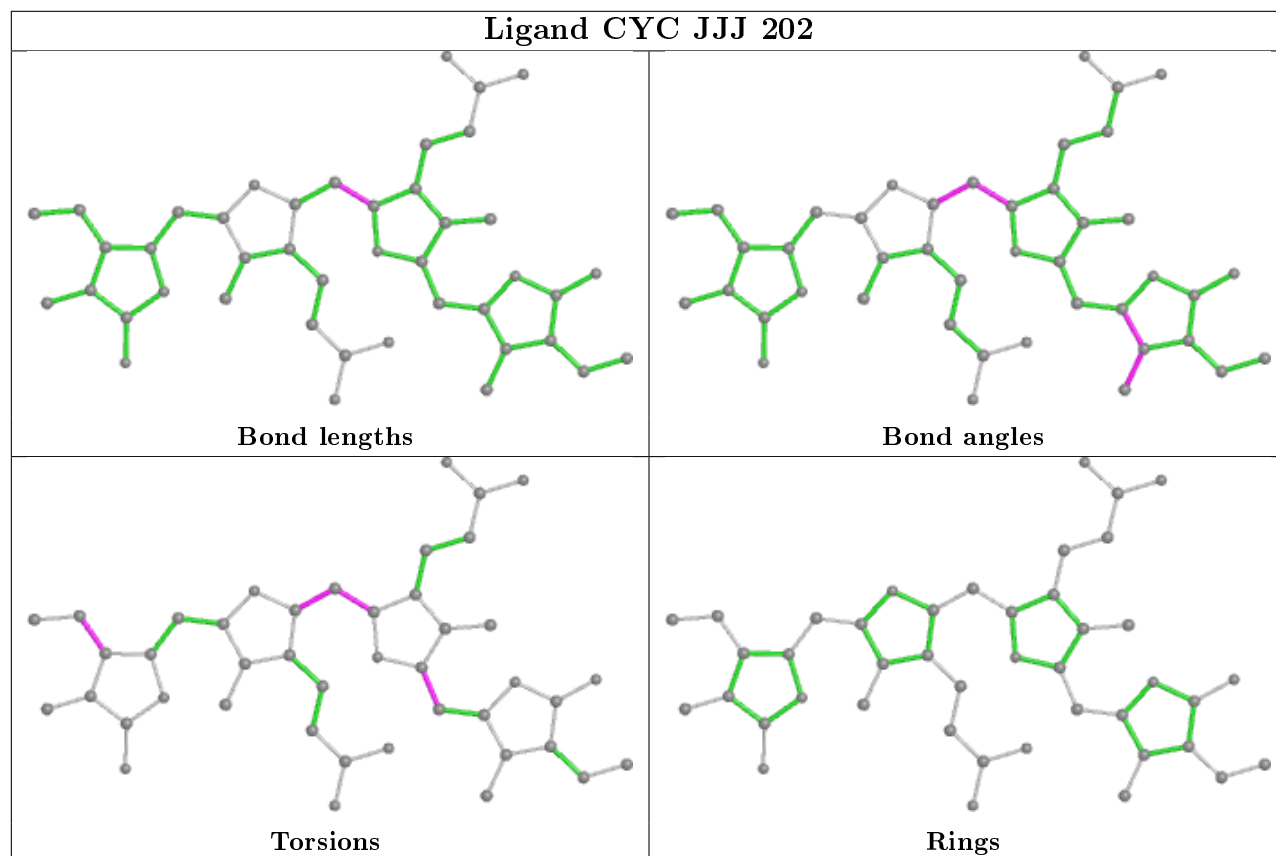
Ligand CYC AAA 201



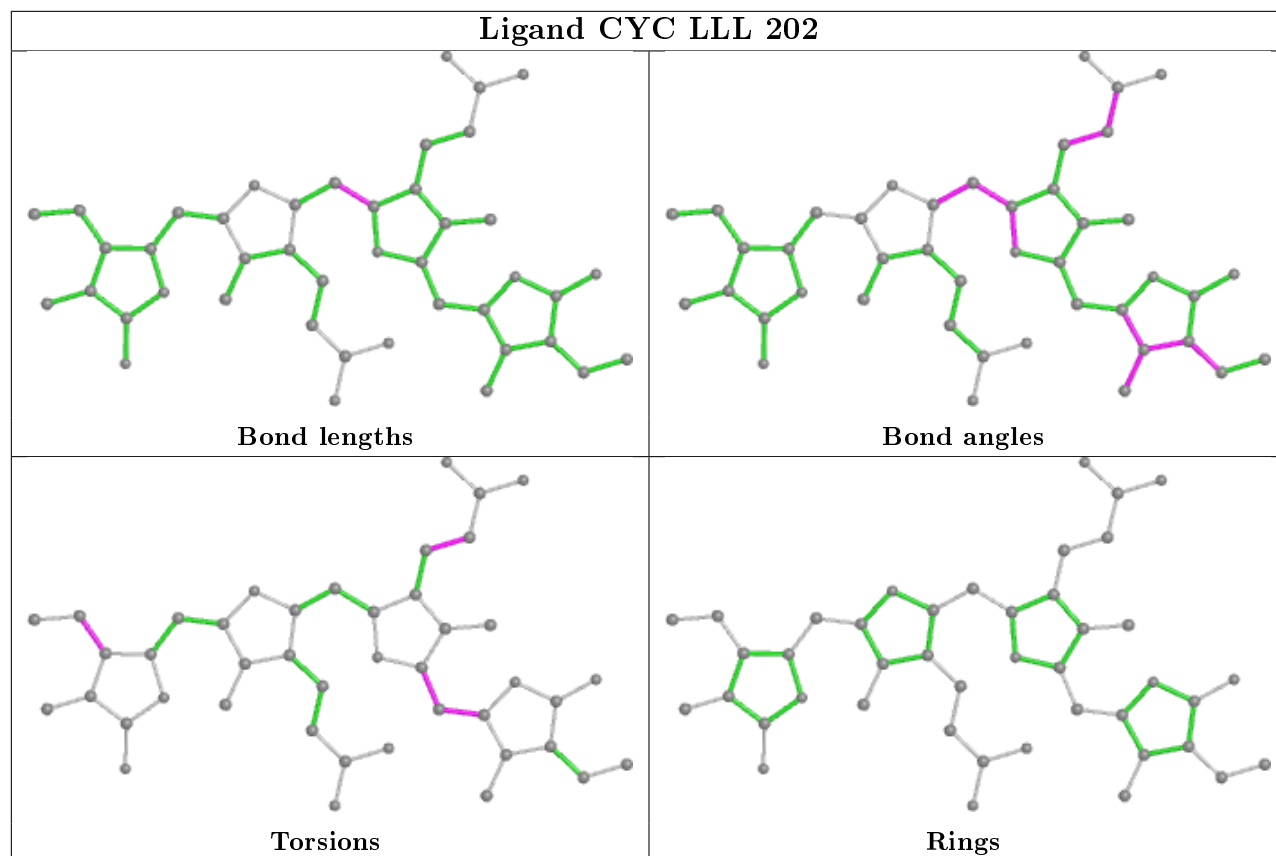
Ligand CYC DDD 201



