



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:42 AM UTC

PDB ID : 9T05 / pdb_00009t05
Title : X-ray structure of the adduct formed by dirhodium tetraacetate with a C-phycocyanin
Authors : Merlino, A.; Ferraro, G.
Deposited on : 2025-10-16
Resolution : 2.17 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

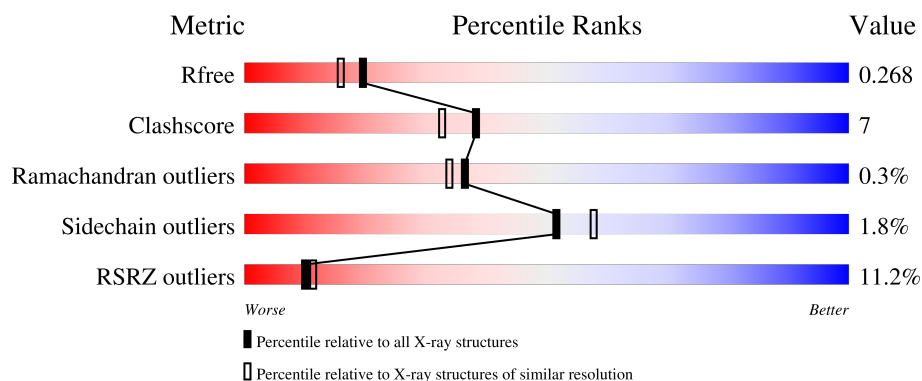
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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.



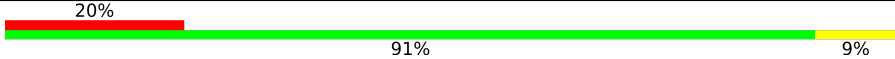
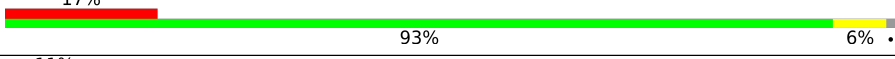
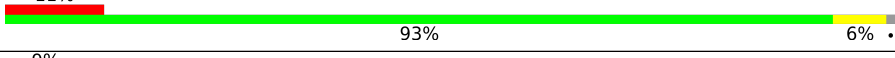
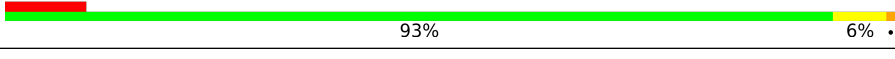
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	12% 93% 6%
1	CCC	162	3% 94% 6%
1	EEE	162	8% 91% 8%
1	GGG	162	7% 94% 6%
1	III	162	4% 91% 8%

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Mol	Chain	Length	Quality of chain
1	KKK	162	
2	BBB	173	
2	DDD	173	
2	FFF	173	
2	HHH	173	
2	JJJ	173	
2	LLL	173	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	162	Total	C	N	O	S	0	3	0
			1240	771	217	244	8			
1	CCC	162	Total	C	N	O	S	0	2	0
			1221	760	210	243	8			
1	EEE	162	Total	C	N	O	S	0	3	0
			1237	769	217	243	8			
1	GGG	162	Total	C	N	O	S	0	5	0
			1241	770	214	249	8			
1	III	162	Total	C	N	O	S	0	4	0
			1243	772	218	245	8			
1	KKK	162	Total	C	N	O	S	0	4	0
			1247	775	216	248	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	1	0
			1280	792	225	255	8			
2	FFF	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
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	2	0
			1291	798	228	257	8			
2	LLL	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			

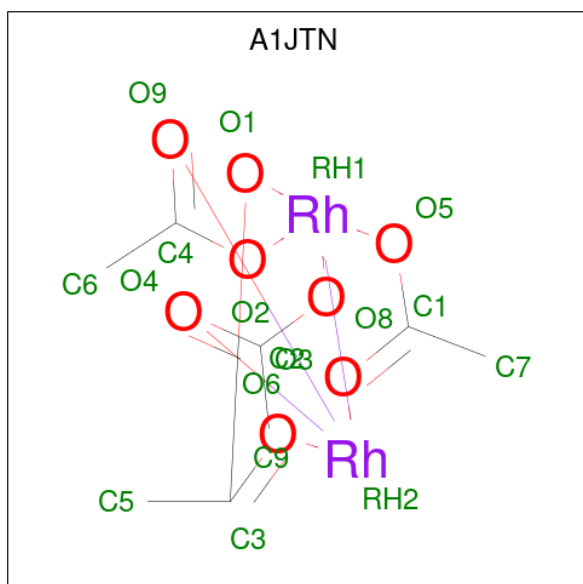
- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆).

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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 dirhodium tetraacetate (CCD ID: A1JTN) (formula: $C_8H_{12}O_8Rh_2$) (labeled as "Ligand of Interest" by depositor).



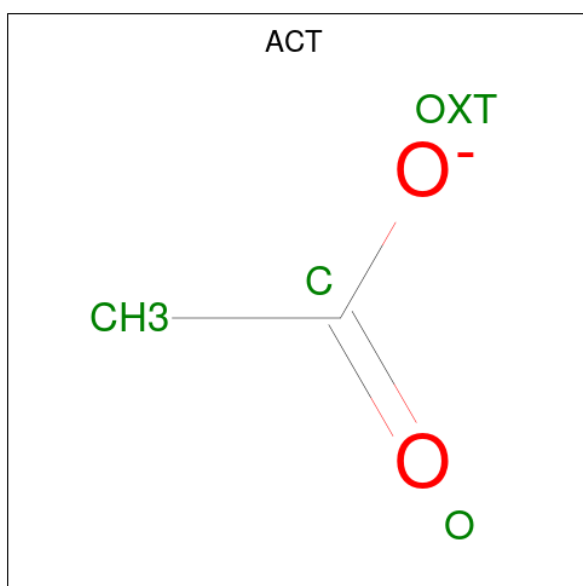
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	Rh			0	0
			2	2				
4	BBB	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	CCC	1	Total	Rh			0	0
			2	2				
4	DDD	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	EEE	1	Total	Rh			0	0
			2	2				
4	FFF	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	GGG	1	Total	Rh			0	0
			2	2				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	HHH	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	III	1	Total	Rh			0	0
			2	2				
4	JJJ	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	KKK	1	Total	Rh			0	0
			2	2				
4	LLL	1	Total	C	O	Rh	0	0
			18	8	8	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	67	Total	O	0	0
			67	67		

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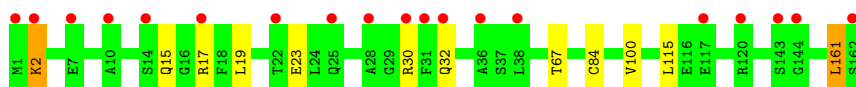
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BBB	48	Total 48	O 48	0	0
6	CCC	68	Total 68	O 68	0	0
6	DDD	41	Total 41	O 41	0	0
6	EEE	49	Total 49	O 49	0	0
6	FFF	21	Total 21	O 21	0	0
6	GGG	37	Total 37	O 37	0	0
6	HHH	28	Total 28	O 28	0	0
6	III	44	Total 44	O 44	0	0
6	JJJ	17	Total 17	O 17	0	0
6	KKK	31	Total 32	O 32	0	1
6	LLL	44	Total 44	O 44	0	0

3 Residue-property plots [i](#)

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

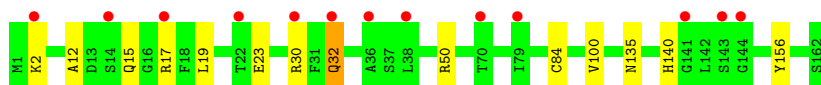
- Molecule 1: C-phycocyanin alpha subunit



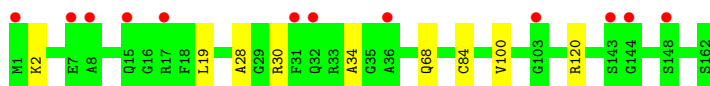
- Molecule 1: C-phycocyanin alpha subunit



- Molecule 1: C-phycocyanin alpha subunit



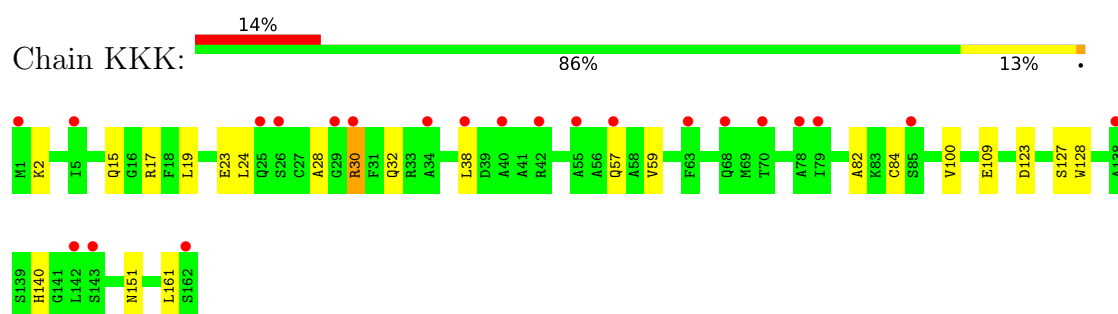
- Molecule 1: C-phycocyanin alpha subunit



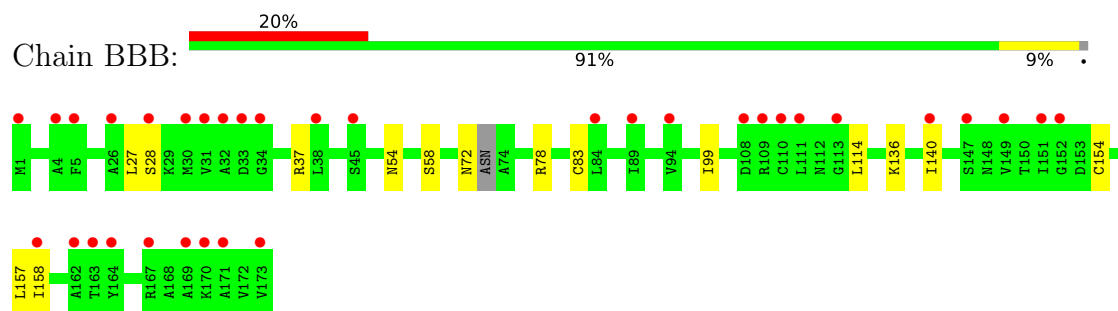
- Molecule 1: C-phycocyanin alpha subunit



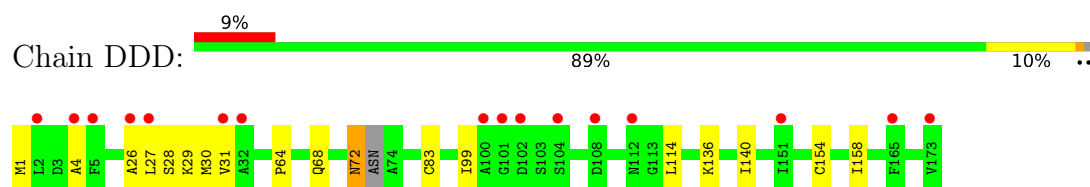
- Molecule 1: C-phycocyanin alpha subunit



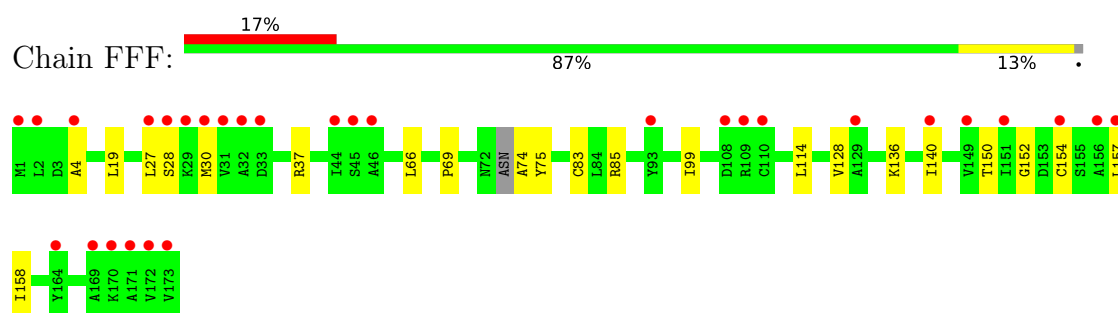
- Molecule 2: C-phycoerythrin beta chain



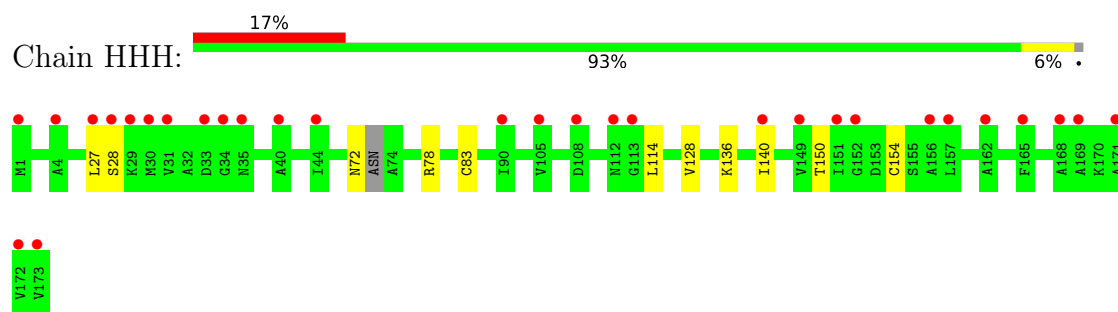
- Molecule 2: C-phycoerythrin beta chain



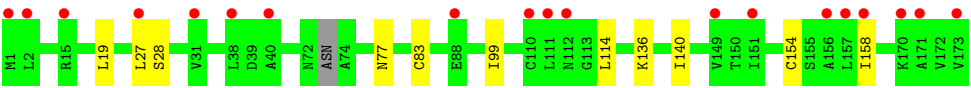
- Molecule 2: C-phycoerythrin beta chain



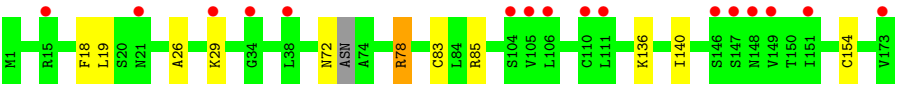
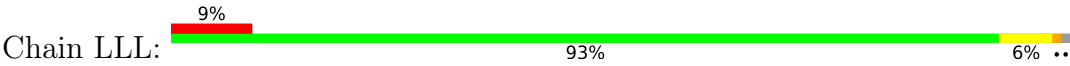
- Molecule 2: C-phycoerythrin beta chain



- Molecule 2: C-phycoerythrin beta chain



● Molecule 2: C-phycoyanin beta chain



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	60.59Å 188.50Å 207.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	139.83 – 2.17 139.44 – 2.17	Depositor EDS
% Data completeness (in resolution range)	81.2 (139.83-2.17) 81.2 (139.44-2.17)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.263 0.230 , 0.268	Depositor DCC
R_{free} test set	5000 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16492	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: MEN, ACT, DOD, CYC, A1JTN

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	1.02	0/1261	1.53	0/1705
1	CCC	1.01	0/1242	1.53	4/1681 (0.2%)
1	EEE	1.03	0/1258	1.51	0/1702
1	GGG	1.05	0/1262	1.51	2/1708 (0.1%)
1	III	0.99	0/1264	1.51	1/1709 (0.1%)
1	KKK	1.01	0/1268	1.52	4/1715 (0.2%)
2	BBB	1.04	0/1279	1.54	0/1730
2	DDD	1.05	0/1282	1.54	0/1735
2	FFF	1.04	0/1273	1.53	0/1722
2	HHH	1.03	0/1273	1.54	0/1722
2	JJJ	1.03	0/1293	1.54	0/1748
2	LLL	1.04	0/1273	1.56	0/1722
All	All	1.03	0/15228	1.53	11/20599 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KKK	161	LEU	CA-C-N	7.81	135.77	121.70
1	KKK	161	LEU	C-N-CA	7.81	135.77	121.70
1	CCC	109	GLU	CB-CG-CD	7.38	125.15	112.60
1	III	39	ASP	CA-CB-CG	6.33	118.93	112.60
1	GGG	28	ALA	CA-C-N	5.68	126.39	120.03