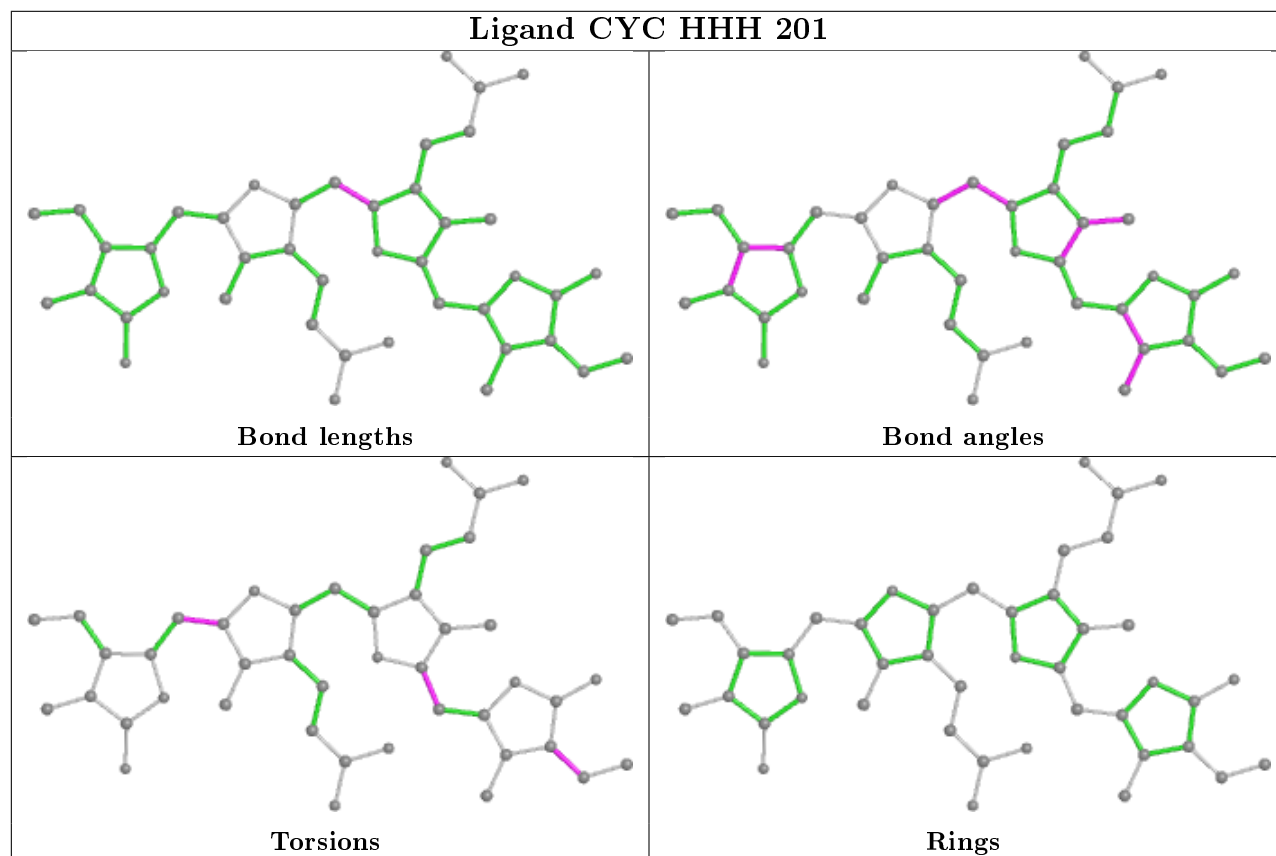
Ligand CYC JJJ 202

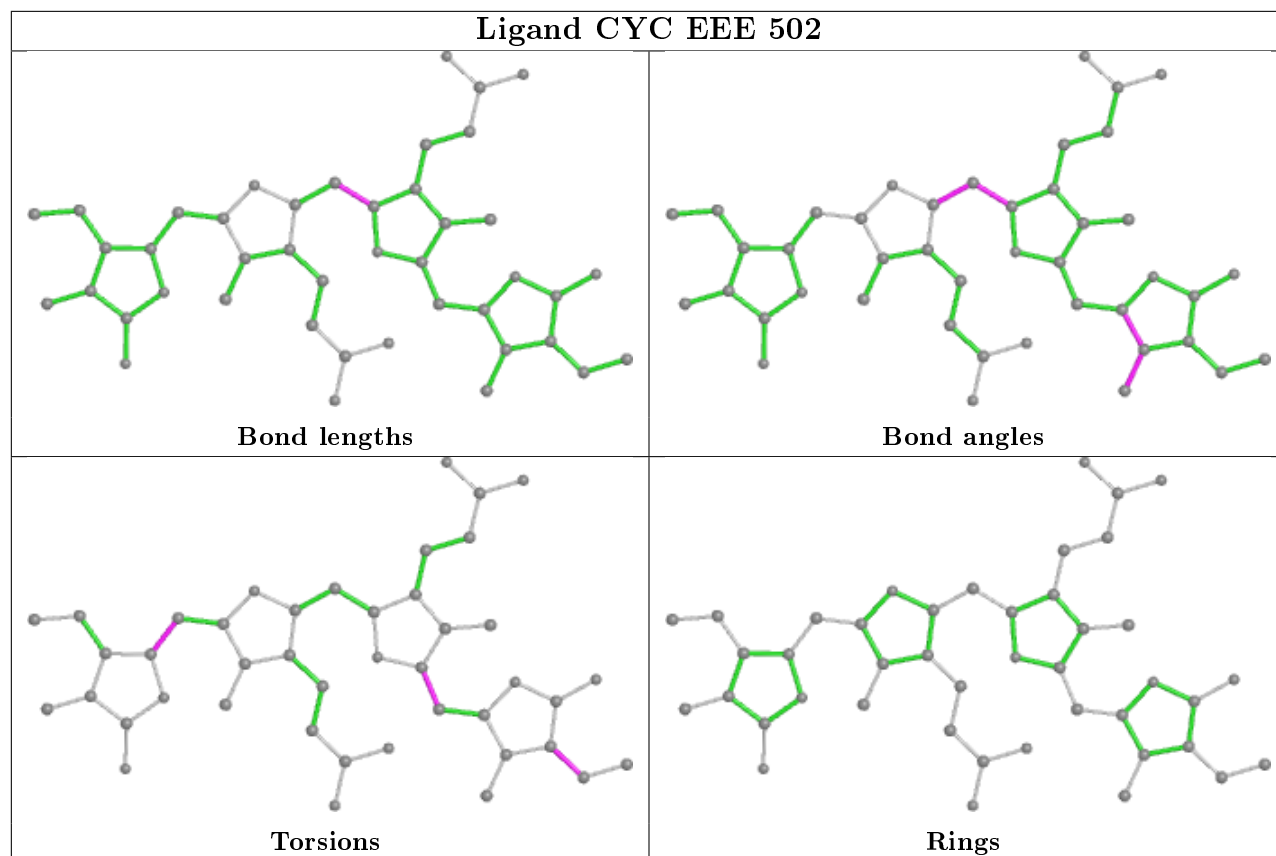
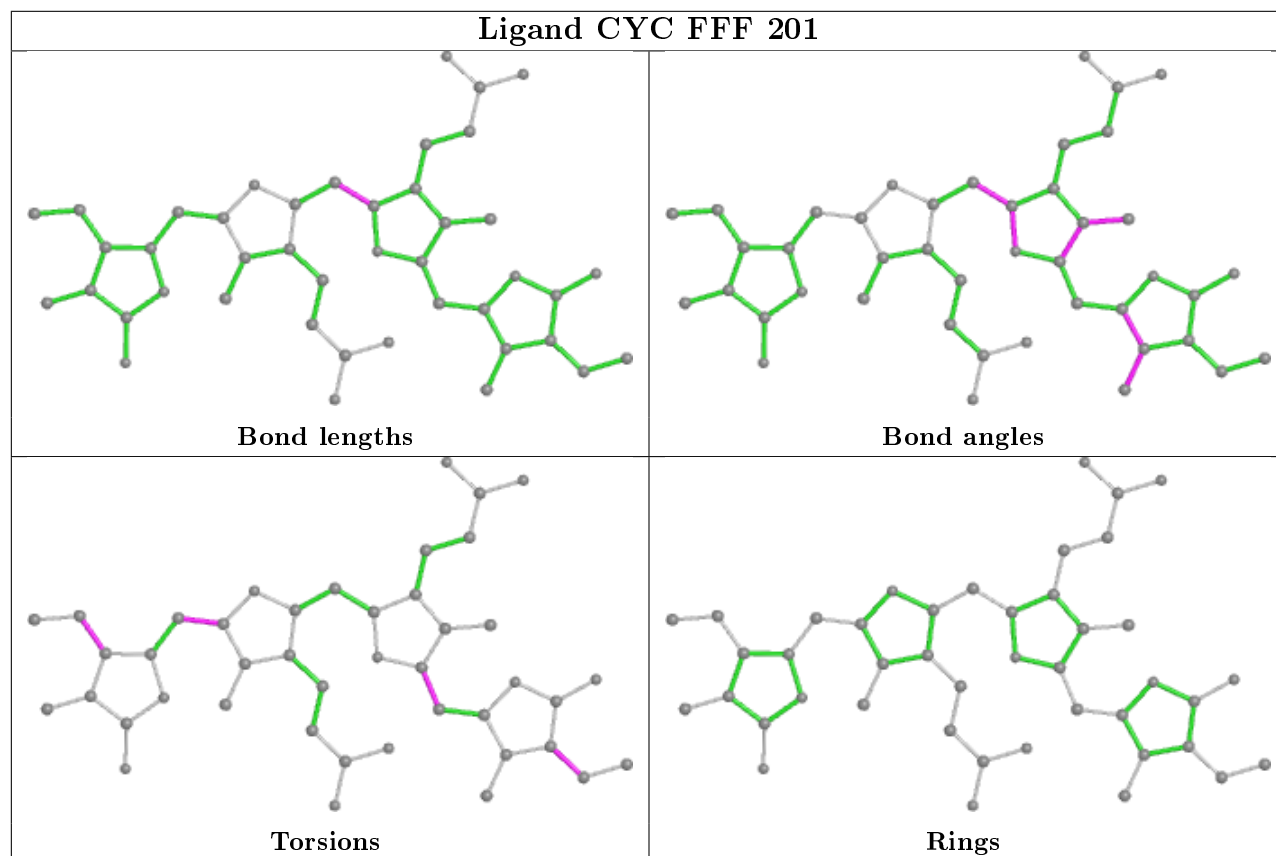