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	AAA	1240	0	1215	24	0
1	CCC	1221	0	1193	9	0
1	EEE	1237	0	1215	23	0
1	GGG	1241	0	1207	13	0
1	III	1243	0	1218	14	0
1	KKK	1247	0	1215	20	0
2	BBB	1277	0	1281	21	0
2	DDD	1280	0	1284	22	0
2	FFF	1271	0	1276	28	0
2	HHH	1271	0	1277	21	0
2	JJJ	1291	0	1294	20	0
2	LLL	1271	0	1277	18	0
3	AAA	43	0	38	8	0
3	BBB	86	0	76	14	0
3	CCC	43	0	37	6	0
3	DDD	86	0	75	17	0
3	EEE	43	0	38	10	0
3	FFF	86	0	76	18	0
3	GGG	43	0	38	8	0
3	HHH	86	0	76	19	0
3	III	43	0	38	3	0
3	JJJ	86	0	76	14	0
3	KKK	43	0	38	6	0
3	LLL	86	0	76	15	0
4	AAA	2	0	0	0	0
4	BBB	18	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	18	0	0	1	0
4	EEE	2	0	0	0	0
4	FFF	18	0	0	0	0
4	GGG	2	0	0	0	0
4	HHH	18	0	0	0	0
4	III	2	0	0	0	0
4	JJJ	18	0	0	0	0
4	KKK	2	0	0	0	0
4	LLL	18	0	0	1	0
5	EEE	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FFF	4	0	3	0	0
5	GGG	4	0	3	0	0
6	AAA	67	0	0	2	0
6	BBB	48	0	0	0	0
6	CCC	68	0	0	2	0
6	DDD	41	0	0	0	0
6	EEE	49	0	0	2	0
6	FFF	21	0	0	0	0
6	GGG	37	0	0	0	0
6	HHH	28	0	0	1	0
6	III	44	0	0	0	0
6	JJJ	17	0	0	0	0
6	KKK	32	0	0	2	0
6	LLL	44	0	0	0	0
All	All	16492	0	15643	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 218 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:GGG:84:CYS:SG	3:GGG:201:CYC:HAC2	1.22	1.71
1:III:84:CYS:SG	3:III:201:CYC:HAC2	1.15	1.70
2:FFF:154:CYS:SG	3:FFF:504:CYC:HAC1	1.28	1.69
2:HHH:154:CYS:SG	3:HHH:203:CYC:HAC1	1.24	1.69
1:AAA:84:CYS:SG	3:AAA:201:CYC:HAC2	1.13	1.68

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	163/162 (101%)	159 (98%)	3 (2%)	1 (1%)	21	15
1	CCC	162/162 (100%)	158 (98%)	3 (2%)	1 (1%)	21	15
1	EEE	163/162 (101%)	159 (98%)	3 (2%)	1 (1%)	21	15
1	GGG	165/162 (102%)	161 (98%)	3 (2%)	1 (1%)	21	15
1	III	164/162 (101%)	160 (98%)	3 (2%)	1 (1%)	21	15
1	KKK	164/162 (101%)	160 (98%)	3 (2%)	1 (1%)	21	15
2	BBB	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
2	DDD	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
2	FFF	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
2	HHH	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
2	JJJ	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
2	LLL	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	1999/2010 (100%)	1957 (98%)	36 (2%)	6 (0%)	36	34

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	III	2	LYS
1	KKK	2	LYS
1	AAA	2	LYS
1	CCC	2	LYS
1	EEE	2	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	126/123 (102%)	123 (98%)	3 (2%)	43	47
1	CCC	125/123 (102%)	124 (99%)	1 (1%)	73	79
1	EEE	126/123 (102%)	122 (97%)	4 (3%)	34	36
1	GGG	128/123 (104%)	126 (98%)	2 (2%)	55	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	III	127/123 (103%)	123 (97%)	4 (3%)	35	37
1	KKK	127/123 (103%)	118 (93%)	9 (7%)	13	8
2	BBB	131/131 (100%)	130 (99%)	1 (1%)	73	79
2	DDD	131/131 (100%)	128 (98%)	3 (2%)	44	49
2	FFF	130/131 (99%)	129 (99%)	1 (1%)	73	79
2	HHH	130/131 (99%)	129 (99%)	1 (1%)	73	79
2	JJJ	132/131 (101%)	131 (99%)	1 (1%)	73	79
2	LLL	130/131 (99%)	128 (98%)	2 (2%)	57	64
All	All	1543/1524 (101%)	1511 (98%)	32 (2%)	51	52

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KKK	123	ASP
1	KKK	127	SER
2	FFF	28	SER
1	EEE	50	ARG
2	LLL	29	LYS

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	DDD	72	2	7,8,9	0.92	1 (14%)	4,9,11	0.60	0
2	MEN	LLL	72	2	7,8,9	0.84	1 (14%)	4,9,11	0.23	0
2	MEN	BBB	72	2	7,8,9	0.85	1 (14%)	4,9,11	0.91	0
2	MEN	HHH	72	2	7,8,9	0.71	0	4,9,11	0.30	0
2	MEN	FFF	72	2	7,8,9	0.71	0	4,9,11	0.33	0
2	MEN	JJJ	72	2	7,8,9	0.68	0	4,9,11	0.31	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	DDD	72	2	-	2/7/8/10	-
2	MEN	LLL	72	2	-	5/7/8/10	-
2	MEN	BBB	72	2	-	2/7/8/10	-
2	MEN	HHH	72	2	-	3/7/8/10	-
2	MEN	FFF	72	2	-	2/7/8/10	-
2	MEN	JJJ	72	2	-	4/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	72	MEN	O-C	2.18	1.28	1.20
2	LLL	72	MEN	O-C	2.18	1.28	1.20
2	BBB	72	MEN	O-C	2.11	1.28	1.20

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	72	MEN	O-C-CA-CB
2	JJJ	72	MEN	CB-CG-ND2-CE2
2	LLL	72	MEN	O-C-CA-CB
2	LLL	72	MEN	CB-CG-ND2-CE2
2	JJJ	72	MEN	OD1-CG-ND2-CE2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	72	MEN	1	0
2	HHH	72	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 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	A1JTN	III	202	1	0,1,21	-	-	-		
3	CYC	KKK	201	-	46,46,46	1.00	1 (2%)	63,67,67	1.11	3 (4%)
4	A1JTN	EEE	203	1	0,1,21	-	-	-		
4	A1JTN	AAA	202	1	0,1,21	-	-	-		
3	CYC	JJJ	202	-	46,46,46	0.88	2 (4%)	63,67,67	1.15	4 (6%)
3	CYC	BBB	202	-	46,46,46	0.85	1 (2%)	63,67,67	1.31	8 (12%)
3	CYC	CCC	201	-	46,46,46	0.82	0	63,67,67	1.15	4 (6%)
3	CYC	GGG	201	-	46,46,46	1.05	3 (6%)	63,67,67	1.10	2 (3%)
3	CYC	BBB	203	-	46,46,46	0.95	1 (2%)	63,67,67	1.09	4 (6%)
4	A1JTN	HHH	201	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.36	0
4	A1JTN	BBB	201	2,6	4,21,21	1.46	1 (25%)	4,40,40	1.75	1 (25%)
4	A1JTN	KKK	202	1	0,1,21	-	-	-		
5	ACT	FFF	501	-	3,3,3	1.41	0	3,3,3	0.56	0
4	A1JTN	JJJ	201	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.55	1 (25%)
3	CYC	LLL	202	-	46,46,46	0.85	1 (2%)	63,67,67	1.10	4 (6%)
4	A1JTN	LLL	201	2,6	4,21,21	1.48	1 (25%)	4,40,40	1.84	1 (25%)
3	CYC	HHH	202	-	46,46,46	0.82	0	63,67,67	1.26	6 (9%)
3	CYC	HHH	203	-	46,46,46	0.80	1 (2%)	63,67,67	1.00	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JTN	GGG	203	1	0,1,21	-	-	-		
3	CYC	DDD	202	-	46,46,46	1.01	4 (8%)	63,67,67	1.26	5 (7%)
4	A1JTN	CCC	202	1	0,1,21	-	-	-		
3	CYC	JJJ	203	-	46,46,46	0.76	2 (4%)	63,67,67	1.11	3 (4%)
3	CYC	EEE	201	-	46,46,46	0.95	3 (6%)	63,67,67	1.03	3 (4%)
4	A1JTN	FFF	502	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.38	1 (25%)
3	CYC	AAA	201	-	46,46,46	0.92	3 (6%)	63,67,67	1.08	1 (1%)
3	CYC	FFF	504	-	46,46,46	0.75	0	63,67,67	1.03	2 (3%)
3	CYC	DDD	203	-	46,46,46	0.88	2 (4%)	63,67,67	0.99	5 (7%)
3	CYC	III	201	-	46,46,46	1.23	3 (6%)	63,67,67	1.20	6 (9%)
4	A1JTN	DDD	201	2,6	4,21,21	1.49	1 (25%)	4,40,40	1.94	1 (25%)
3	CYC	FFF	503	-	46,46,46	0.79	0	63,67,67	1.31	5 (7%)
5	ACT	EEE	202	-	3,3,3	1.13	0	3,3,3	0.75	0
3	CYC	LLL	203	-	46,46,46	0.73	0	63,67,67	1.09	3 (4%)
5	ACT	GGG	202	-	3,3,3	1.03	0	3,3,3	1.39	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
3	CYC	KKK	201	-	-	10/26/74/74	0/4/4/4
3	CYC	JJJ	202	-	-	8/26/74/74	0/4/4/4
3	CYC	BBB	202	-	-	12/26/74/74	0/4/4/4
3	CYC	CCC	201	-	-	7/26/74/74	0/4/4/4
3	CYC	GGG	201	-	-	11/26/74/74	0/4/4/4
3	CYC	BBB	203	-	-	9/26/74/74	0/4/4/4
4	A1JTN	HHH	201	2,6	-	-	0/4/4/4
4	A1JTN	BBB	201	2,6	-	-	0/4/4/4
4	A1JTN	JJJ	201	2,6	-	-	0/4/4/4
3	CYC	LLL	202	-	-	7/26/74/74	0/4/4/4
4	A1JTN	LLL	201	2,6	-	-	0/4/4/4
3	CYC	HHH	202	-	-	10/26/74/74	0/4/4/4
3	CYC	HHH	203	-	-	10/26/74/74	0/4/4/4
3	CYC	DDD	202	-	-	8/26/74/74	0/4/4/4
3	CYC	JJJ	203	-	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	EEE	201	-	-	10/26/74/74	0/4/4/4
4	A1JTN	FFF	502	2,6	-	-	0/4/4/4
3	CYC	AAA	201	-	-	9/26/74/74	0/4/4/4
3	CYC	FFF	504	-	-	16/26/74/74	0/4/4/4
3	CYC	DDD	203	-	-	9/26/74/74	0/4/4/4
3	CYC	III	201	-	-	9/26/74/74	0/4/4/4
4	A1JTN	DDD	201	2,6	-	-	0/4/4/4
3	CYC	FFF	503	-	-	10/26/74/74	0/4/4/4
3	CYC	LLL	203	-	-	13/26/74/74	0/4/4/4

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	III	201	CYC	CHD-C4C	4.49	1.43	1.36
3	KKK	201	CYC	CHD-C4C	3.39	1.42	1.36
3	GGG	201	CYC	CHD-C4C	3.36	1.42	1.36
3	III	201	CYC	C1B-C2B	-3.24	1.39	1.45
3	GGG	201	CYC	C1B-NB	3.16	1.43	1.37

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	JJJ	203	CYC	CMB-C2B-C1B	4.87	130.08	124.16
3	FFF	503	CYC	CMB-C2B-C1B	4.40	129.51	124.16
3	BBB	203	CYC	CMB-C2B-C1B	4.35	129.45	124.16
3	HHH	202	CYC	CMB-C2B-C1B	4.25	129.33	124.16
3	CCC	201	CYC	CMB-C2B-C1B	4.11	129.16	124.16

There are no chirality outliers.

5 of 180 torsion outliers are listed below:

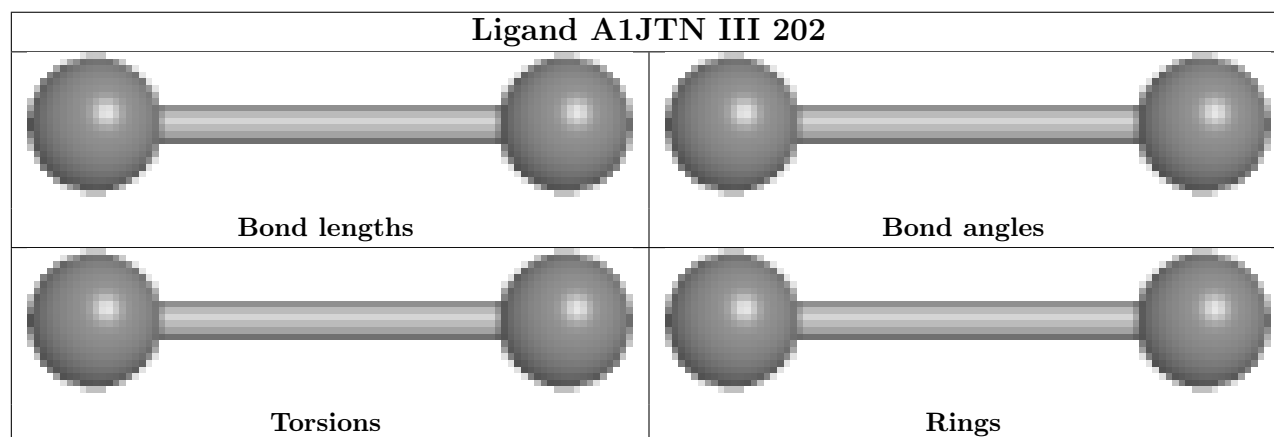
Mol	Chain	Res	Type	Atoms
3	AAA	201	CYC	NA-C4A-CHB-C1B
3	AAA	201	CYC	C3A-C4A-CHB-C1B
3	AAA	201	CYC	NC-C4C-CHD-C1D
3	AAA	201	CYC	C3C-C4C-CHD-C1D
3	BBB	202	CYC	NA-C4A-CHB-C1B

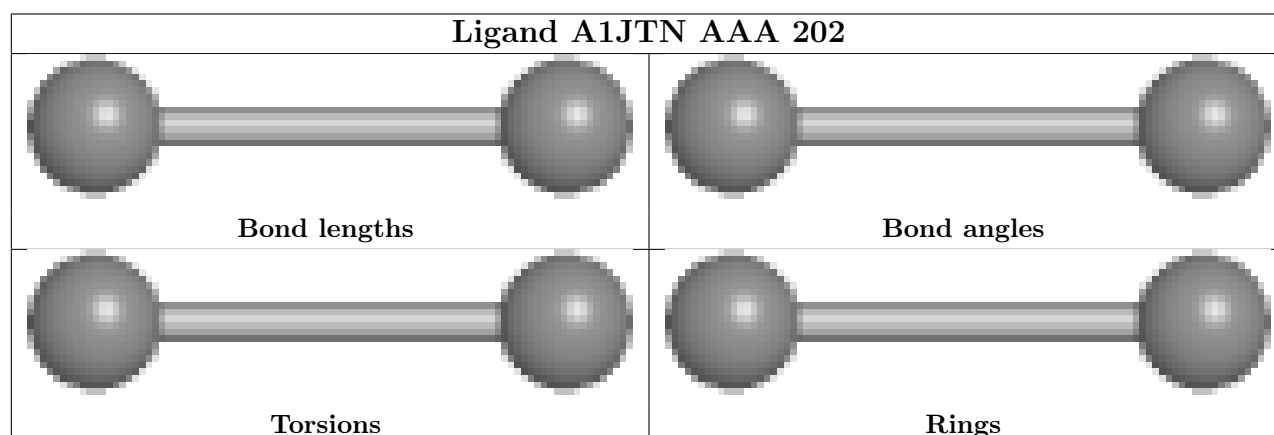
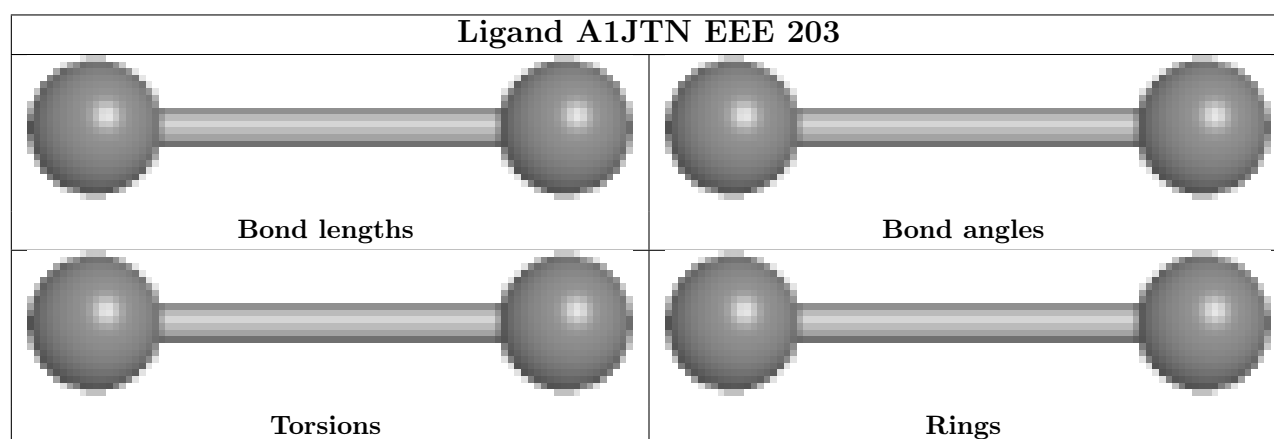
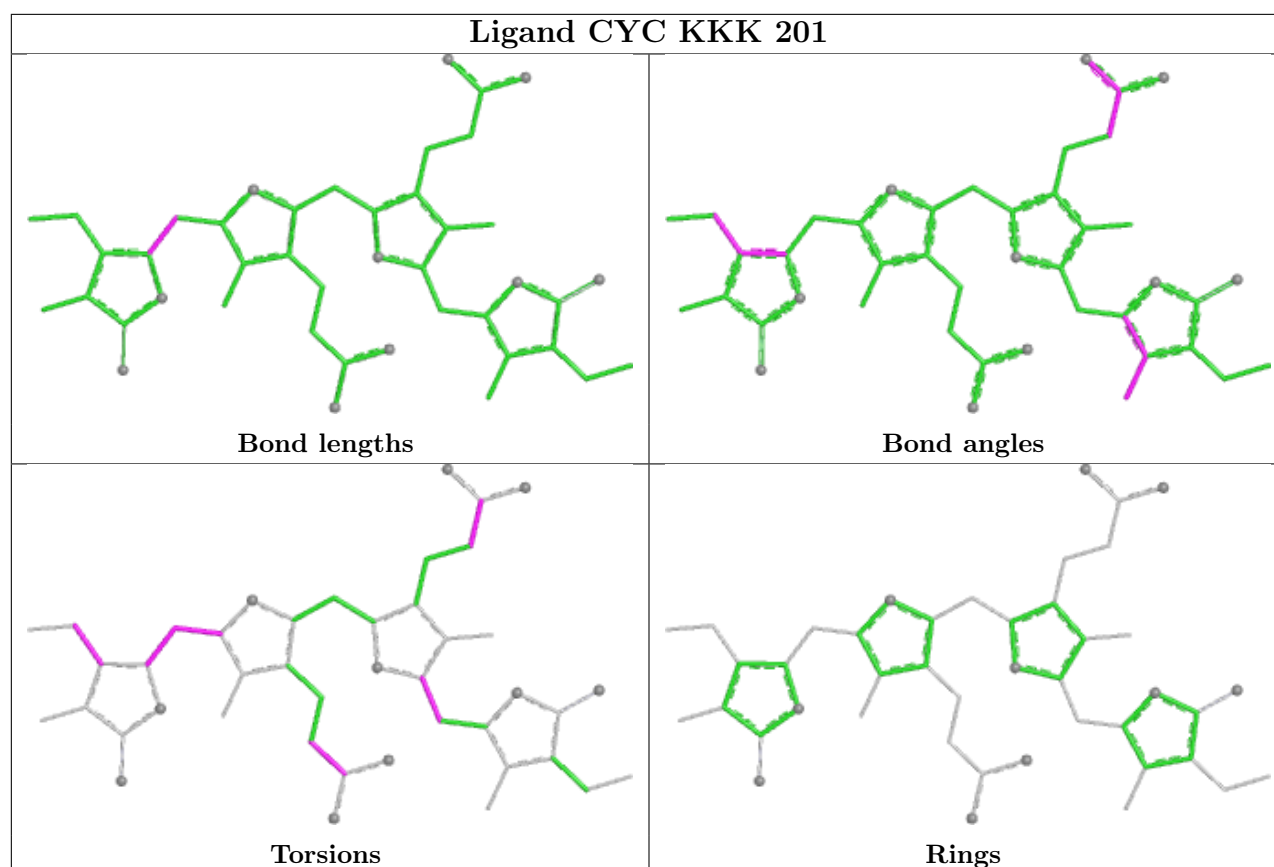
There are no ring outliers.

20 monomers are involved in 140 short contacts:

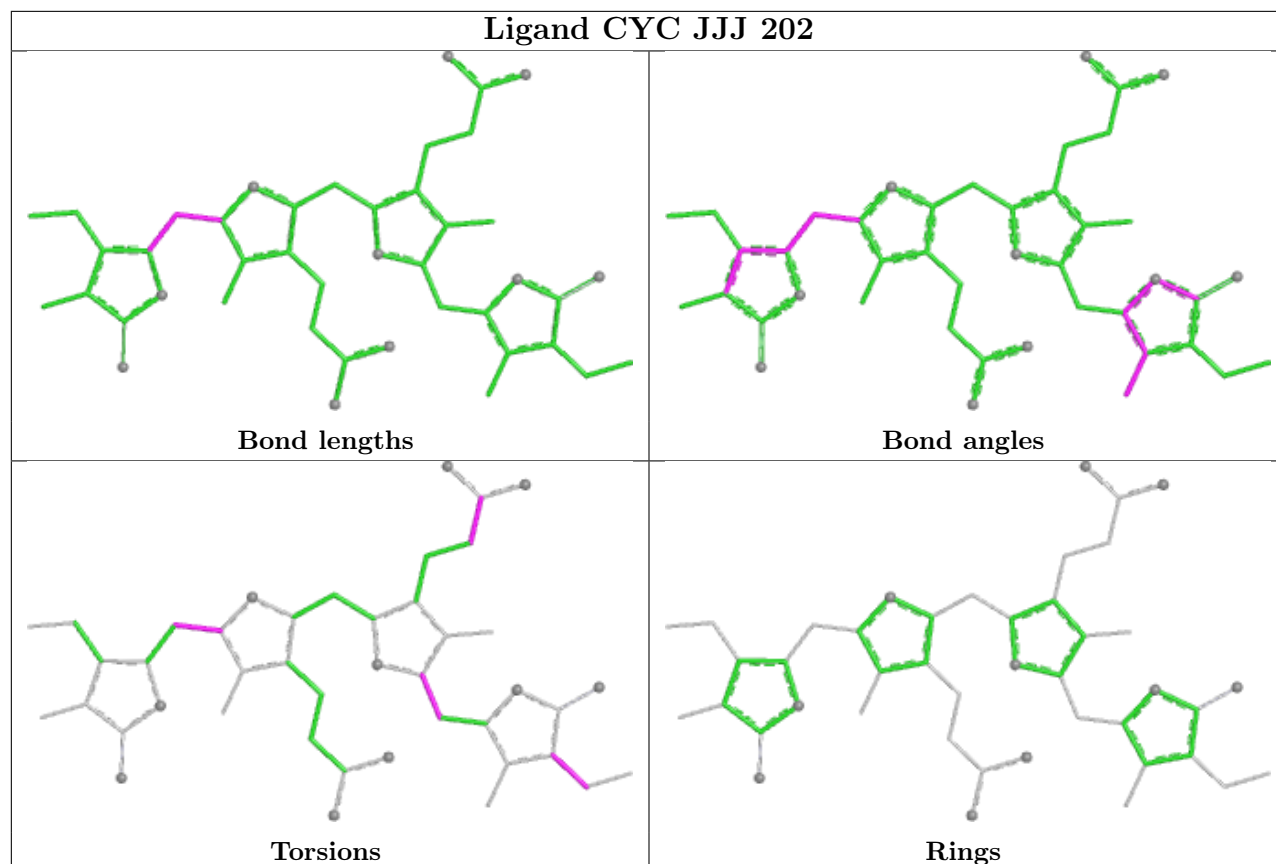
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	KKK	201	CYC	6	0
3	JJJ	202	CYC	9	0
3	BBB	202	CYC	7	0
3	CCC	201	CYC	6	0
3	GGG	201	CYC	8	0
3	BBB	203	CYC	7	0
3	LLL	202	CYC	7	0
4	LLL	201	A1JTN	1	0
3	HHH	202	CYC	12	0
3	HHH	203	CYC	7	0
3	DDD	202	CYC	10	0
3	JJJ	203	CYC	5	0
3	EEE	201	CYC	10	0
3	AAA	201	CYC	8	0
3	FFF	504	CYC	9	0
3	DDD	203	CYC	7	0
3	III	201	CYC	3	0
4	DDD	201	A1JTN	1	0
3	FFF	503	CYC	9	0
3	LLL	203	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.

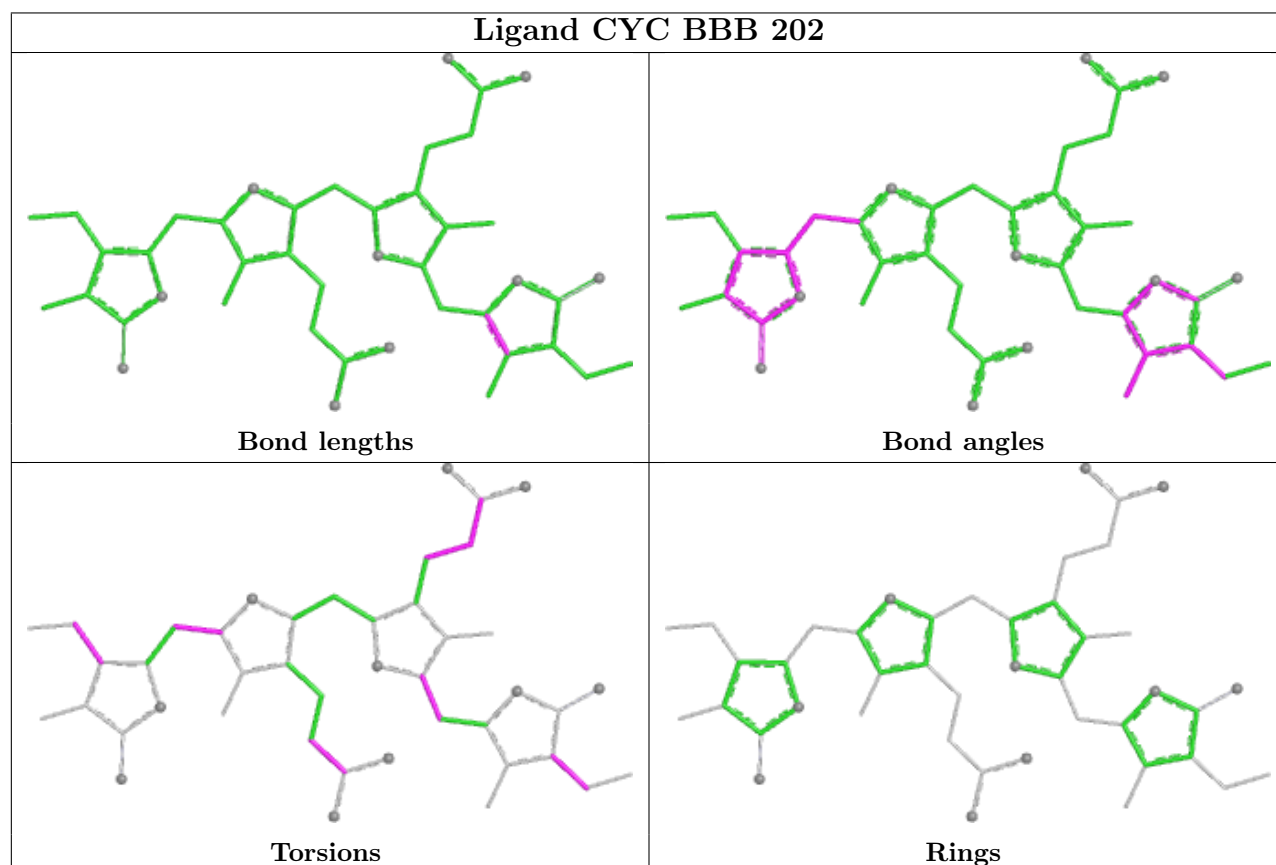


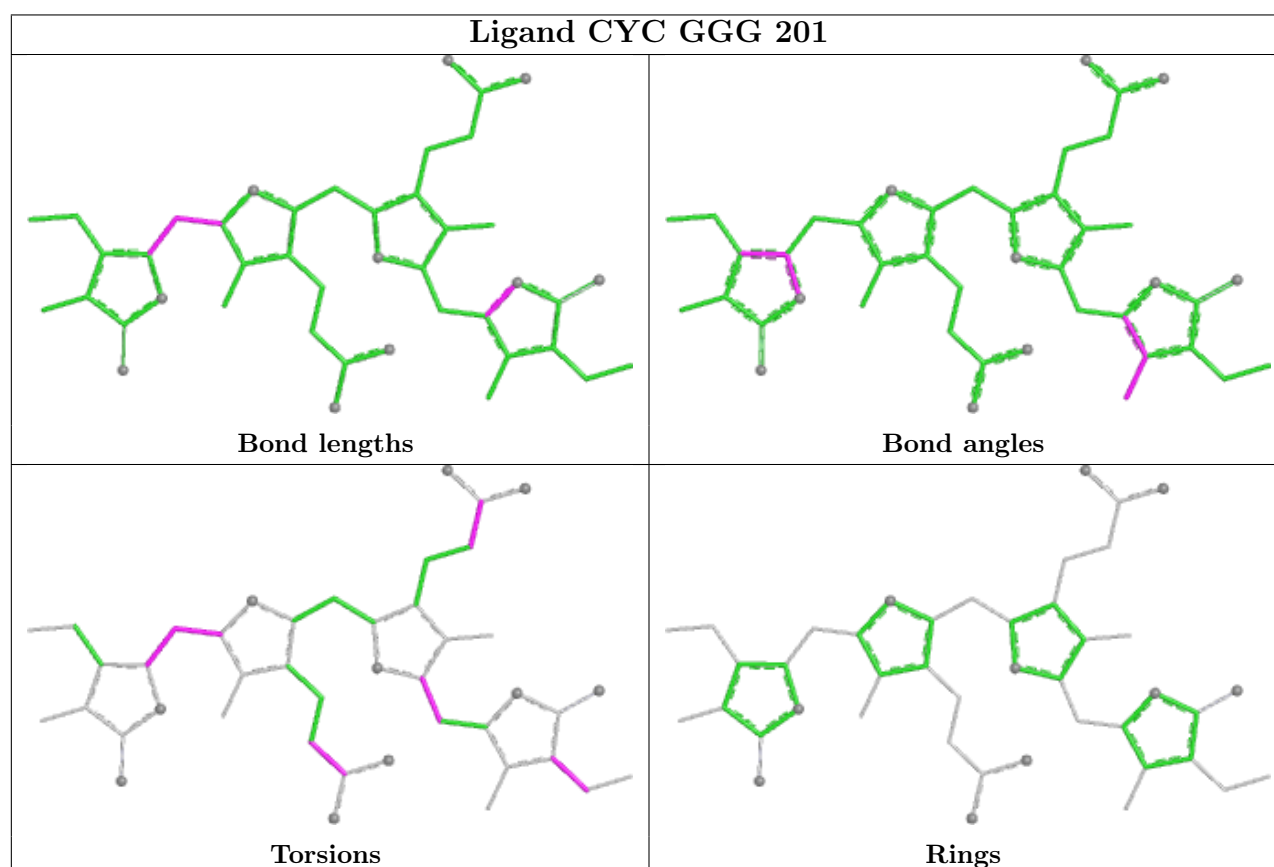
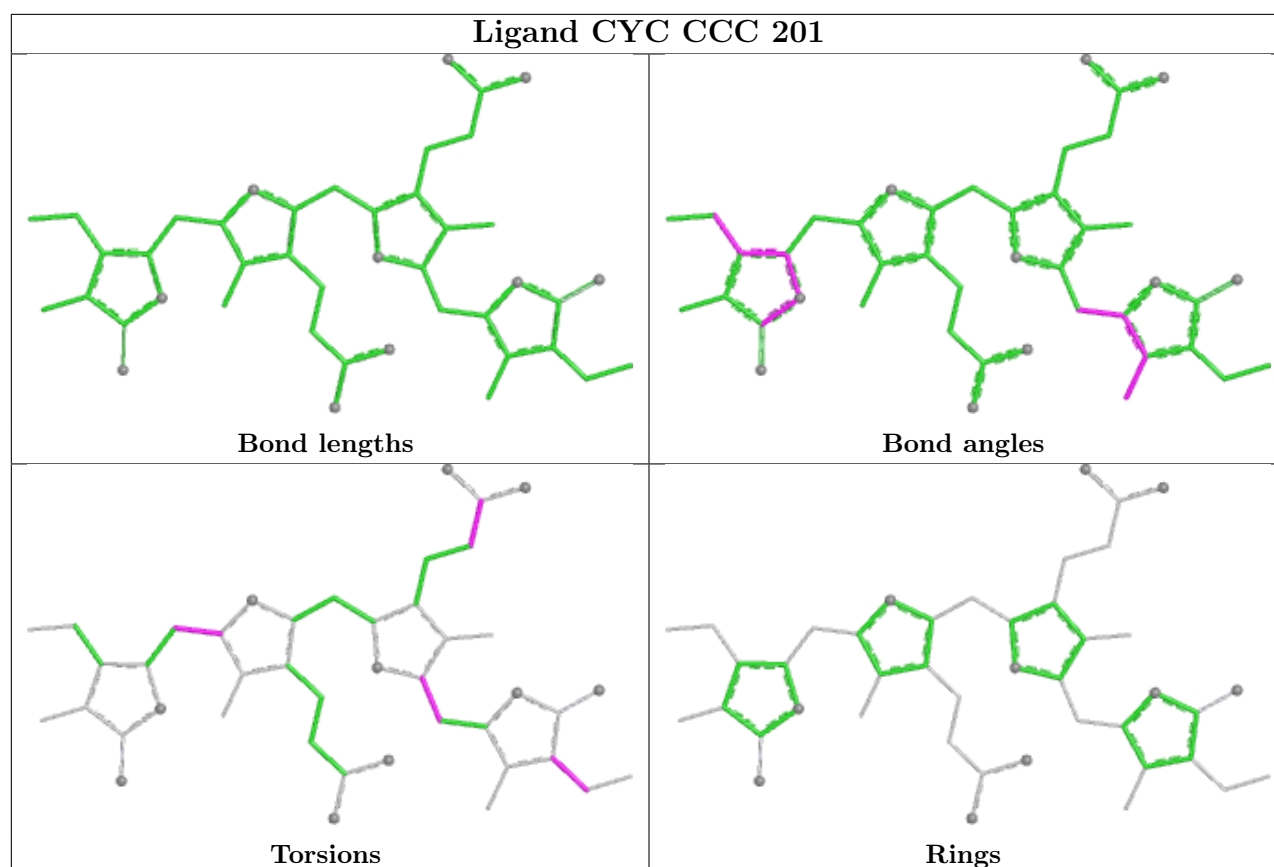