Ligand CYC LLL 202

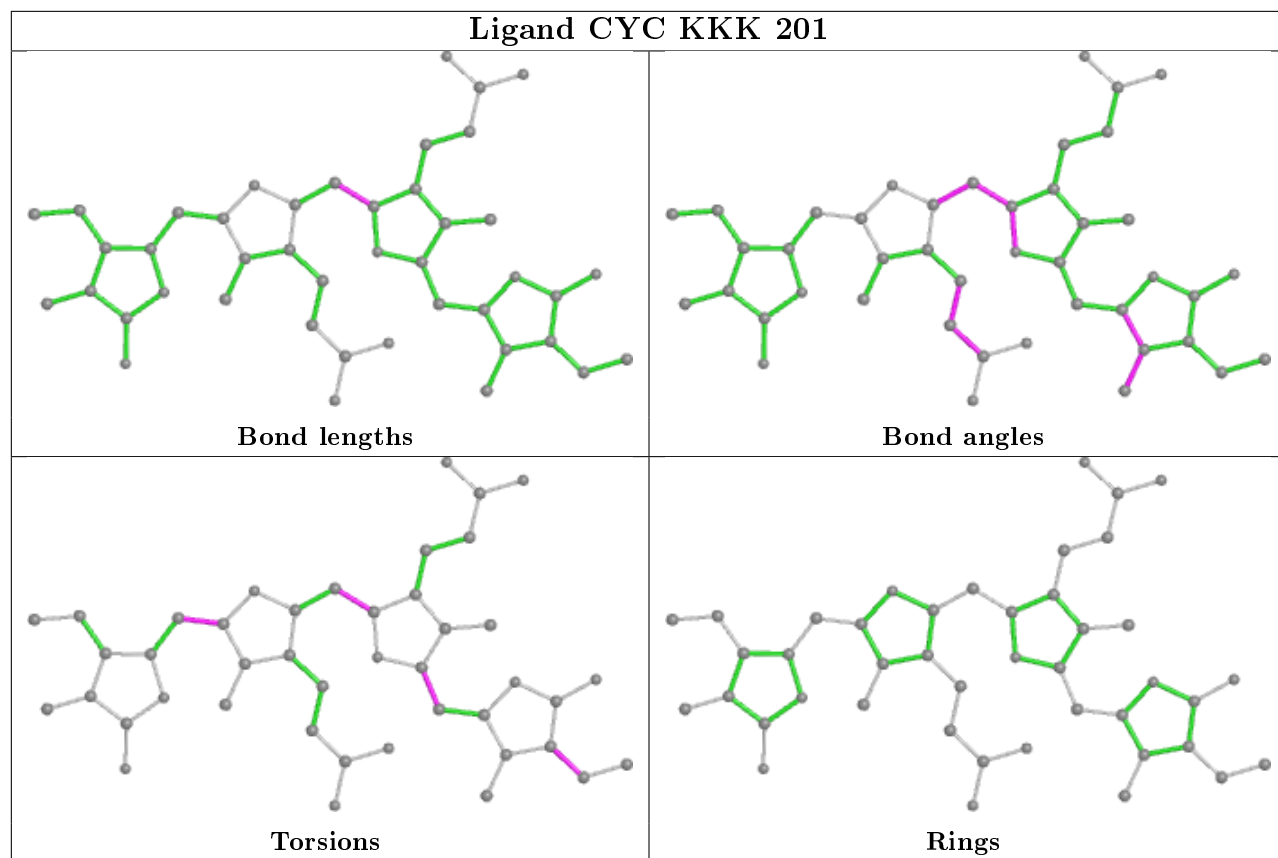


Ligand CYC HHH 201

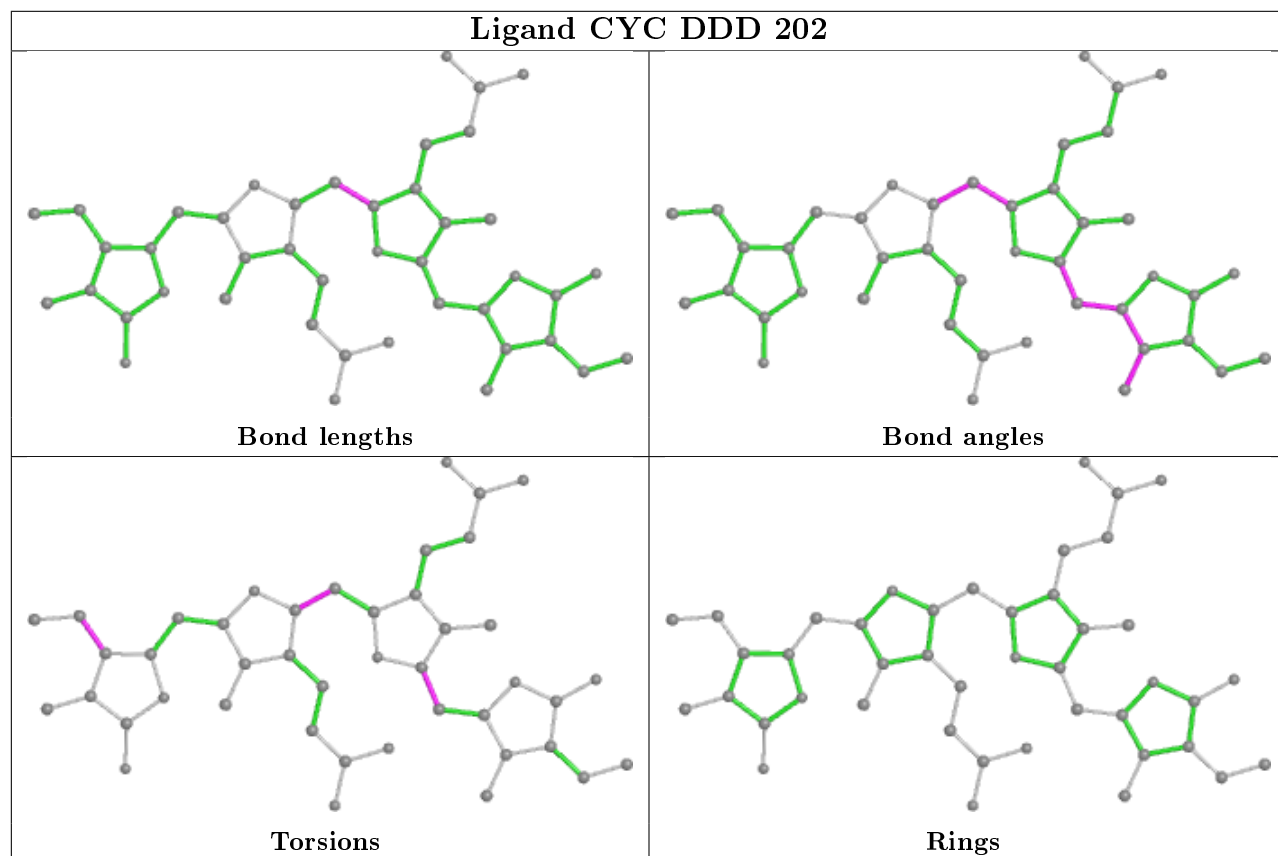


Ligand CYC EEE 502**Ligand CYC FFF 201**

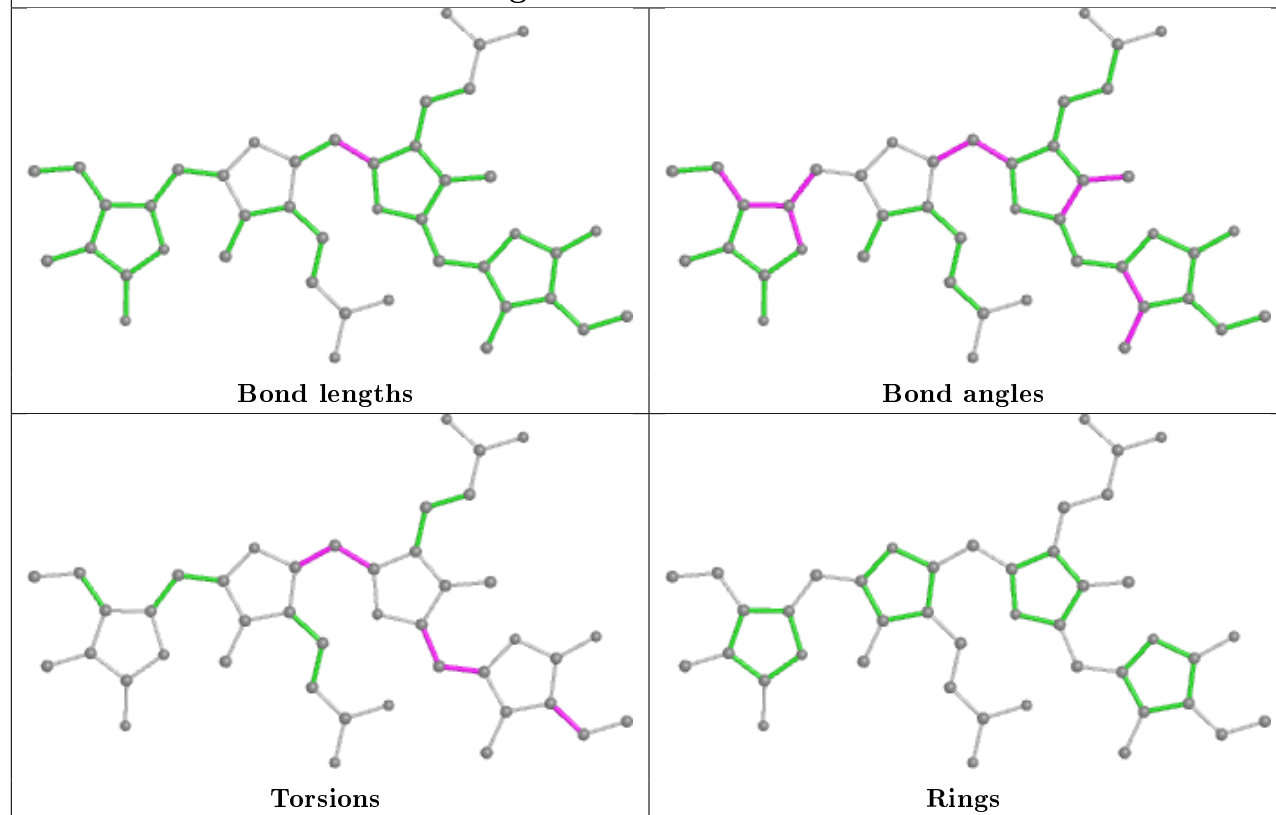
Ligand CYC KKK 201



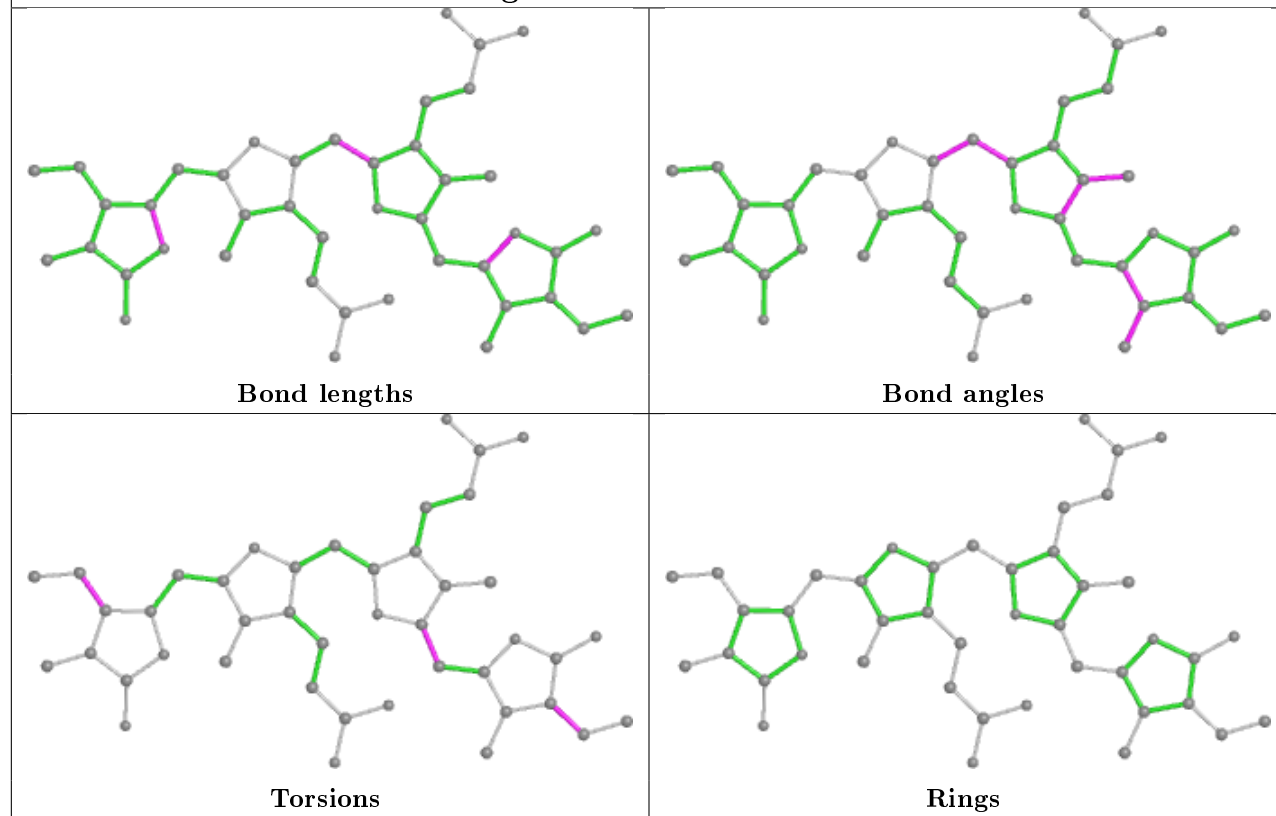
Ligand CYC DDD 202



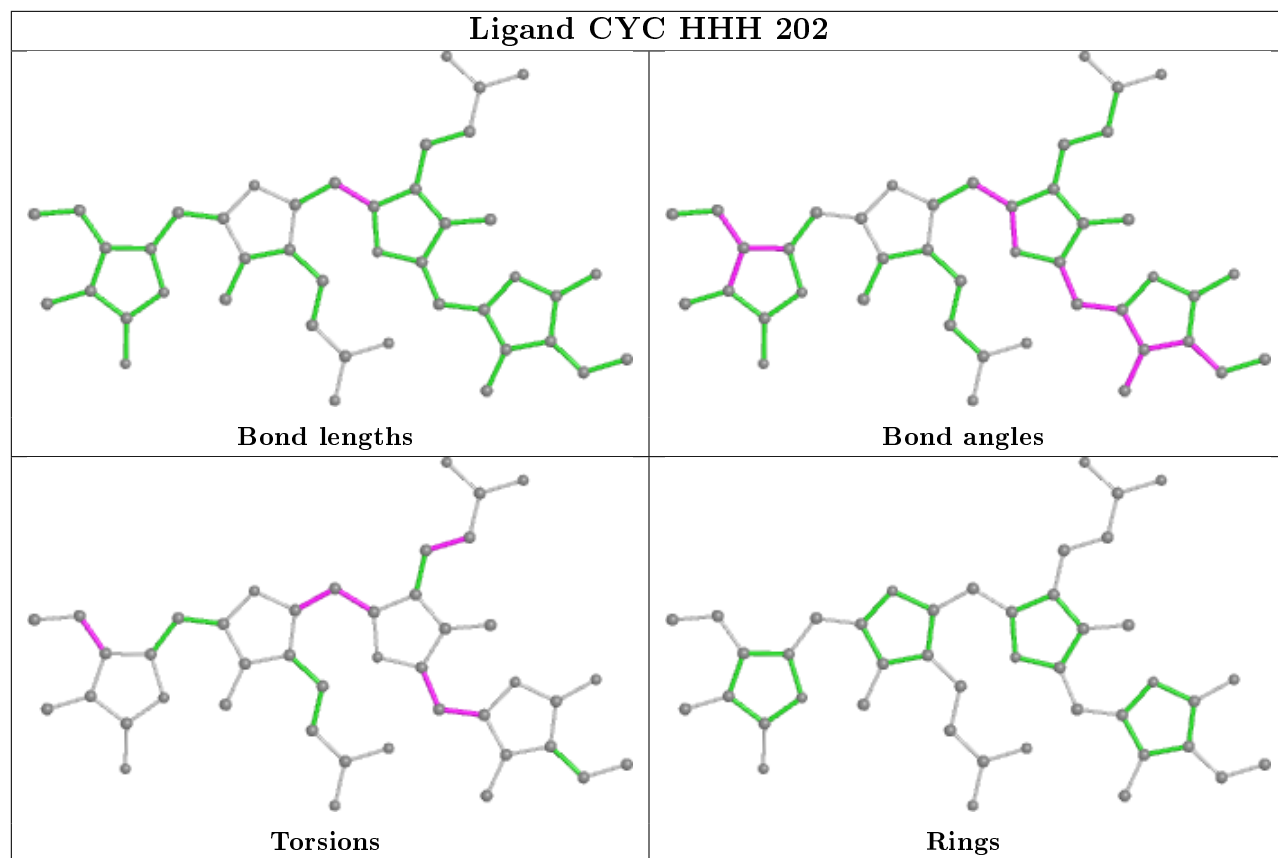
Ligand CYC FFF 202



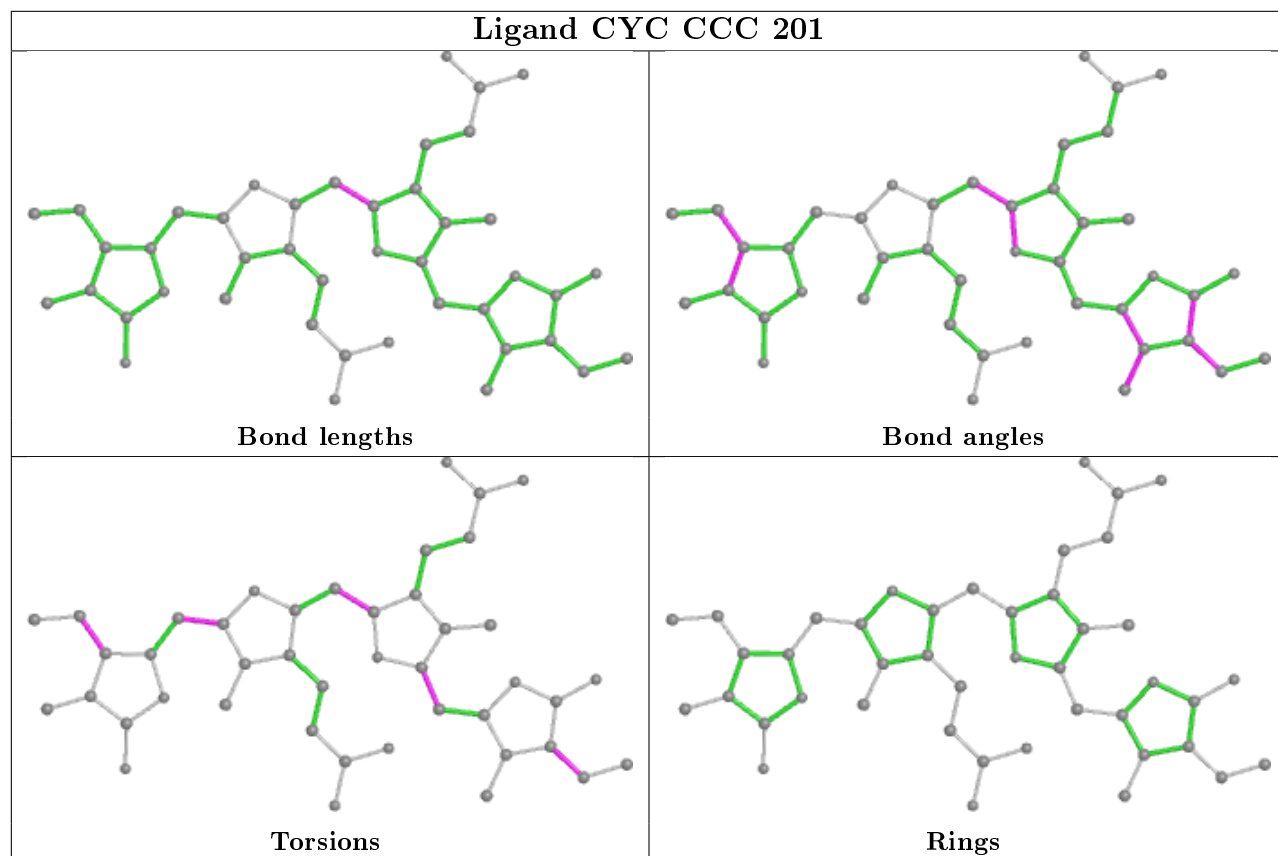
Ligand CYC GGG 201



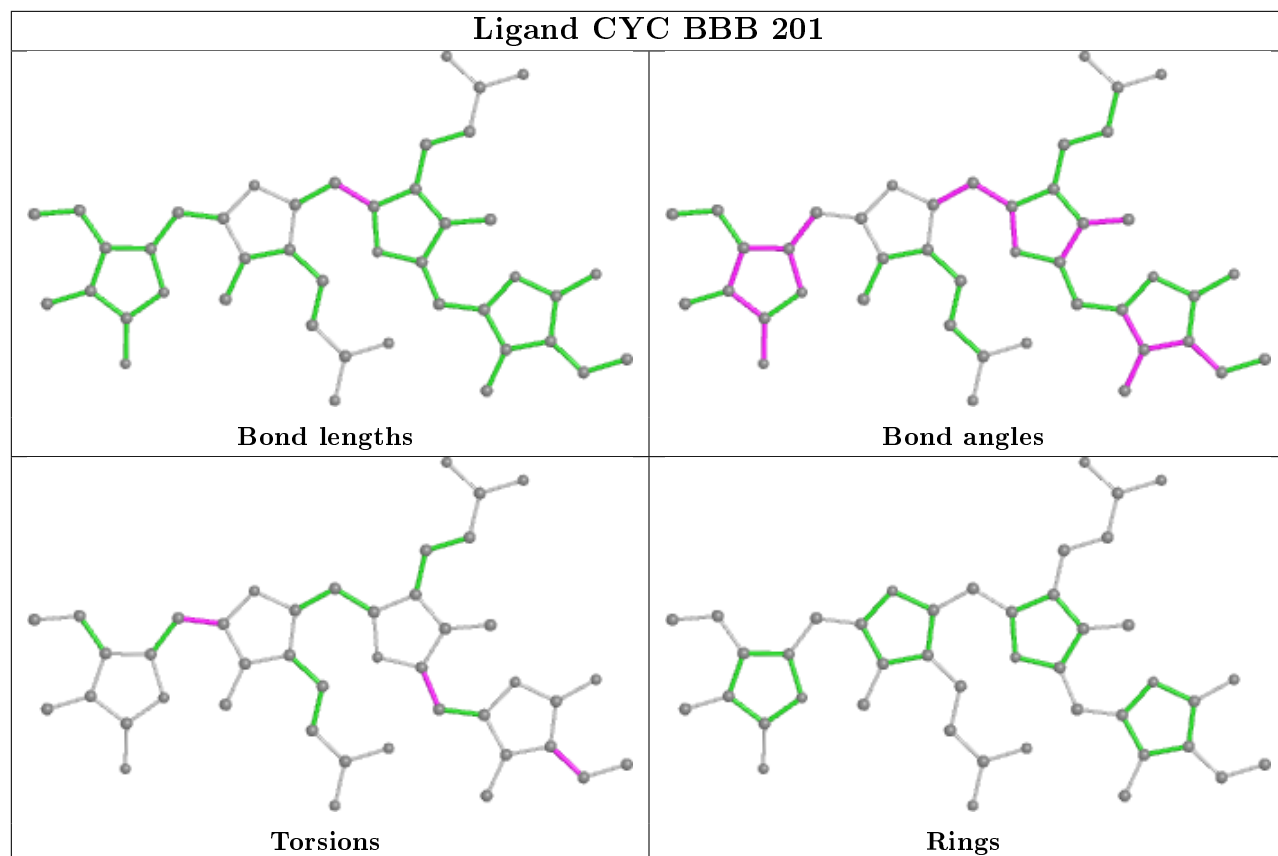
Ligand CYC HHH 202



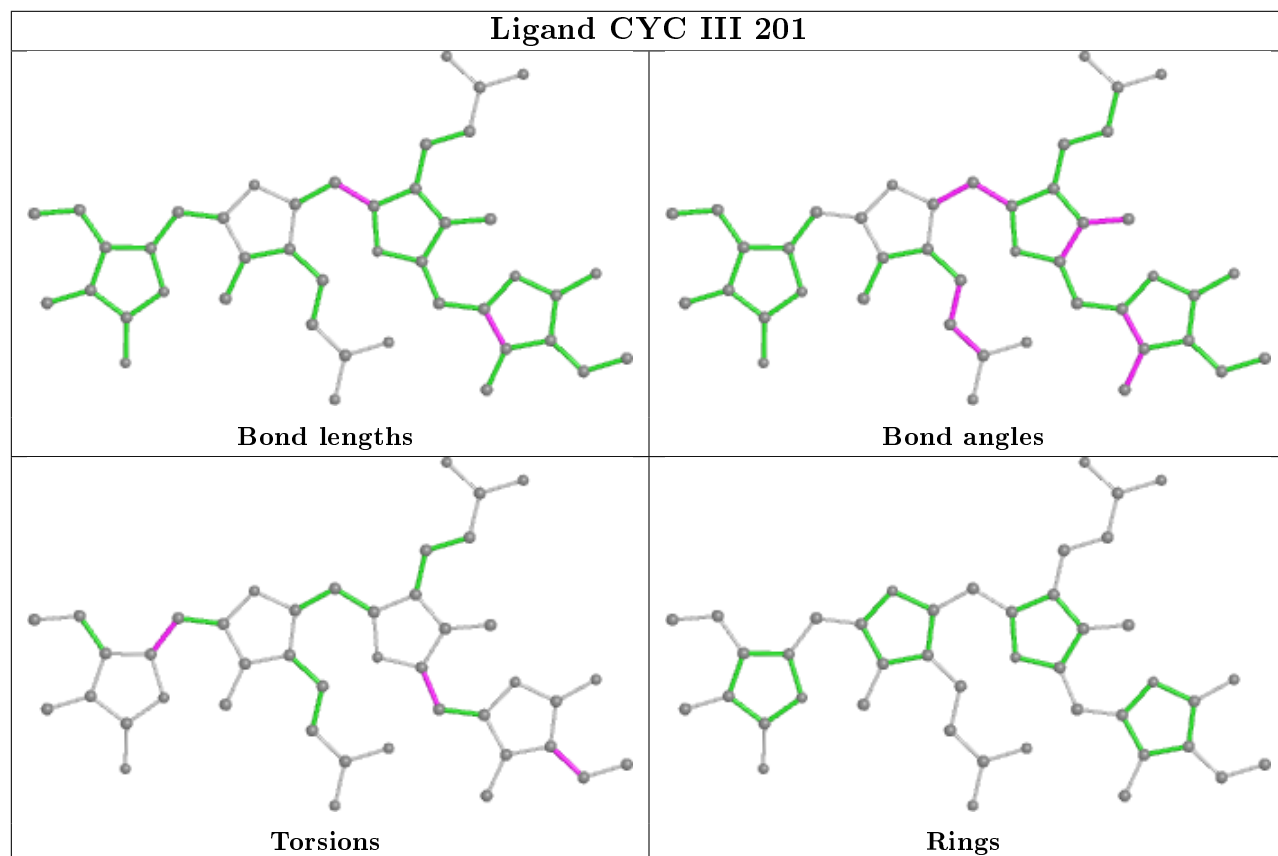
Ligand CYC CCC 201

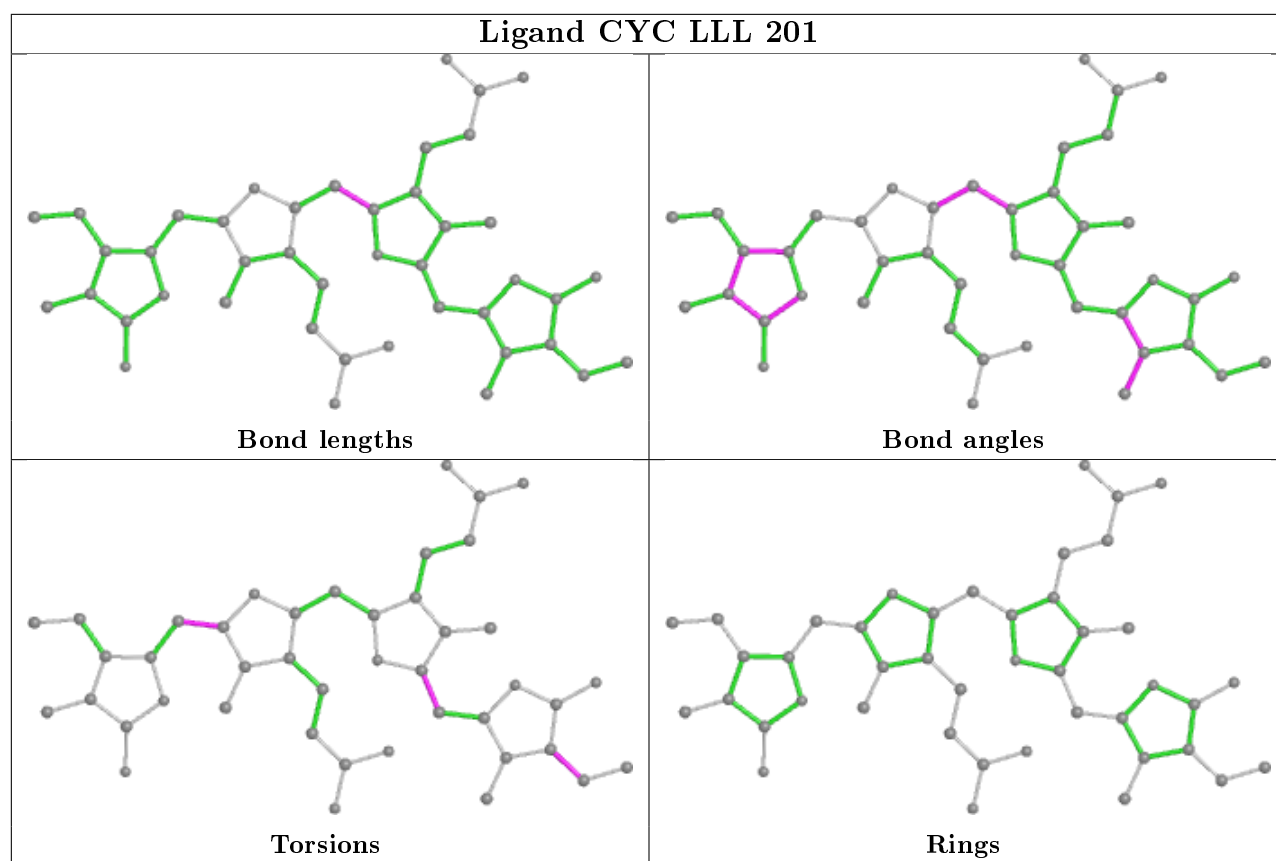


Ligand CYC BBB 201



Ligand CYC III 201





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	AAA	162/162 (100%)	-0.42	0	100	100	19, 28, 40, 55	0
1	CCC	162/162 (100%)	-0.41	0	100	100	20, 27, 39, 46	0
1	EEE	162/162 (100%)	-0.41	0	100	100	21, 30, 40, 52	0
1	GGG	162/162 (100%)	-0.40	0	100	100	19, 27, 40, 52	0
1	III	162/162 (100%)	-0.42	0	100	100	20, 29, 43, 66	0
1	KKK	162/162 (100%)	-0.37	1 (0%)	89	87	24, 33, 46, 64	0