Ligand CYC JJJ 202

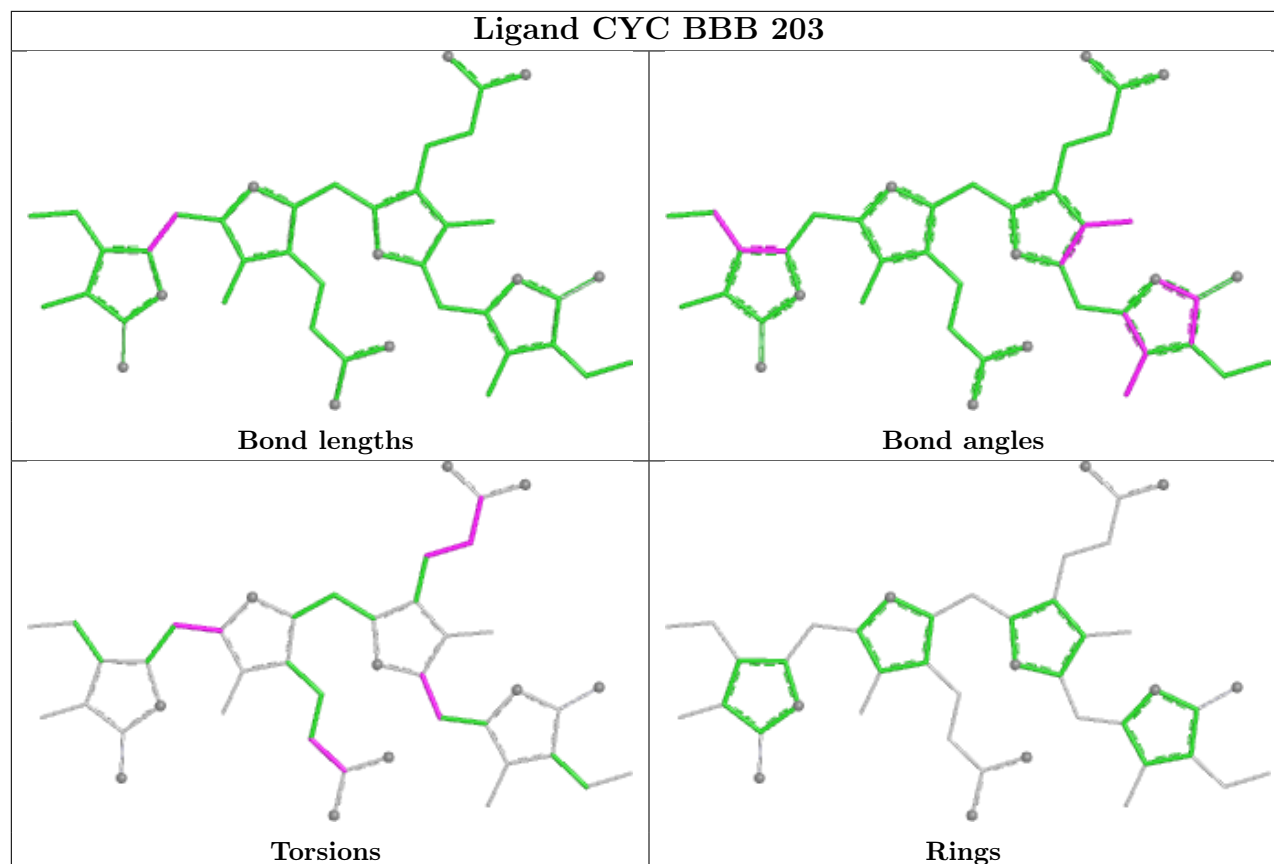


Ligand CYC BBB 202

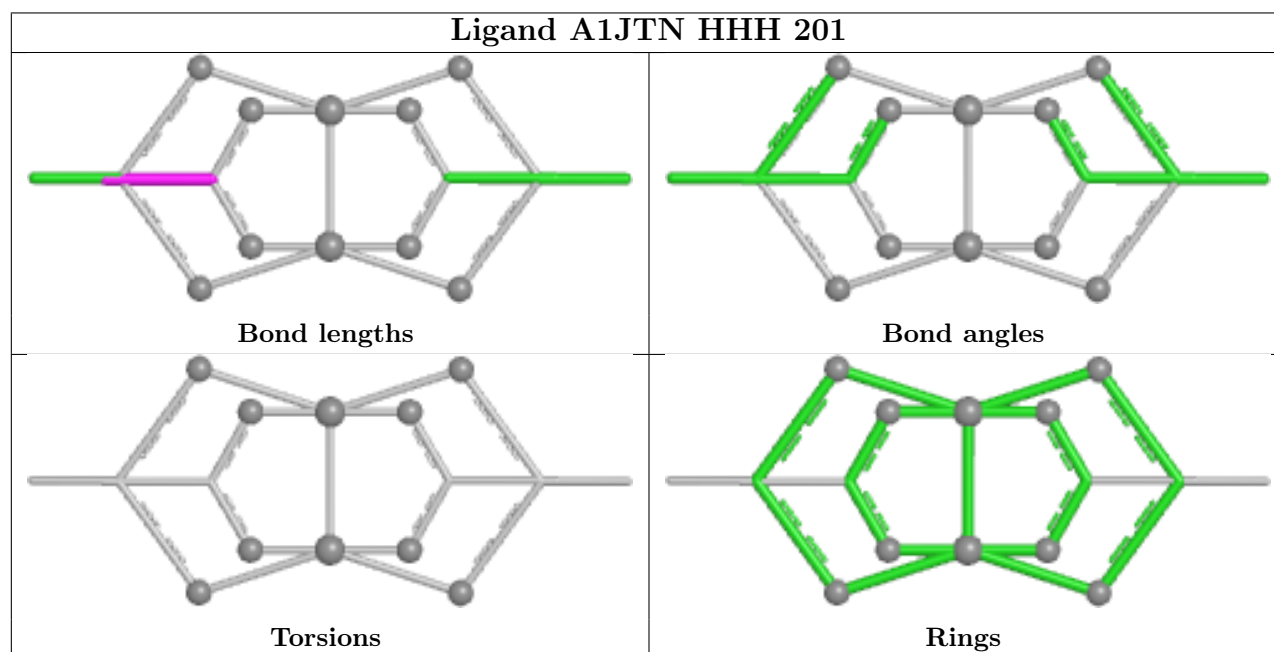


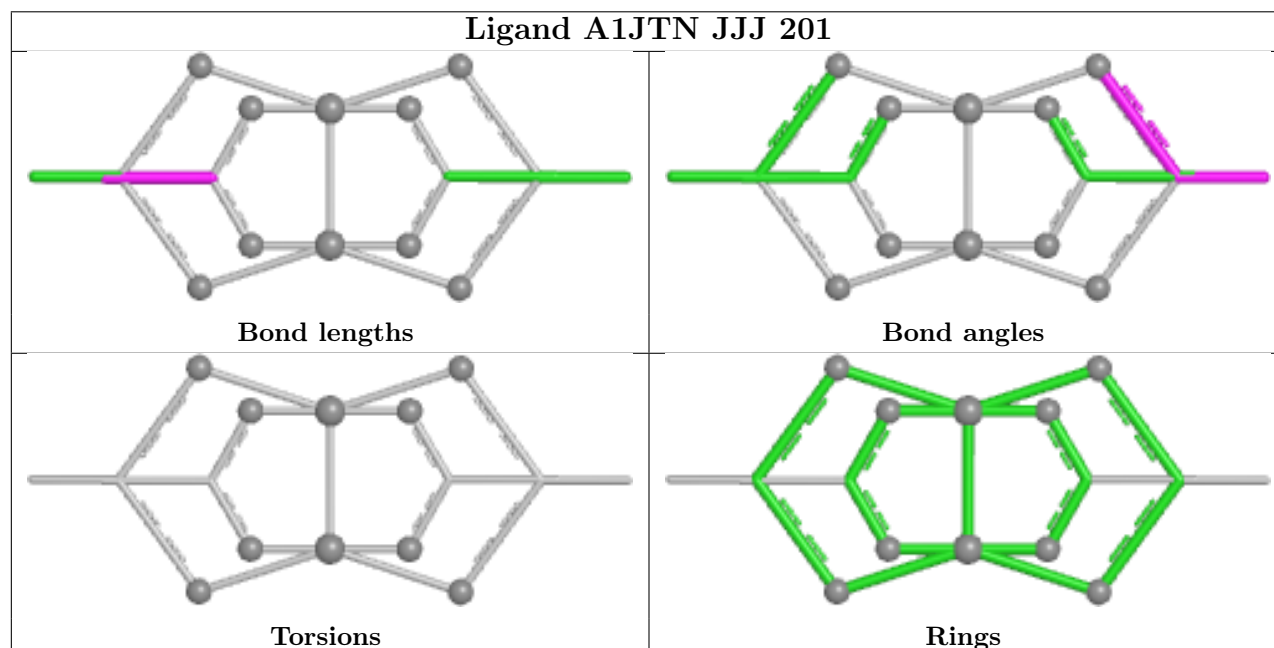
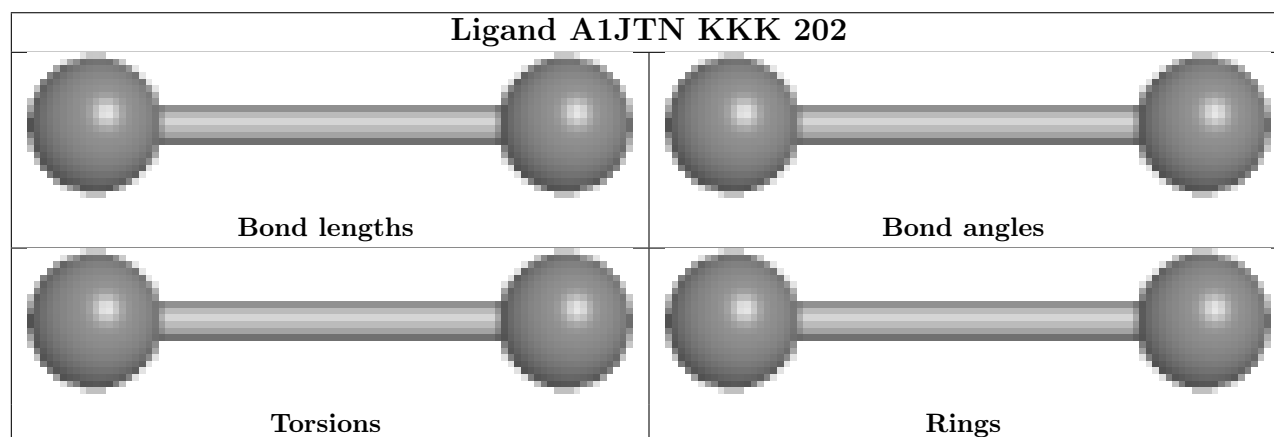
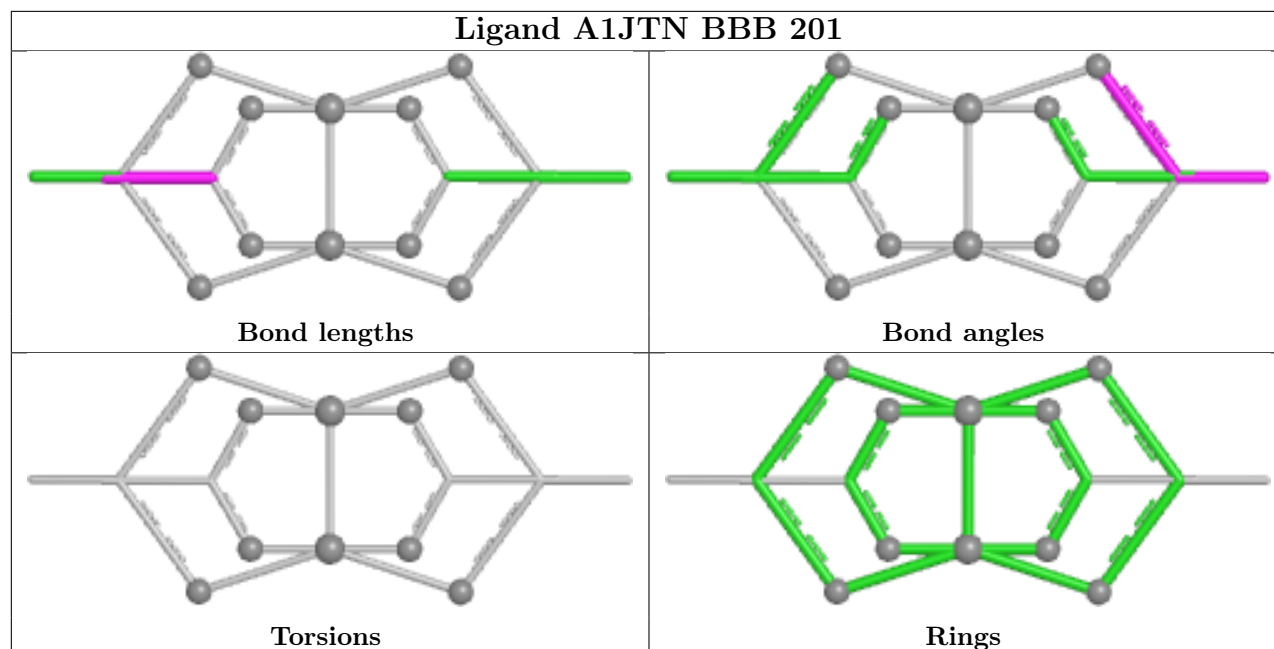


Ligand CYC BBB 203

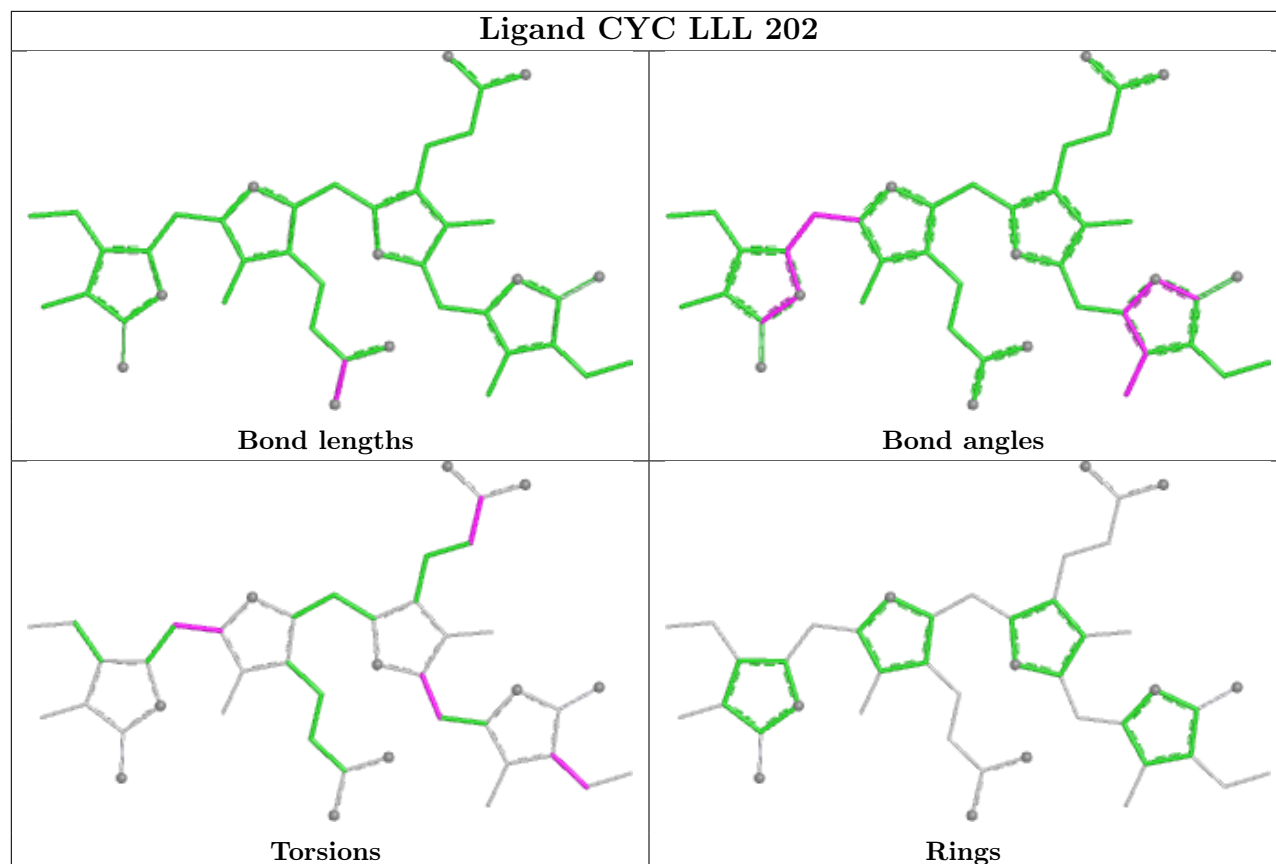


Ligand A1JTN HHH 201

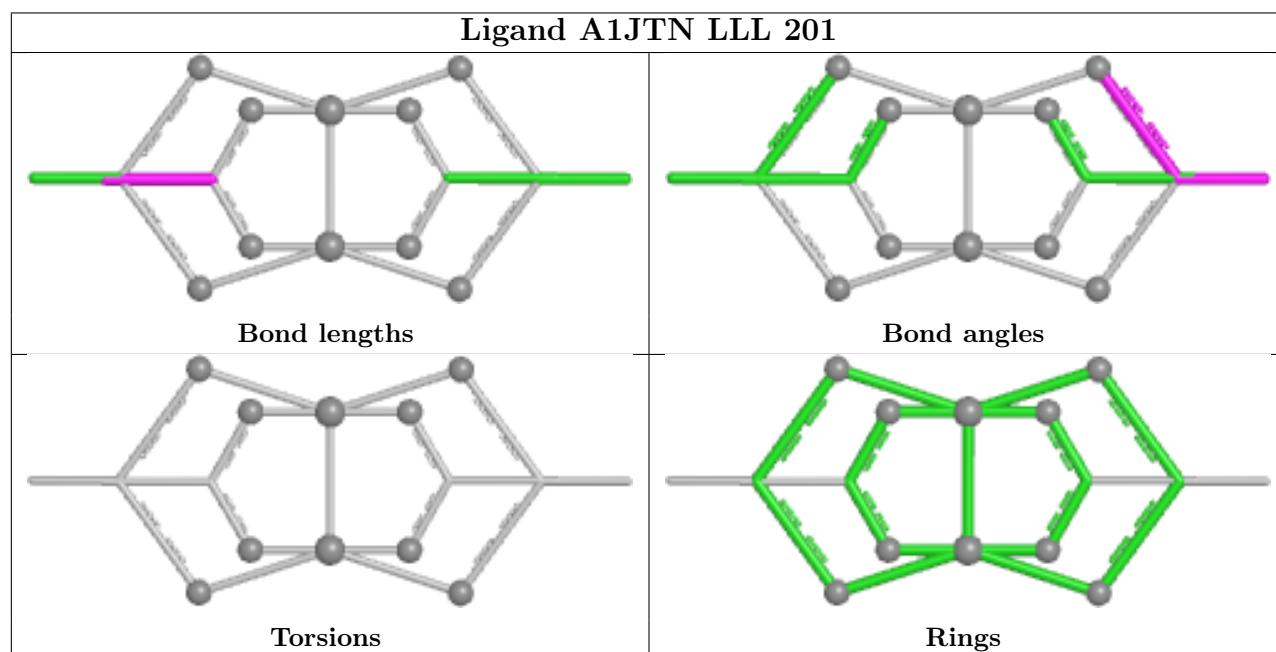




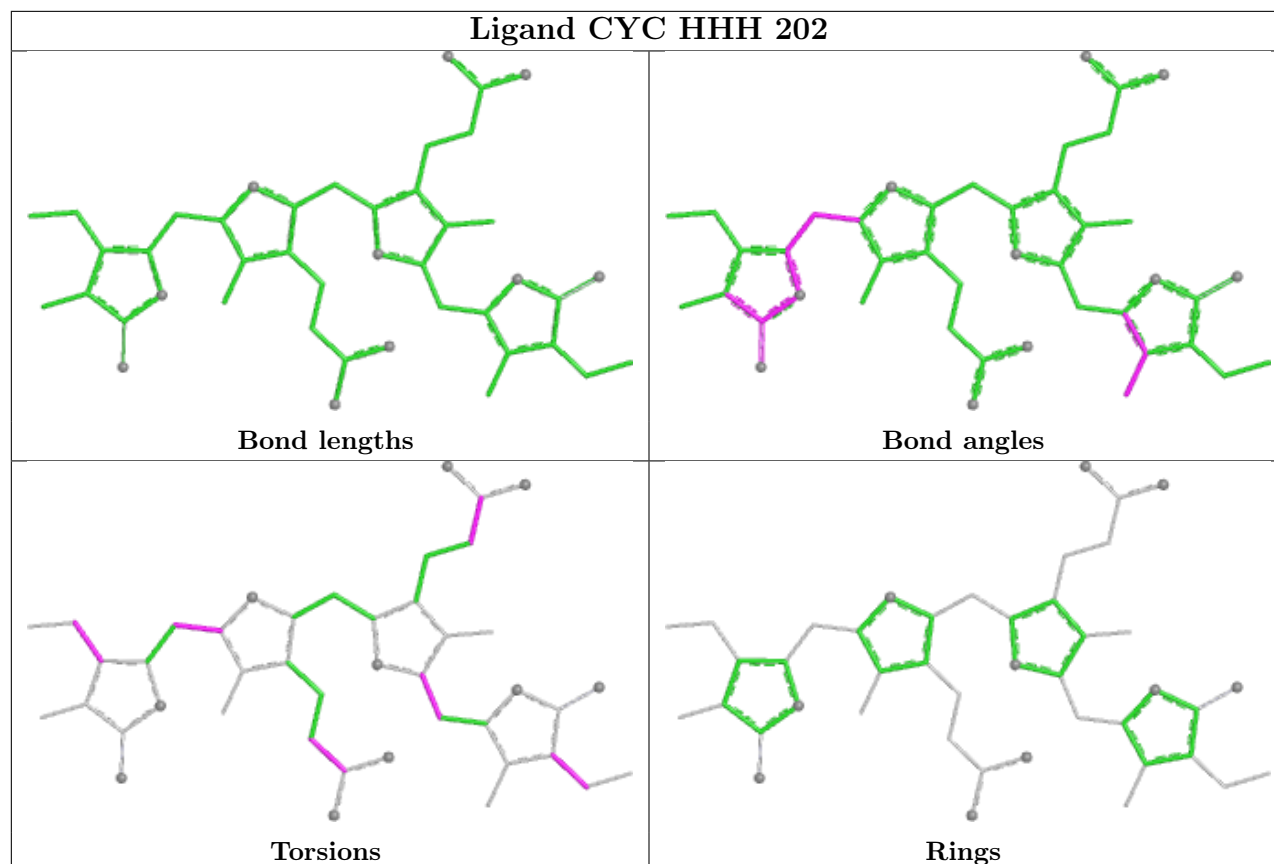
Ligand CYC LLL 202



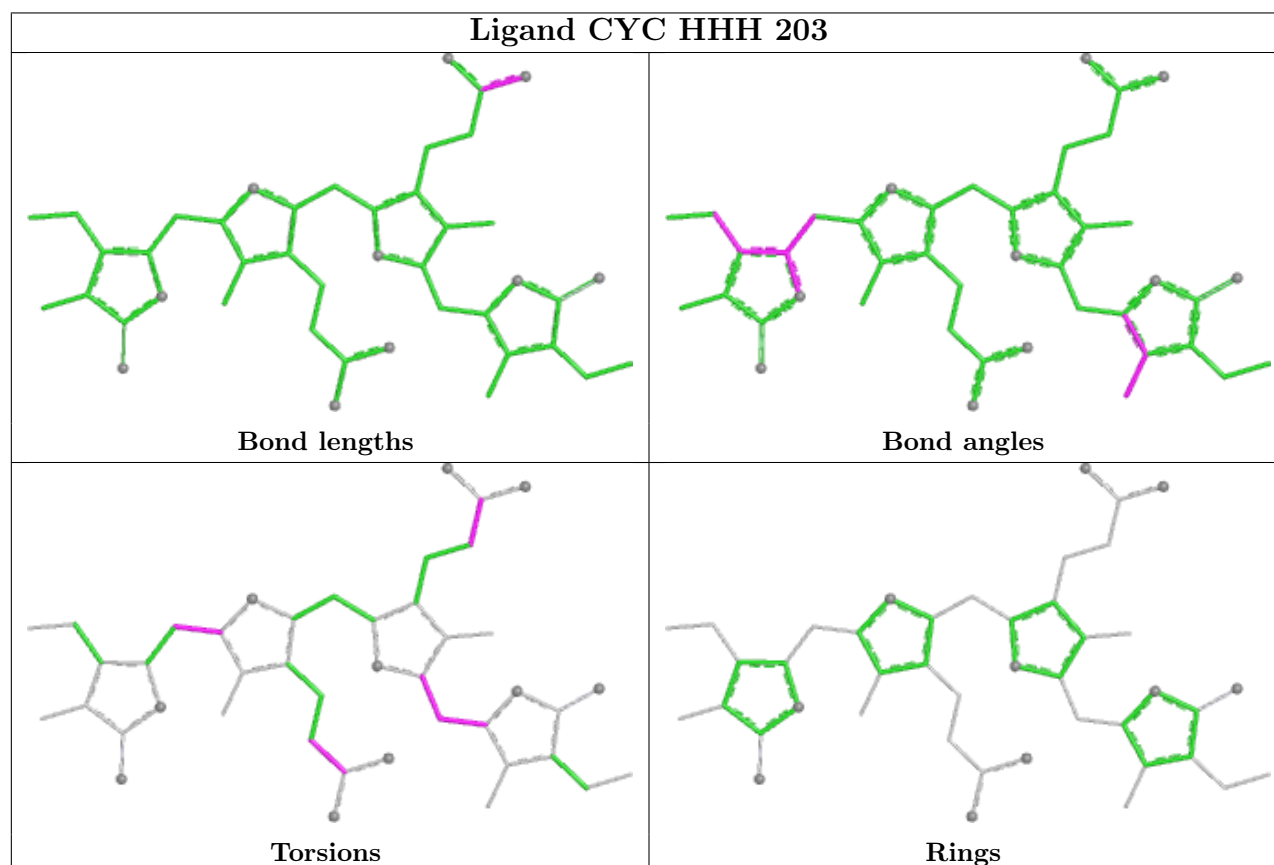
Ligand A1JTN LLL 201

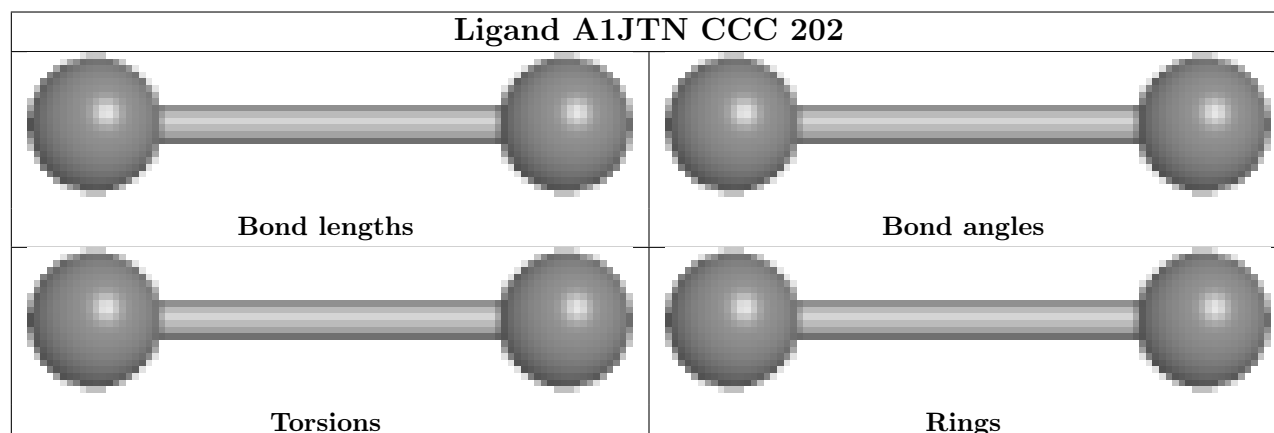