2	BBB	171/172 (99%)	-0.30	0	100	100	22, 32, 50, 59	0
2	DDD	171/172 (99%)	-0.37	0	100	100	21, 30, 43, 57	0
2	FFF	171/172 (99%)	-0.30	0	100	100	25, 37, 52, 64	0
2	HHH	171/172 (99%)	-0.30	0	100	100	24, 34, 50, 61	0
2	JJJ	171/172 (99%)	-0.26	0	100	100	22, 36, 54, 64	0
2	LLL	171/172 (99%)	-0.27	1 (0%)	89	87	23, 32, 50, 67	0
All	All	1998/2004 (99%)	-0.35	2 (0%)	95	93	19, 31, 48, 67	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	LLL	147	ASN	2.1
1	KKK	162	SER	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, 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(\AA^2)	Q<0.9
2	MEN	JJJ	72	9/10	0.97	0.08	27,28,29,31	0
2	MEN	DDD	72	9/10	0.97	0.07	24,26,27,27	0
2	MEN	FFF	72	9/10	0.97	0.09	29,30,32,32	0
2	MEN	LLL	72	9/10	0.97	0.08	24,29,30,31	0
2	MEN	BBB	72	9/10	0.98	0.08	23,24,25,25	0
2	MEN	HHH	72	9/10	0.98	0.08	27,32,34,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

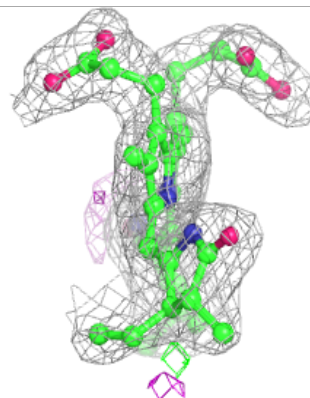
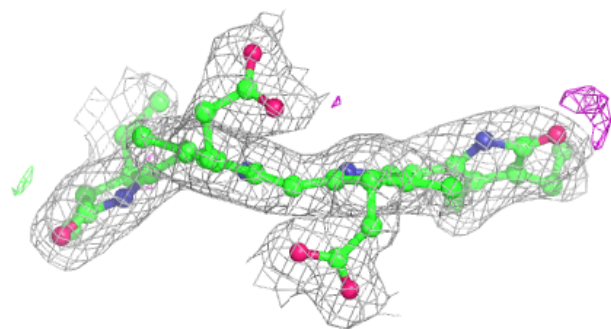
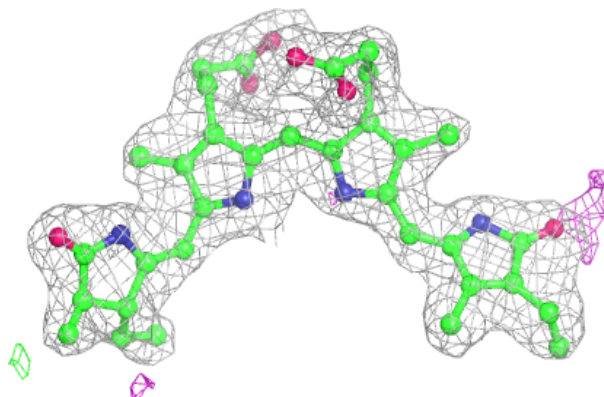