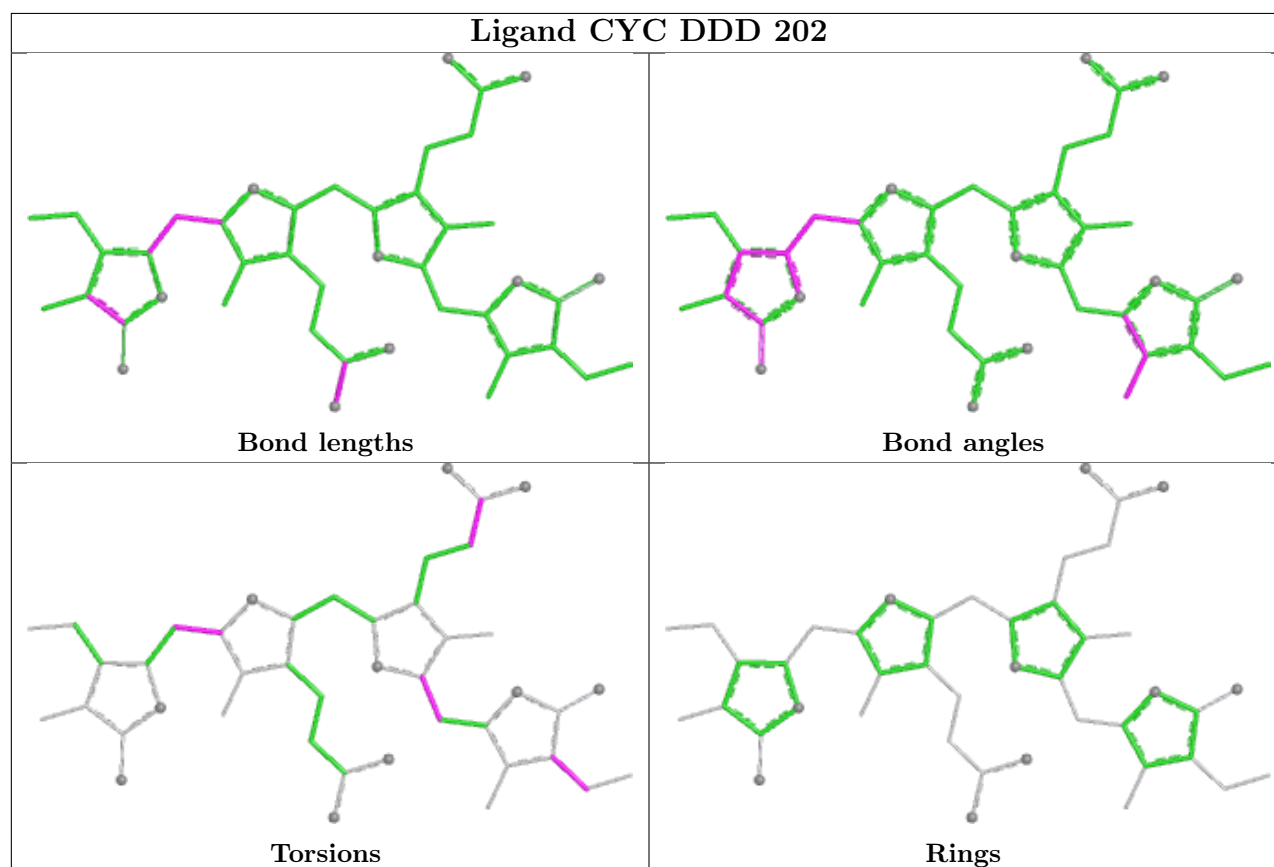
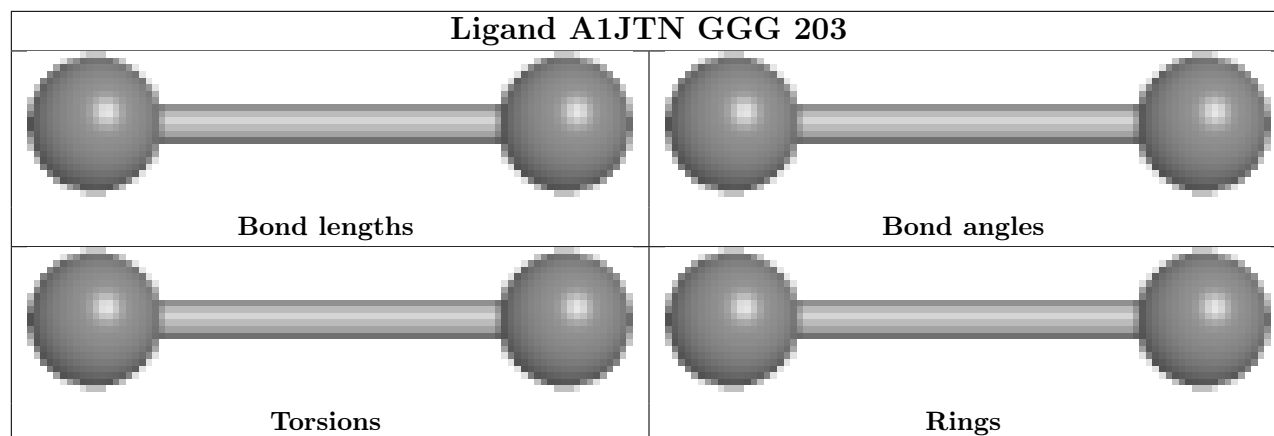


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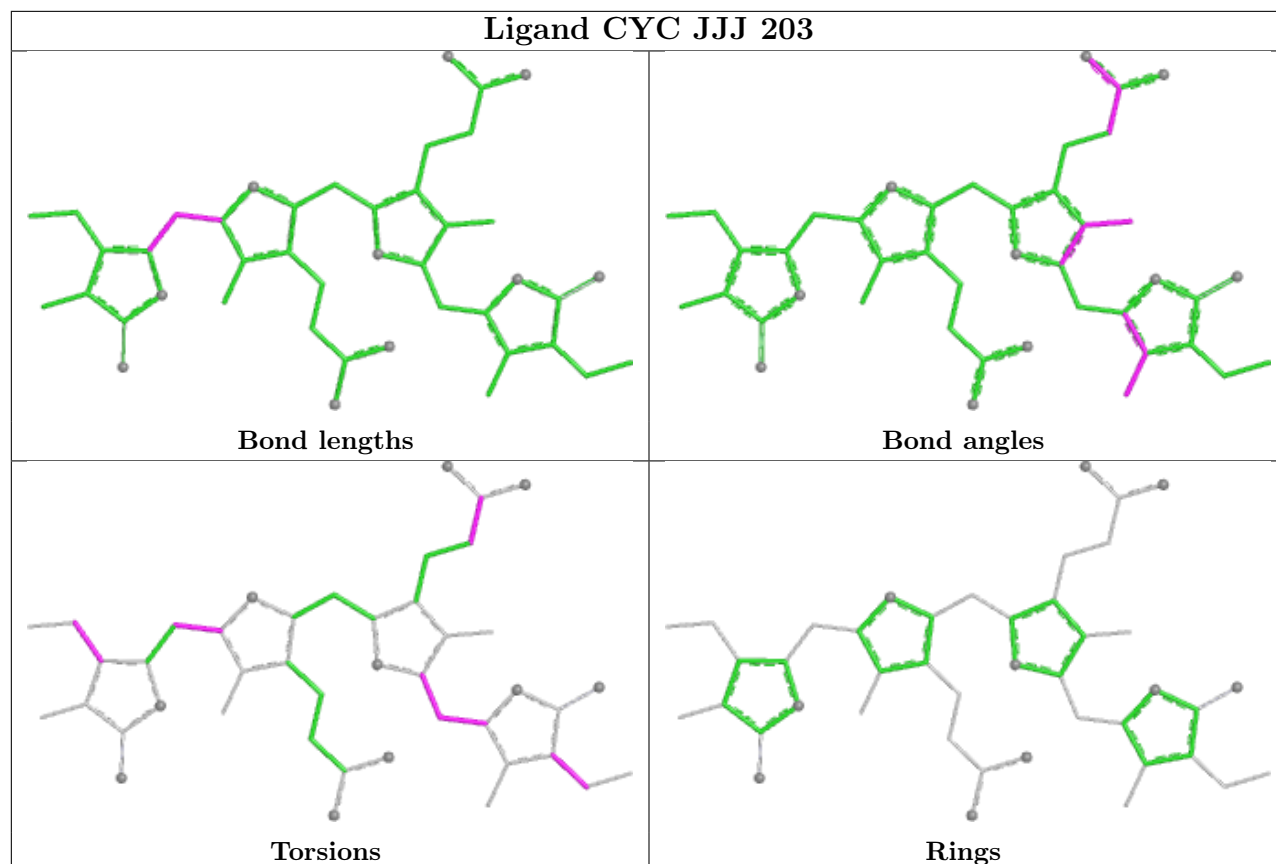


Ligand CYC HHH 203

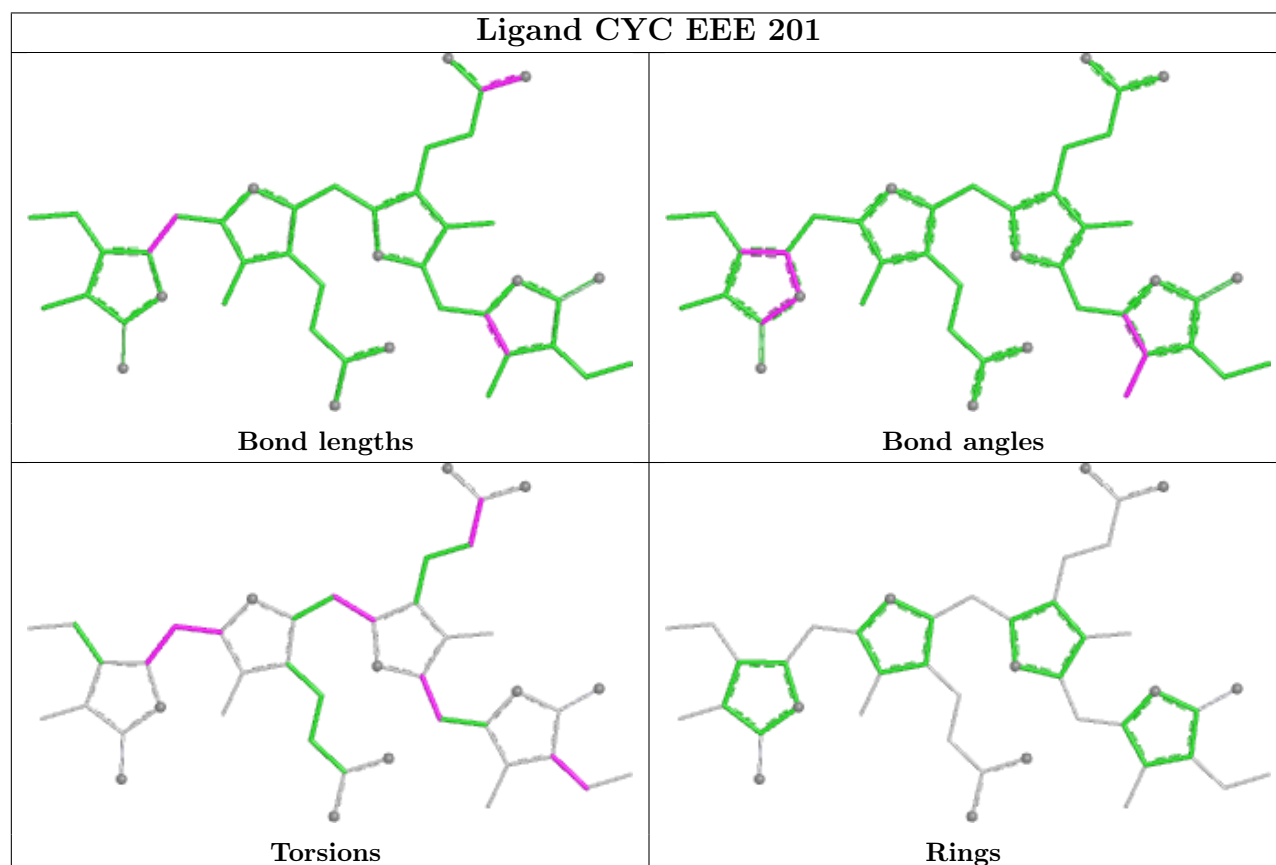


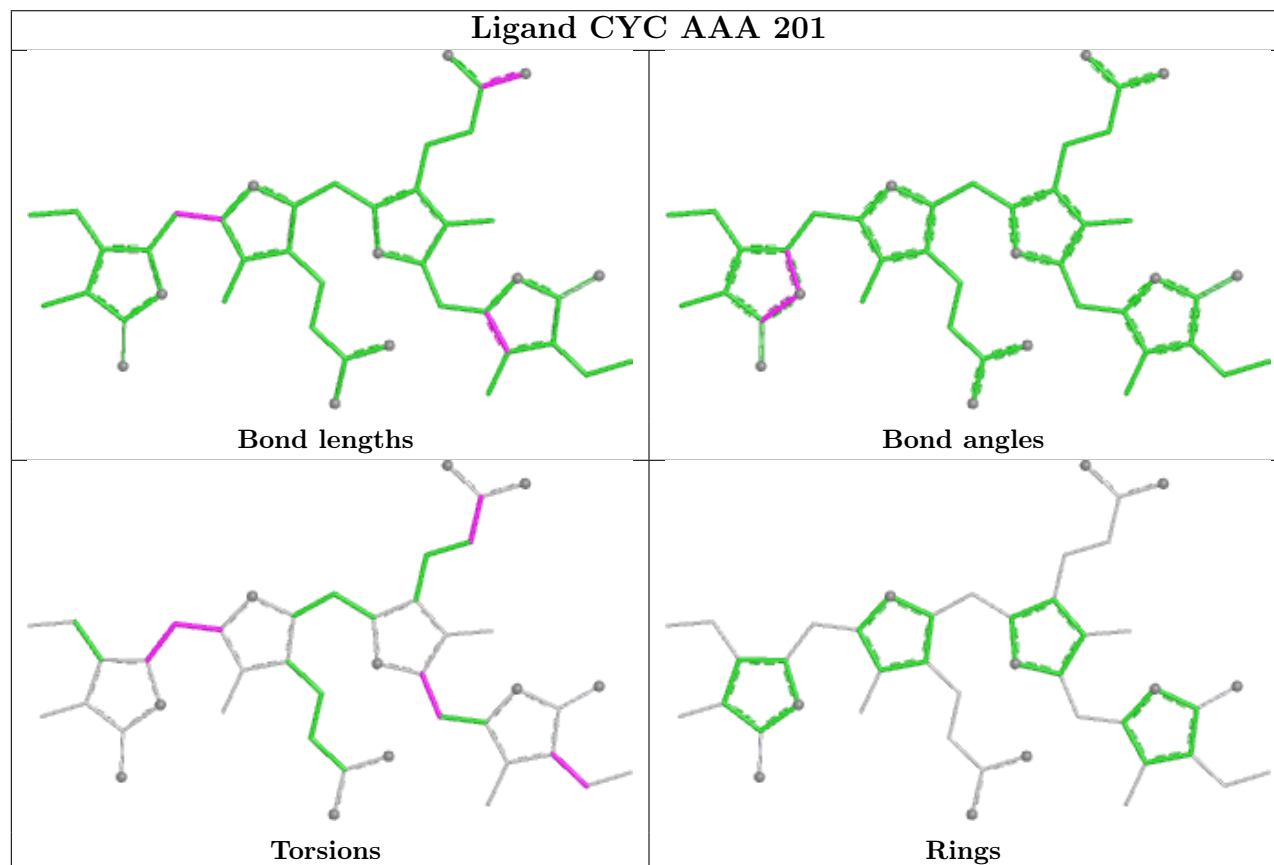
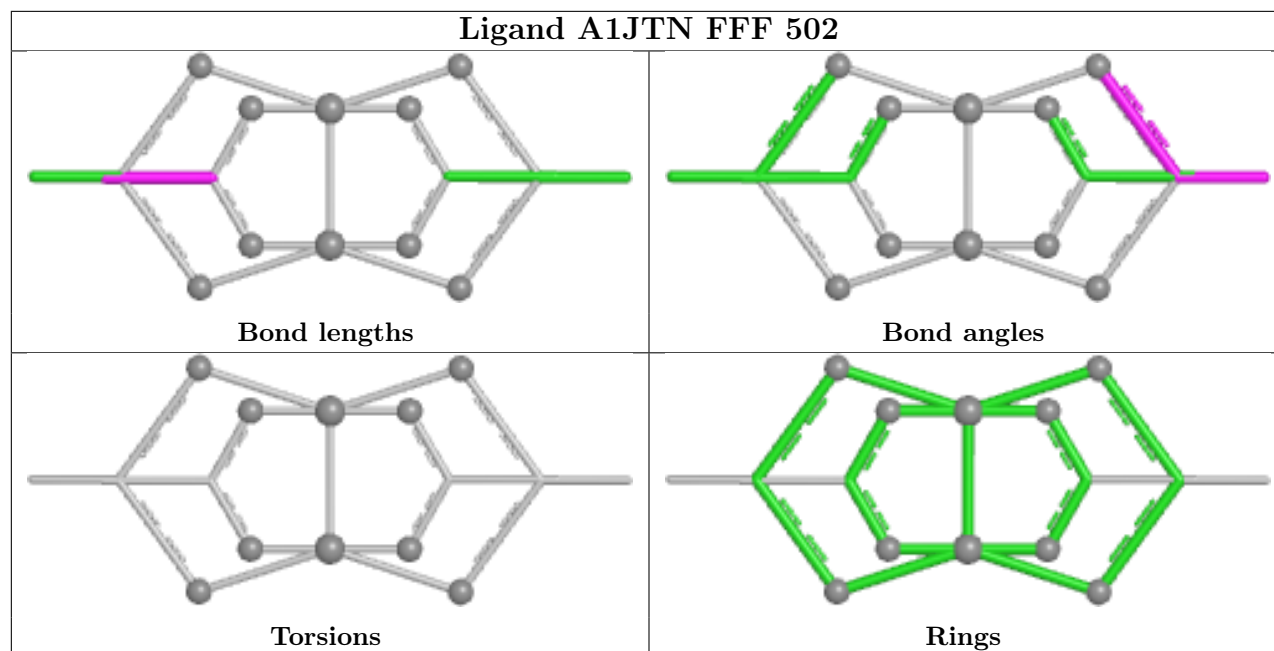


Ligand CYC JJJ 203

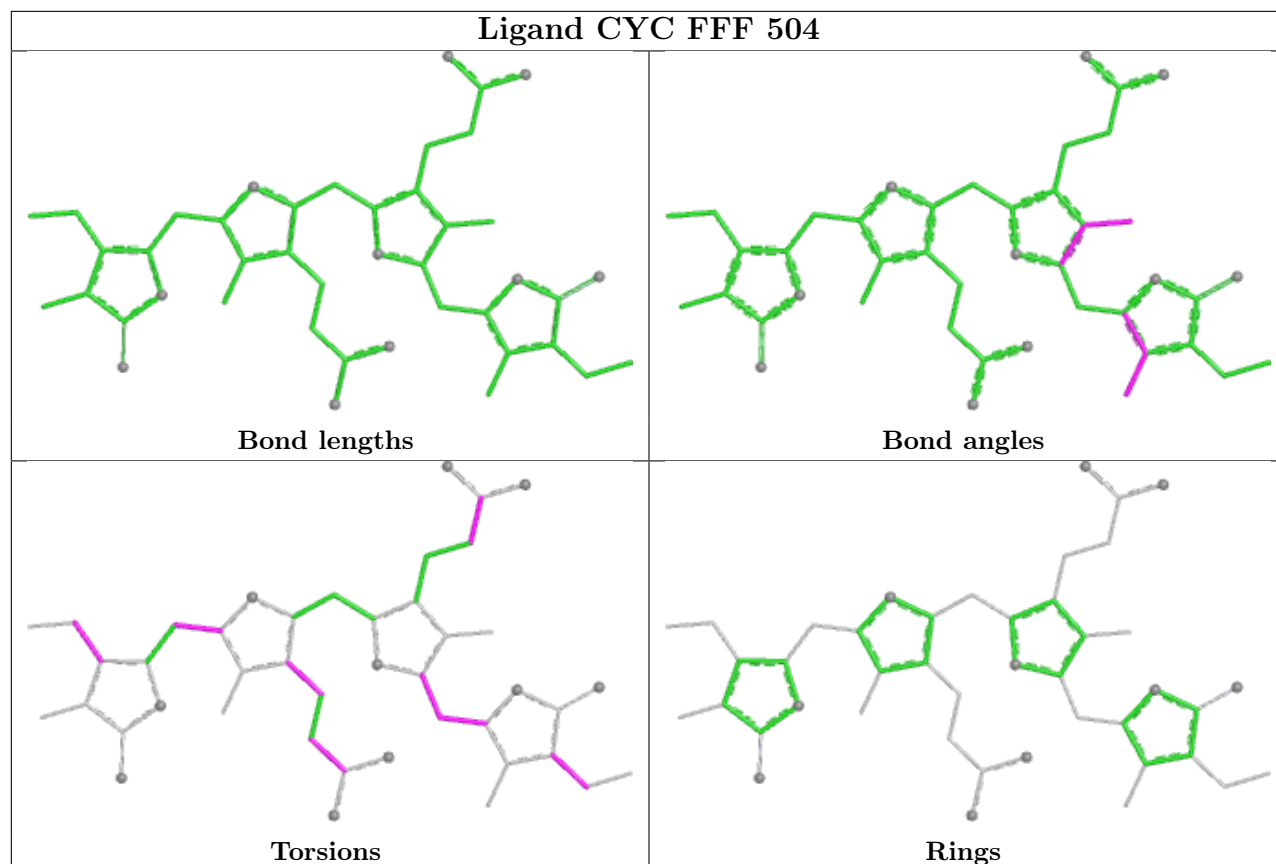


Ligand CYC EEE 201

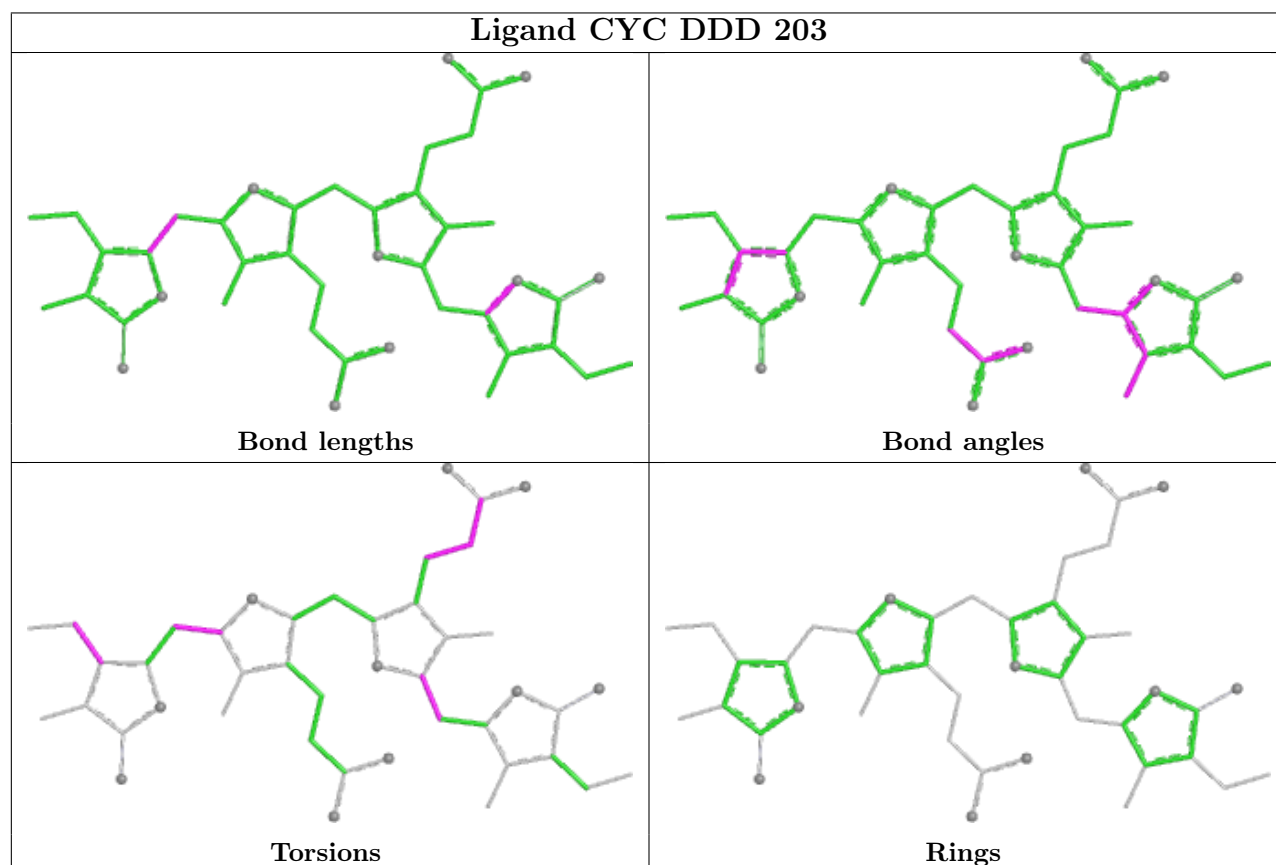




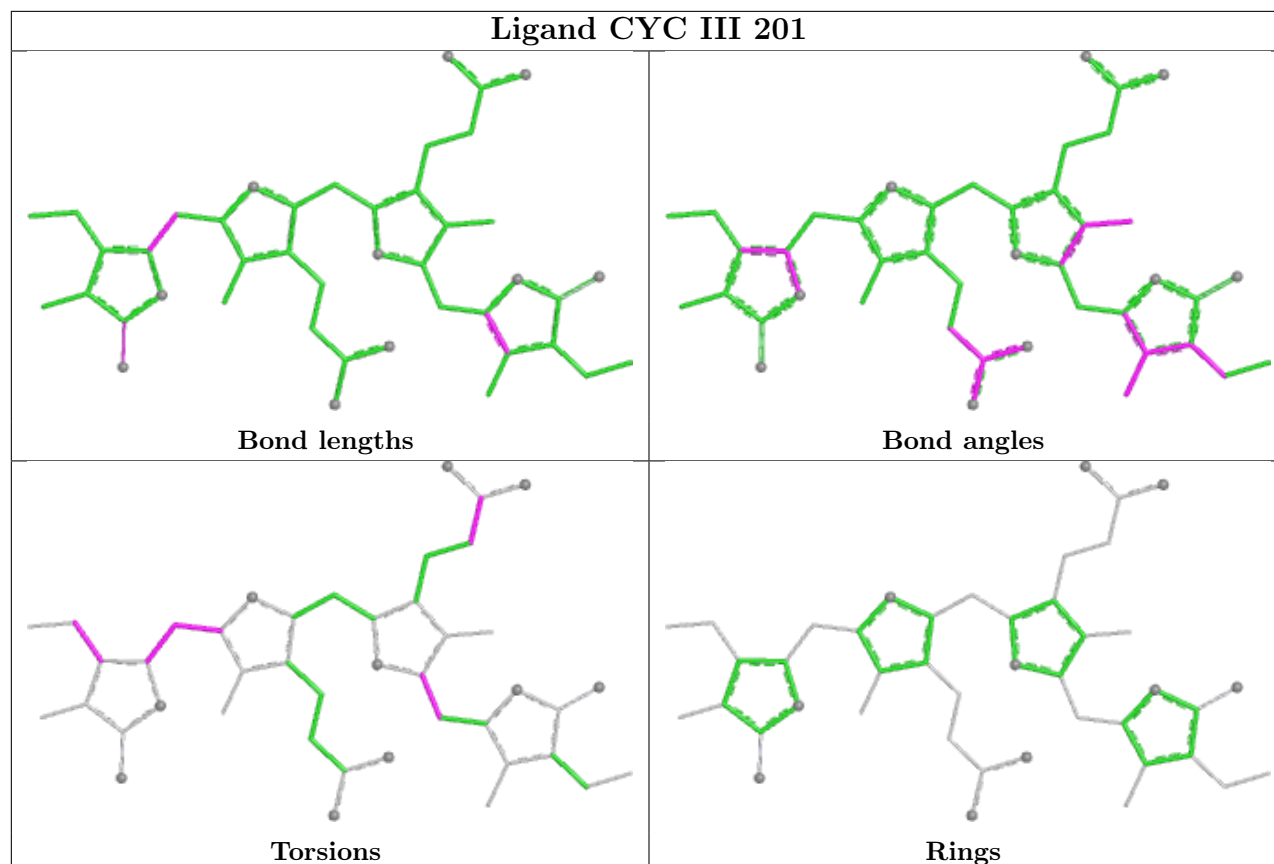
Ligand CYC FFF 504



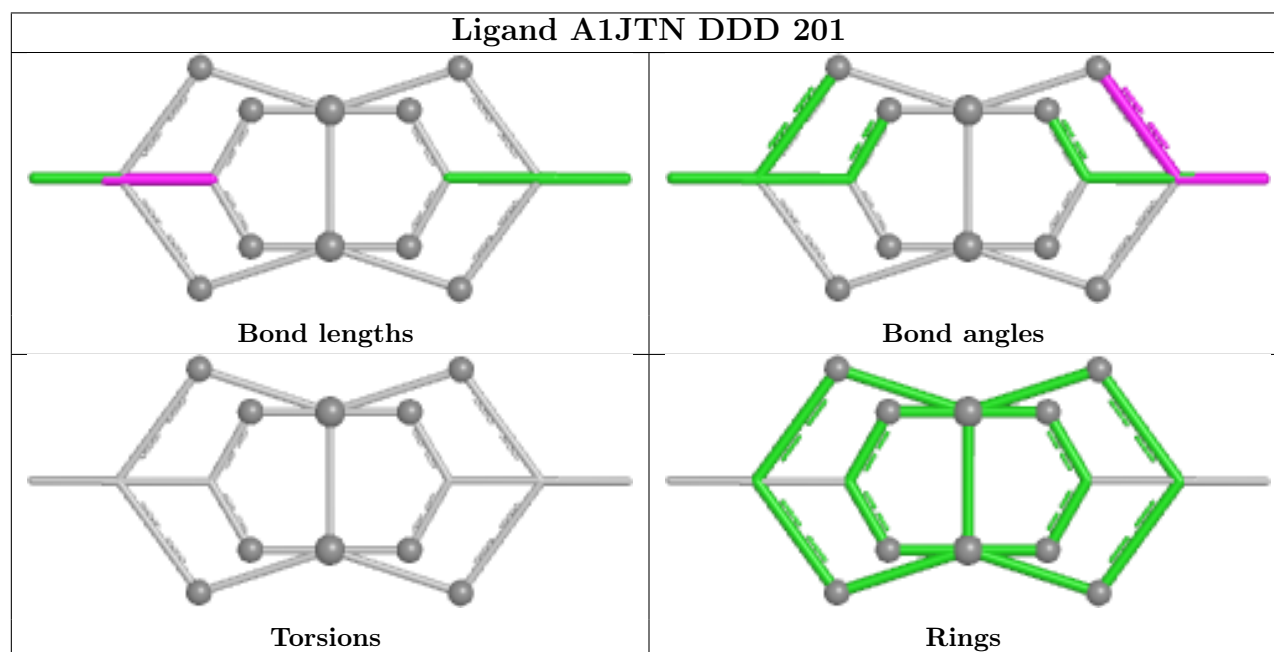
Ligand CYC DDD 203



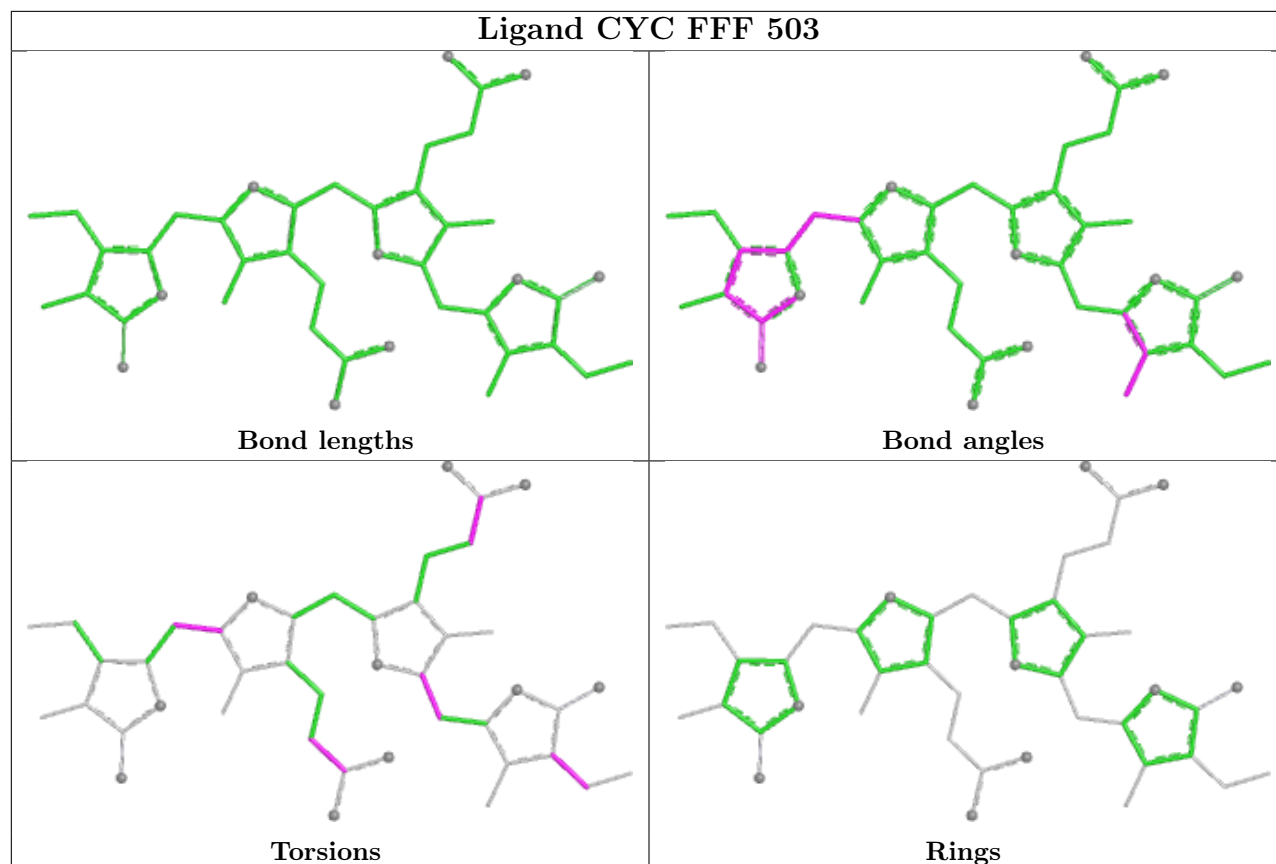
Ligand CYC III 201



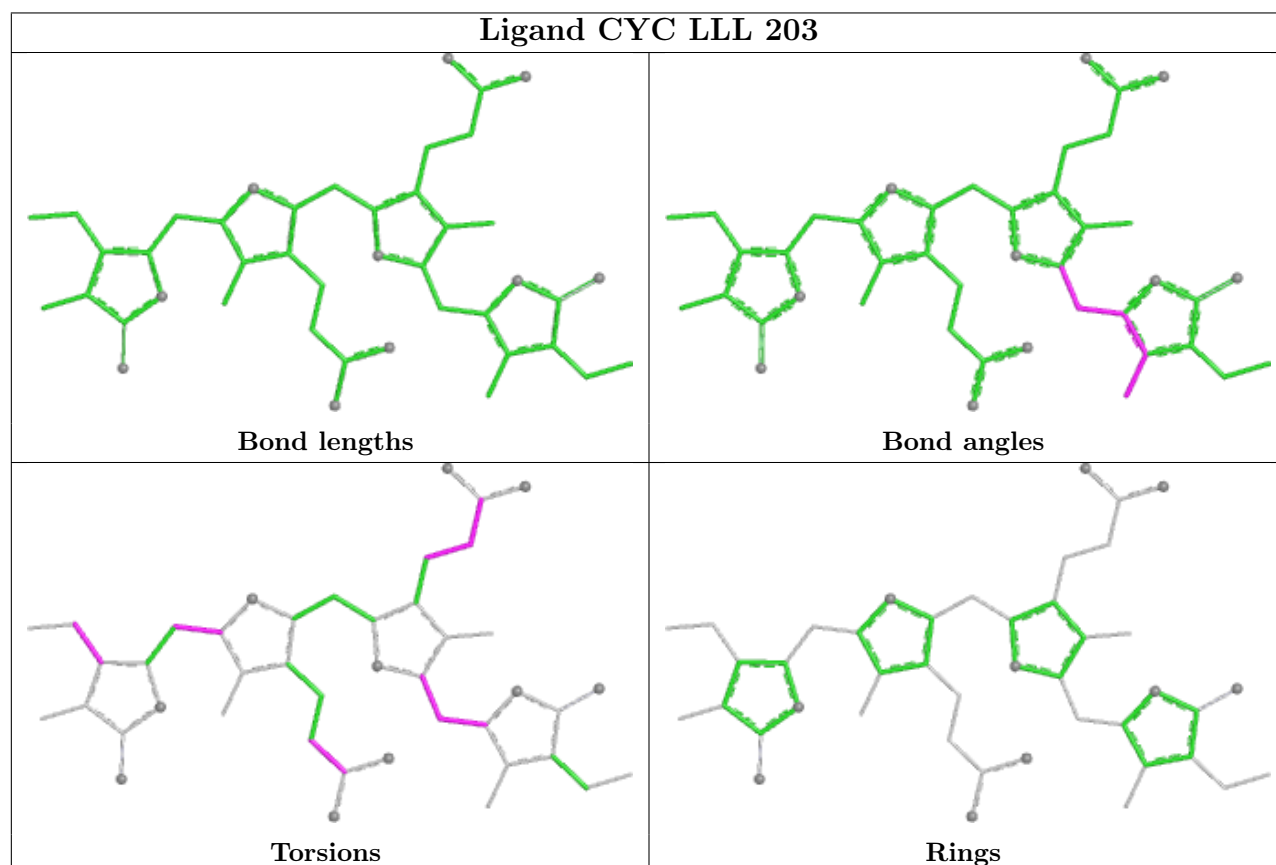
Ligand A1JTN DDD 201



Ligand CYC FFF 503



Ligand CYC LLL 203



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.71	19 (11%)	9 10	14, 29, 54, 84	3 (1%)
1	CCC	162/162 (100%)	0.51	5 (3%)	51 55	12, 30, 48, 64	2 (1%)
1	EEE	162/162 (100%)	0.85	13 (8%)	18 20	15, 35, 52, 66	3 (1%)
1	GGG	162/162 (100%)	0.57	12 (7%)	20 23	10, 30, 54, 74	5 (3%)
1	III	162/162 (100%)	0.56	7 (4%)	40 45	17, 29, 48, 62	4 (2%)
1	KKK	162/162 (100%)	1.18	22 (13%)	7 7	15, 40, 58, 67	4 (2%)
2	BBB	171/173 (98%)	1.15	34 (19%)	3 3	15, 40, 67, 75	1 (0%)
2	DDD	171/173 (98%)	0.78	16 (9%)	14 15	14, 36, 55, 71	1 (0%)
2	FFF	171/173 (98%)	1.19	30 (17%)	4 4	26, 45, 66, 85	0
2	HHH	171/173 (98%)	1.16	30 (17%)	4 4	22, 42, 64, 76	0
2	JJJ	171/173 (98%)	0.96	19 (11%)	10 11	17, 41, 63, 83	2 (1%)
2	LLL	171/173 (98%)	0.72	16 (9%)	14 15	20, 35, 62, 72	0
All	All	1998/2010 (99%)	0.86	223 (11%)	10 11	10, 37, 61, 85	25 (1%)

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	172	VAL	6.6
2	BBB	34	GLY	5.2
2	FFF	169	ALA	4.9
1	KKK	30[A]	ARG	4.7
2	HHH	34	GLY	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MEN	JJJ	72	9/10	0.92	0.08	20,22,27,29	0
2	MEN	HHH	72	9/10	0.93	0.10	23,27,33,35	0
2	MEN	FFF	72	9/10	0.93	0.11	26,29,35,37	0
2	MEN	DDD	72	9/10	0.94	0.08	22,24,28,29	0
2	MEN	BBB	72	9/10	0.94	0.06	22,24,25,32	0
2	MEN	LLL	72	9/10	0.94	0.07	25,27,30,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	ACT	GGG	202	4/4	0.52	0.34	51,57,61,64	0
5	ACT	FFF	501	4/4	0.63	0.29	57,66,67,70	0
4	A1JTN	CCC	202	2/18	0.70	0.21	47,47,47,52	2
5	ACT	EEE	202	4/4	0.72	0.29	100,102,105,106	0