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	DDD	203	6/6	0.61	0.20	56,62,66,68	0
5	ACT	EEE	501	4/4	0.82	0.12	43,45,47,52	0
5	ACT	LLL	203	4/4	0.89	0.14	39,42,47,50	0
3	CYC	HHH	202	43/43	0.93	0.11	37,41,45,51	0
3	CYC	BBB	202	43/43	0.94	0.11	36,40,47,59	0
3	CYC	FFF	201	43/43	0.94	0.10	27,35,51,52	0
3	CYC	JJJ	202	43/43	0.94	0.11	40,45,50,55	0
3	CYC	DDD	202	43/43	0.94	0.11	27,39,51,60	0
3	CYC	FFF	202	43/43	0.94	0.11	34,42,53,56	0
3	CYC	LLL	202	43/43	0.94	0.11	31,38,43,54	0
3	CYC	HHH	201	43/43	0.94	0.11	23,33,49,62	0
3	CYC	LLL	201	43/43	0.94	0.11	24,33,49,59	0
3	CYC	JJJ	201	43/43	0.95	0.11	26,32,49,57	0
3	CYC	KKK	201	43/43	0.95	0.09	25,29,33,35	0
3	CYC	BBB	201	43/43	0.95	0.10	23,27,45,58	0
3	CYC	DDD	201	43/43	0.95	0.10	22,27,44,57	0
3	CYC	GGG	201	43/43	0.95	0.09	21,23,28,32	0
3	CYC	AAA	201	43/43	0.96	0.09	19,23,27,30	0
3	CYC	III	201	43/43	0.96	0.08	22,25,31,32	0
3	CYC	EEE	502	43/43	0.96	0.08	22,26,29,30	0
3	CYC	CCC	201	43/43	0.96	0.08	21,24,28,30	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.

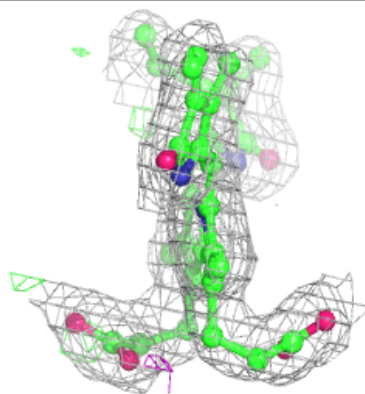
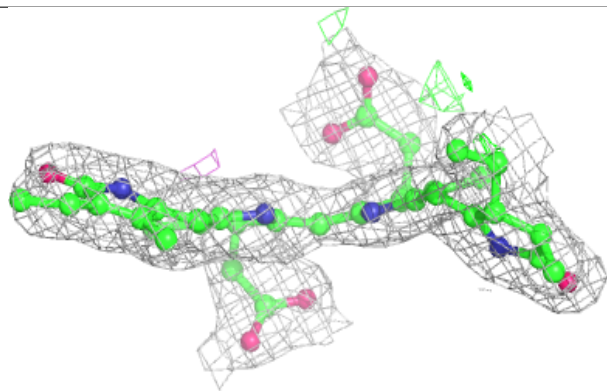
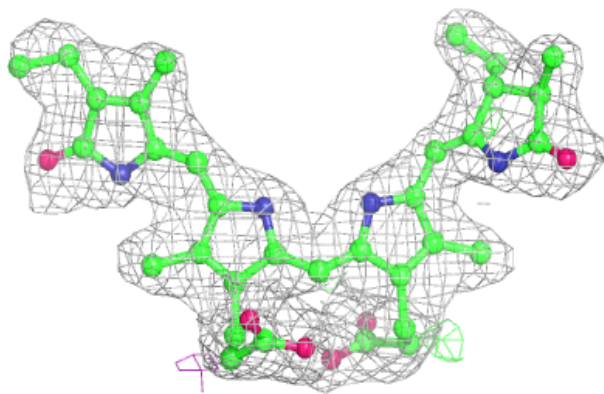
Electron density around CYC HHH 202:

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



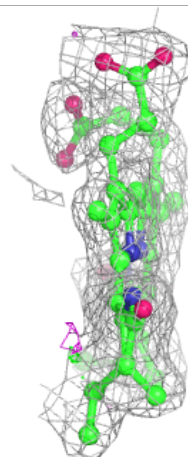
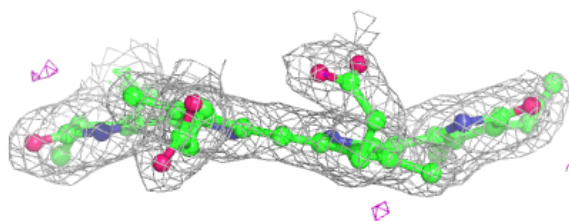
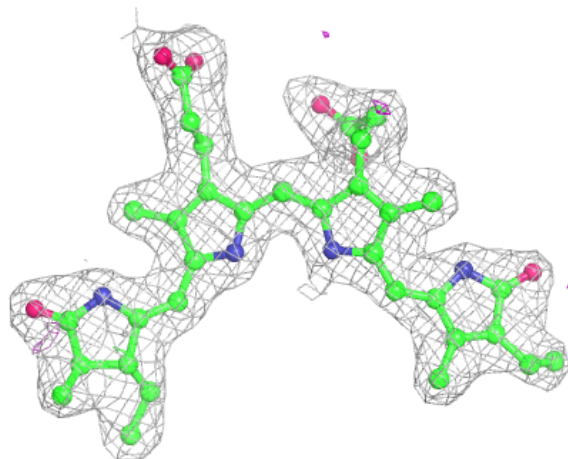
Electron density around CYC BBB 202:

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



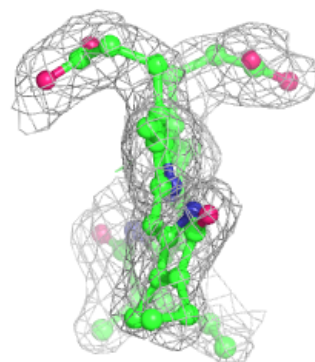
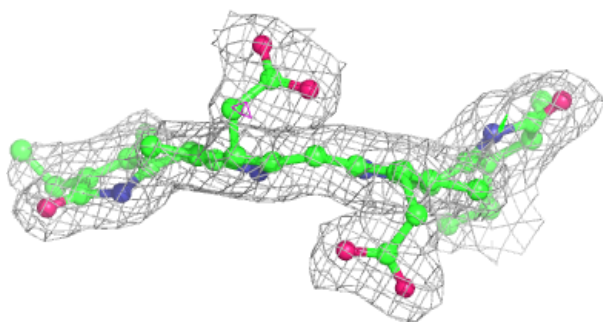
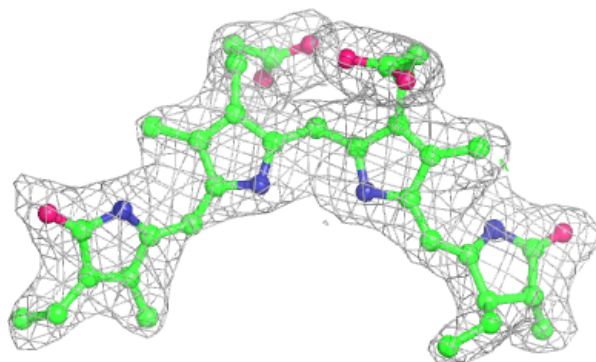
Electron density around CYC FFF 201:

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

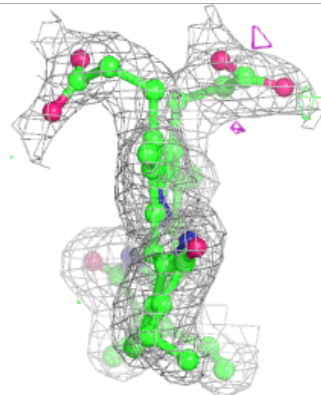
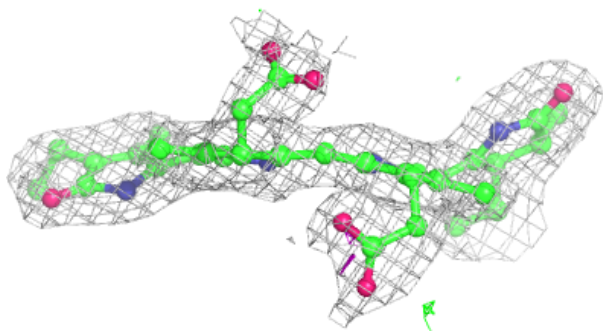
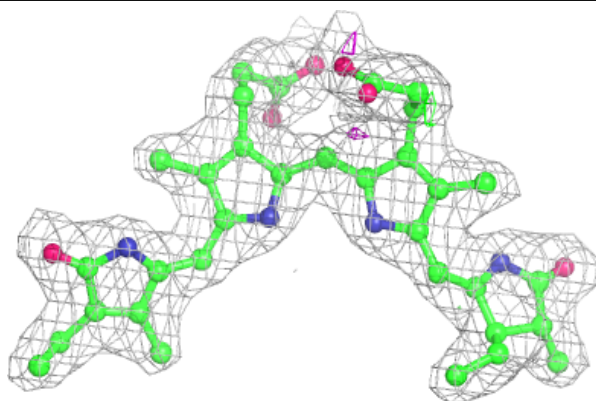


Electron density around CYC JJJ 202:

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

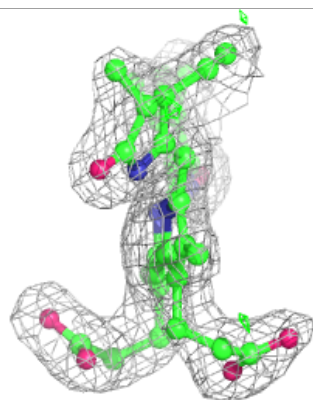
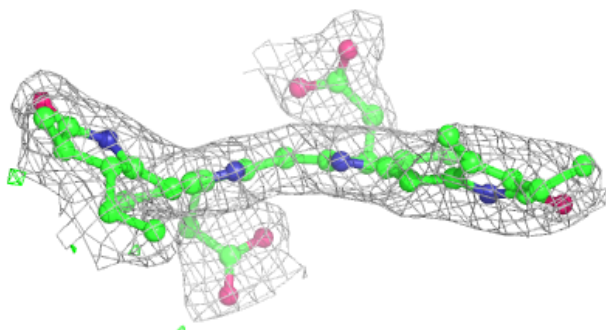
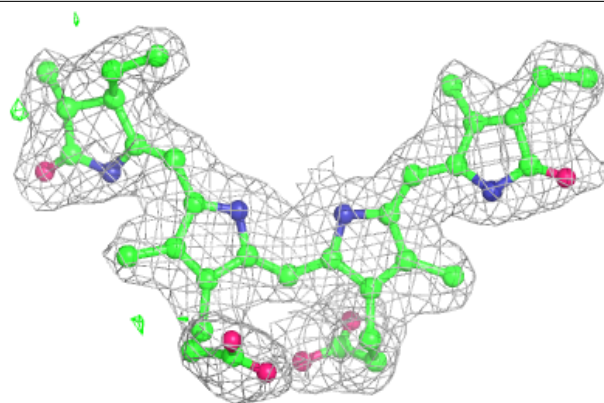
**Electron density around CYC DDD 202:**

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

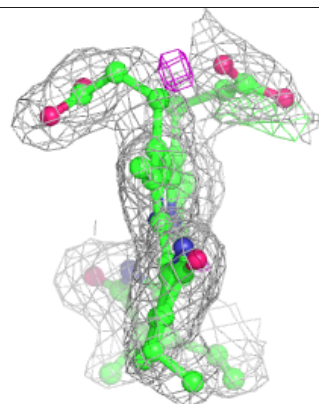
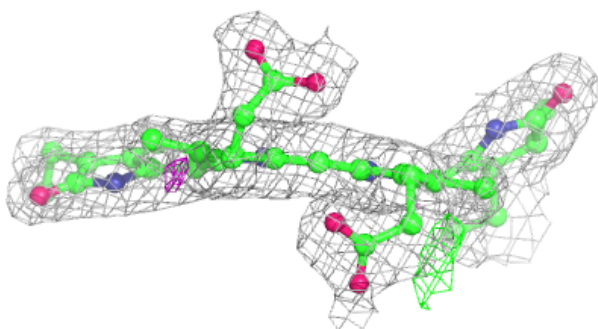
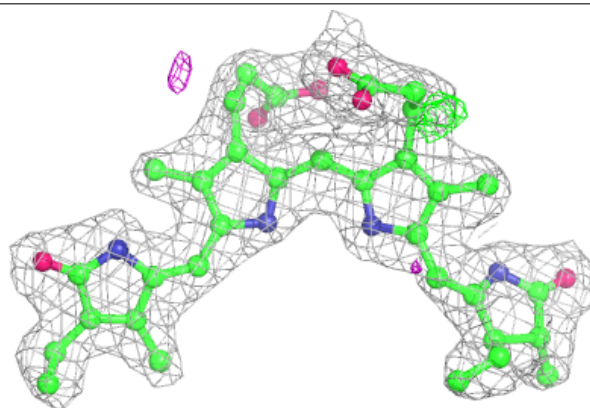


Electron density around CYC FFF 202:

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

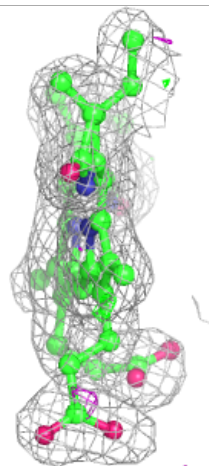
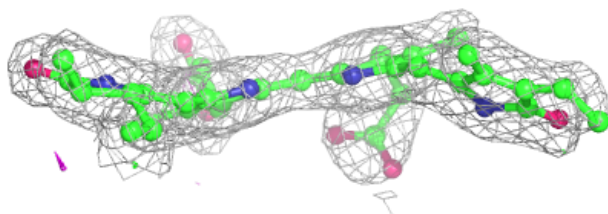
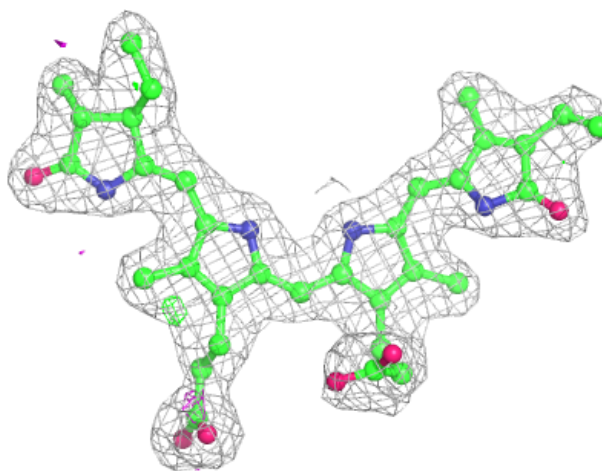
**Electron density around CYC LLL 202:**

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



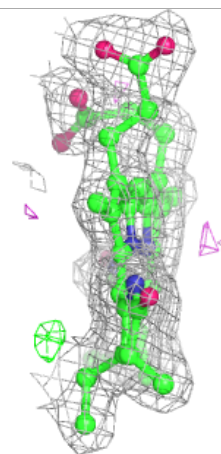
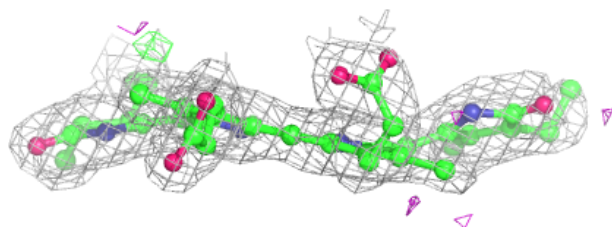
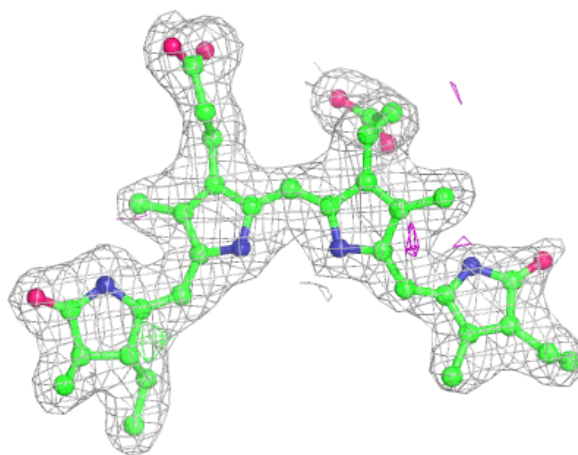
Electron density around CYC HHH 201:

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



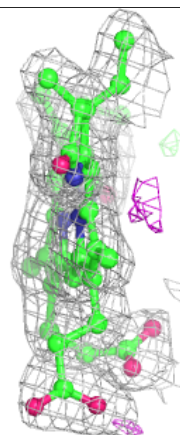
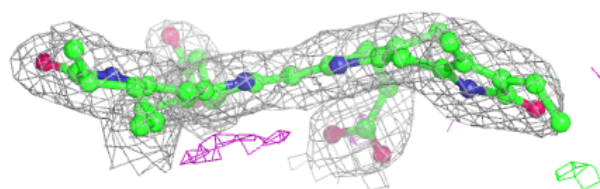
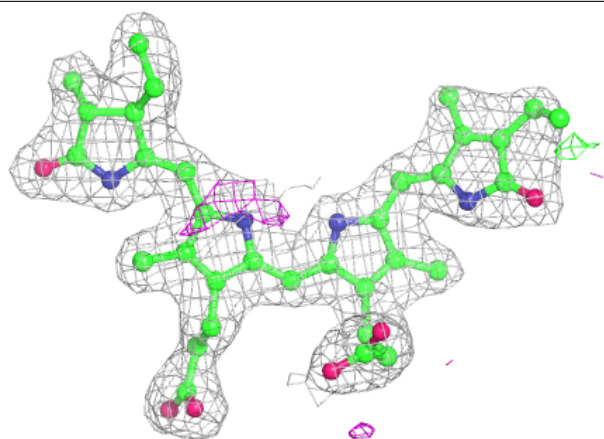
Electron density around CYC LLL 201:

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



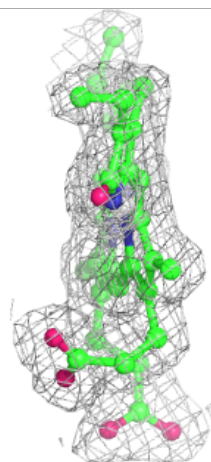
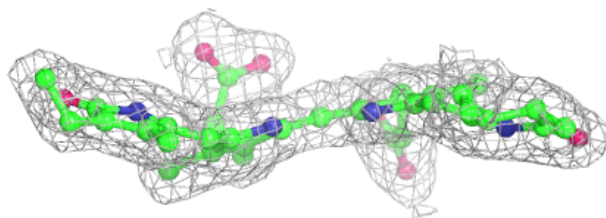
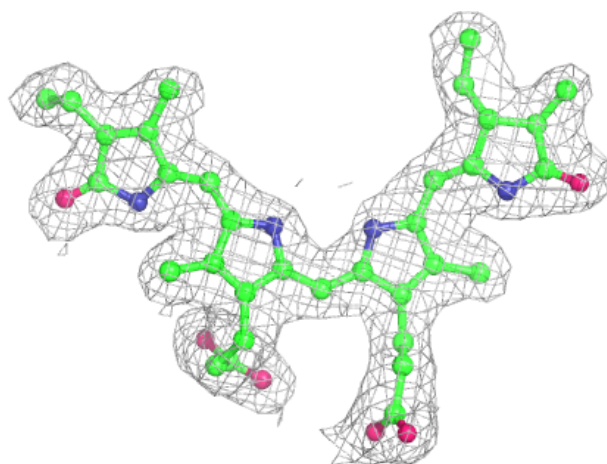
Electron density around CYC JJJ 201:

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



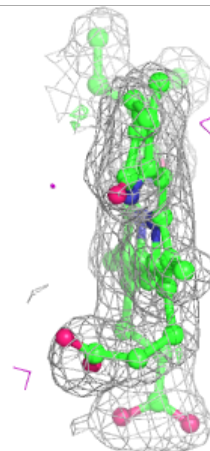
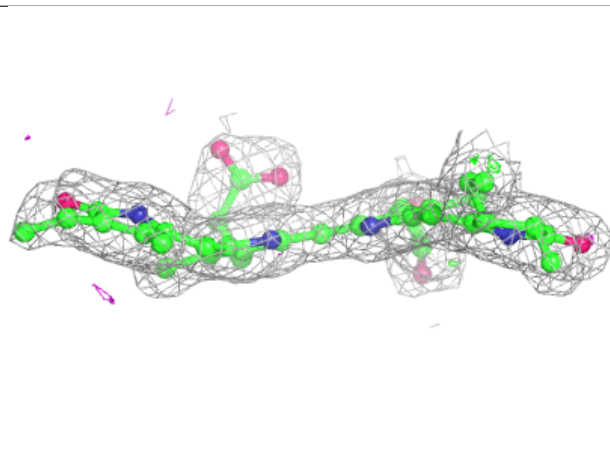
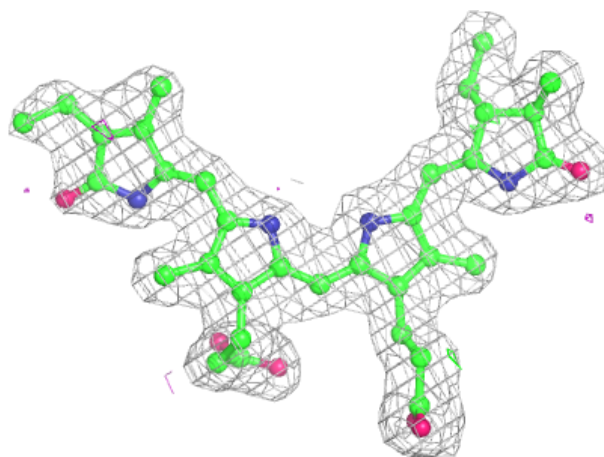
Electron density around CYC KKK 201:

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



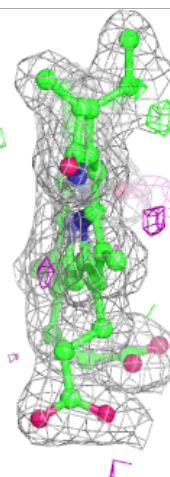
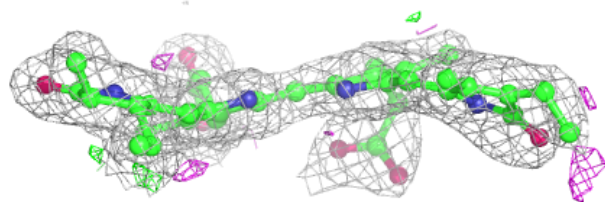
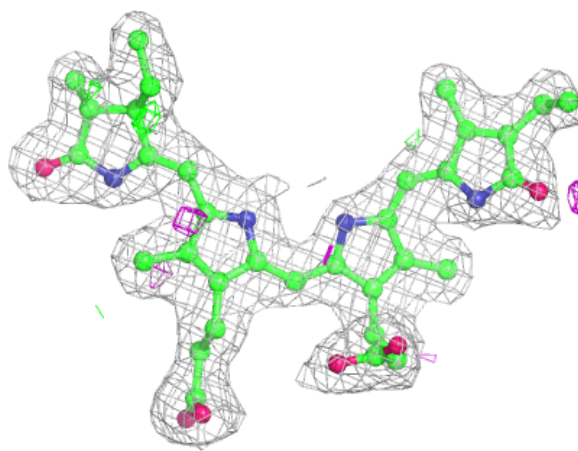
Electron density around CYC BBB 201:

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



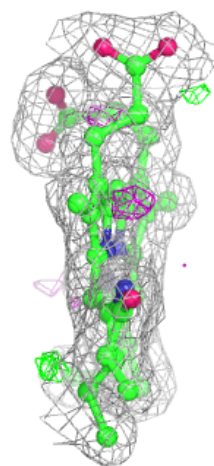
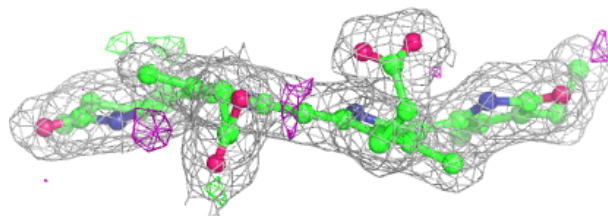
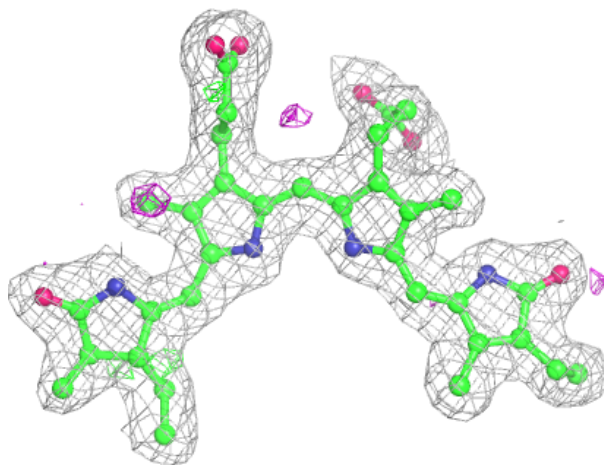
Electron density around CYC DDD 201:

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



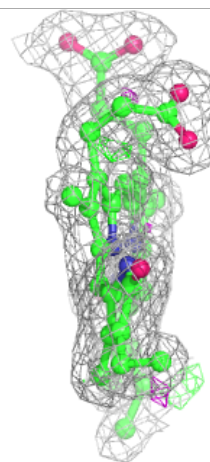
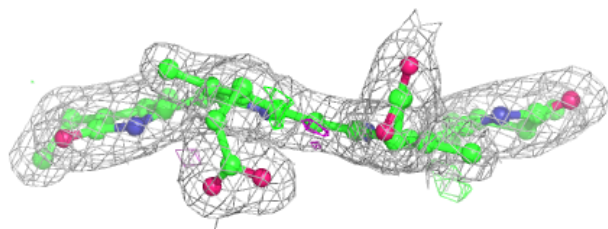
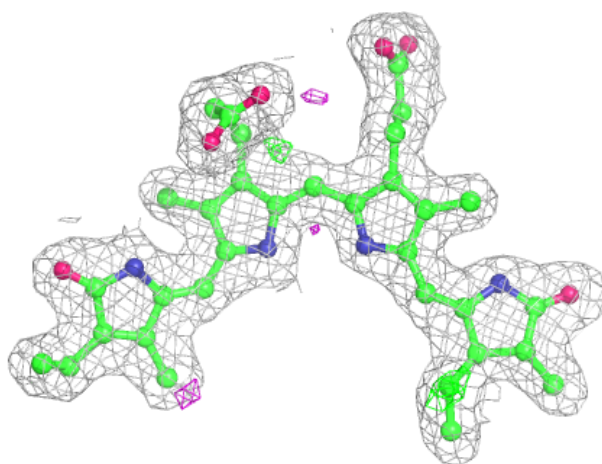
Electron density around CYC GGG 201:

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



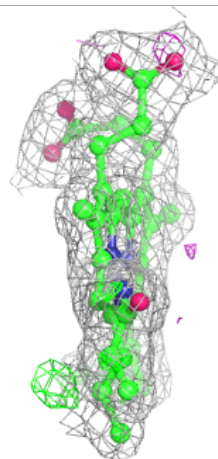
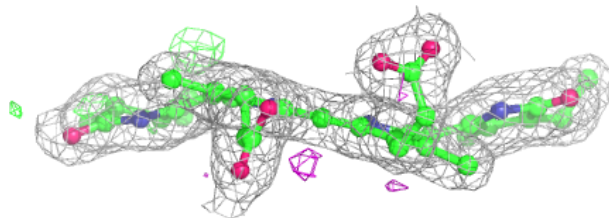
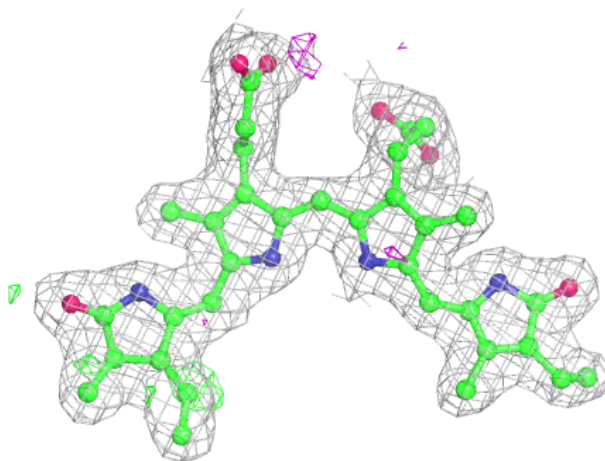
Electron density around CYC AAA 201:

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



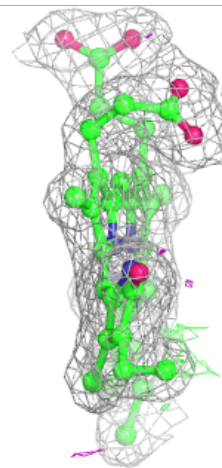
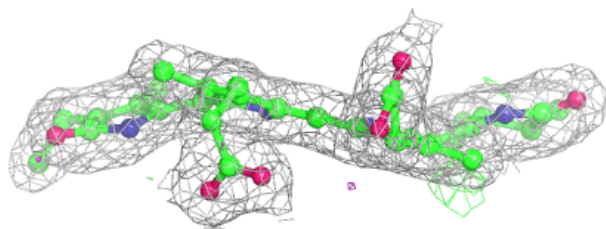
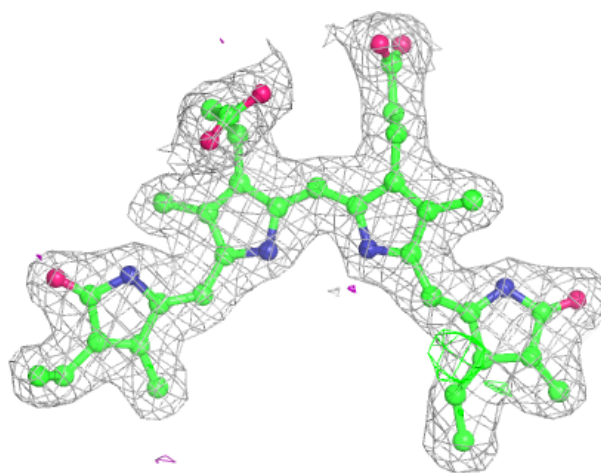
Electron density around CYC III 201:

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



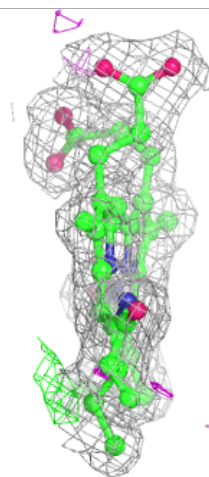
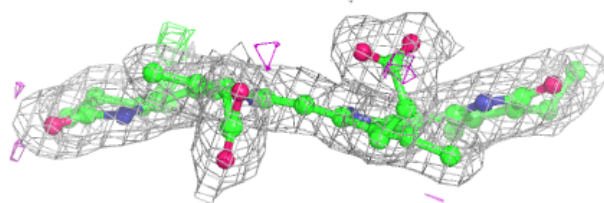
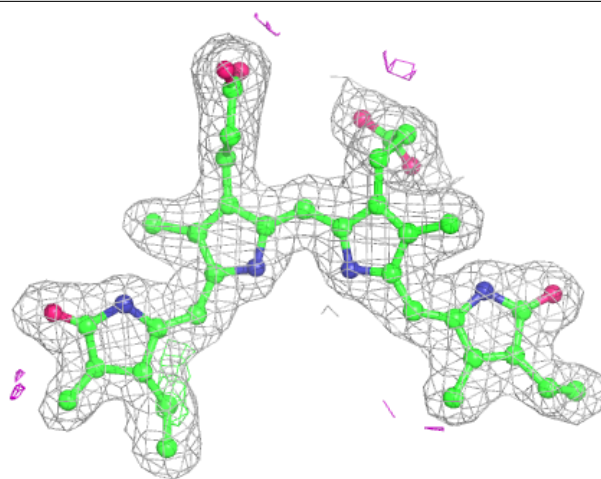
Electron density around CYC EEE 502:

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



Electron density around CYC CCC 201:

$2mF_o-DF_c$ (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.