4	A1JTN	KKK	202	2/18	0.76	0.23	54,54,54,58	2
3	CYC	BBB	203	43/43	0.85	0.12	31,45,59,65	0
3	CYC	FFF	504	43/43	0.87	0.13	40,47,58,62	0
4	A1JTN	EEE	203	2/18	0.88	0.13	48,48,48,61	2
3	CYC	HHH	203	43/43	0.88	0.12	34,49,61,67	0
3	CYC	JJJ	203	43/43	0.88	0.12	42,49,54,62	0
4	A1JTN	AAA	202	2/18	0.88	0.14	37,37,37,62	2
3	CYC	DDD	203	43/43	0.88	0.11	28,34,45,57	0
3	CYC	DDD	202	43/43	0.89	0.11	18,32,46,49	0
4	A1JTN	GGG	203	2/18	0.89	0.14	40,40,40,65	2
3	CYC	FFF	503	43/43	0.90	0.10	27,37,56,67	0
4	A1JTN	III	202	2/18	0.90	0.25	30,30,30,57	2
3	CYC	BBB	202	43/43	0.91	0.11	24,32,50,58	0
3	CYC	HHH	202	43/43	0.91	0.11	24,34,55,58	0
3	CYC	LLL	203	43/43	0.91	0.10	27,38,43,49	0
3	CYC	JJJ	202	43/43	0.92	0.09	25,35,50,56	0

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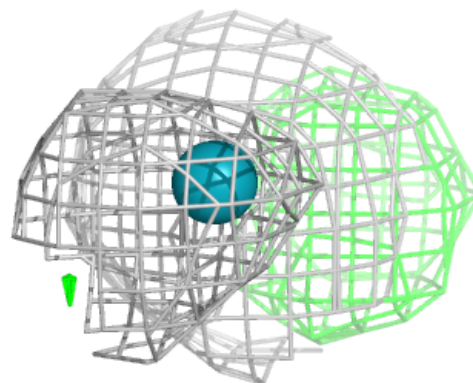
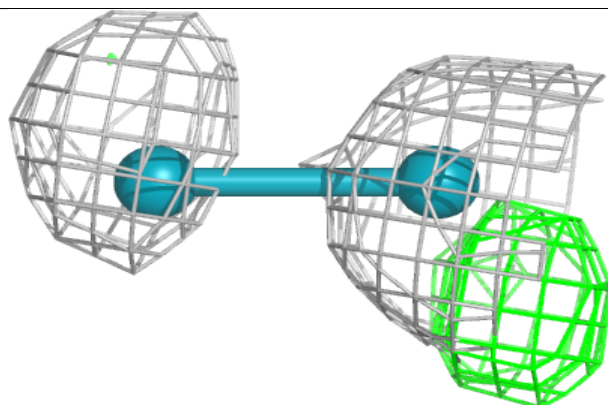
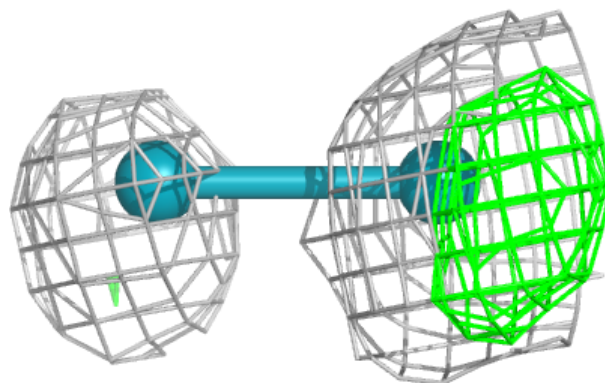
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CYC	LLL	202	43/43	0.92	0.10	22,36,56,63	0
3	CYC	III	201	43/43	0.93	0.08	13,19,23,27	0
3	CYC	GGG	201	43/43	0.93	0.07	16,19,25,26	0
3	CYC	CCC	201	43/43	0.93	0.07	20,23,28,30	0
3	CYC	KKK	201	43/43	0.93	0.08	23,29,33,34	0
3	CYC	EEE	201	43/43	0.93	0.08	19,25,32,38	0
3	CYC	AAA	201	43/43	0.95	0.06	19,22,25,26	0
4	A1JTN	FFF	502	18/18	0.95	0.15	47,56,61,61	18
4	A1JTN	HHH	201	18/18	0.96	0.14	38,43,44,49	18
4	A1JTN	JJJ	201	18/18	0.96	0.14	26,30,33,34	18
4	A1JTN	BBB	201	18/18	0.97	0.14	40,46,52,53	18
4	A1JTN	DDD	201	18/18	0.97	0.13	41,47,50,50	18
4	A1JTN	LLL	201	18/18	0.99	0.08	19,22,24,26	18

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.

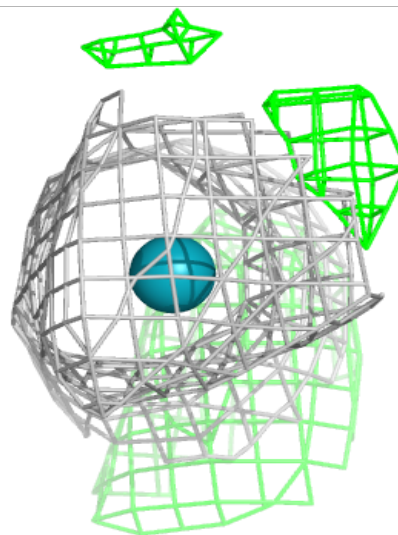
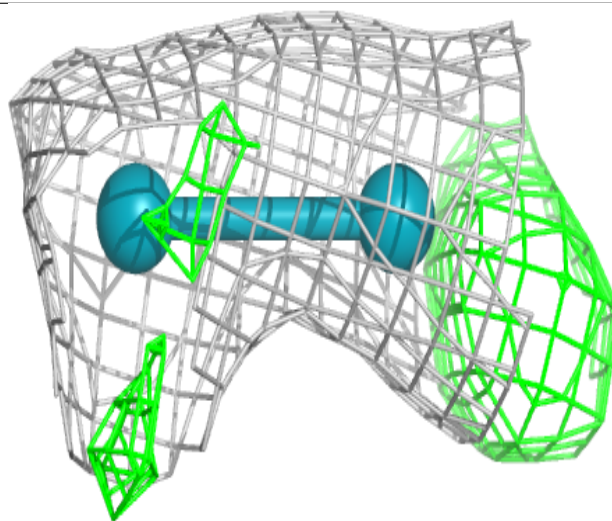
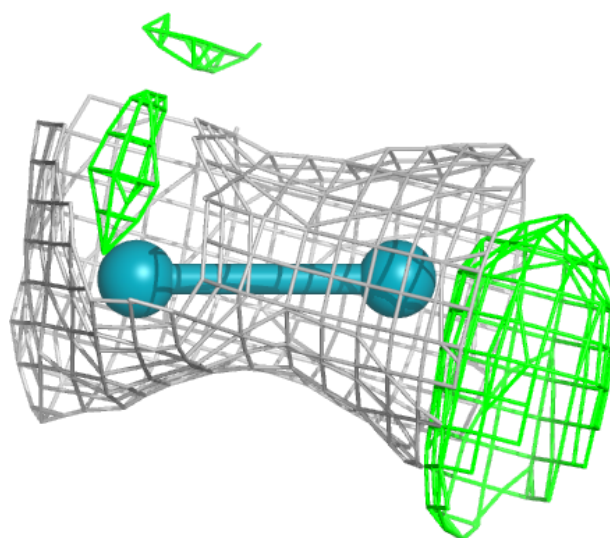
Electron density around A1JTN CCC 202:

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



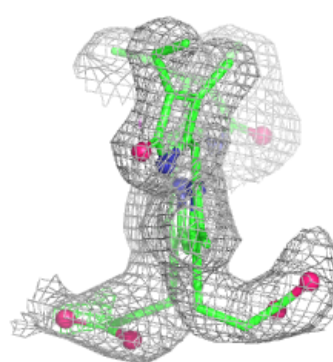
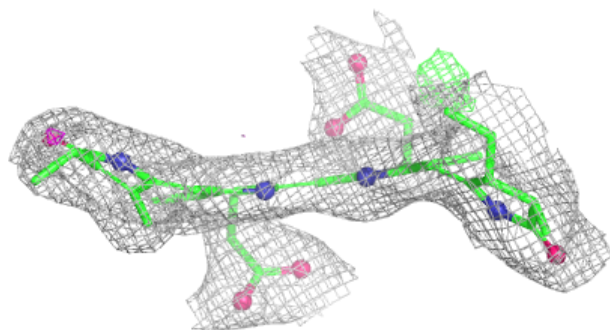
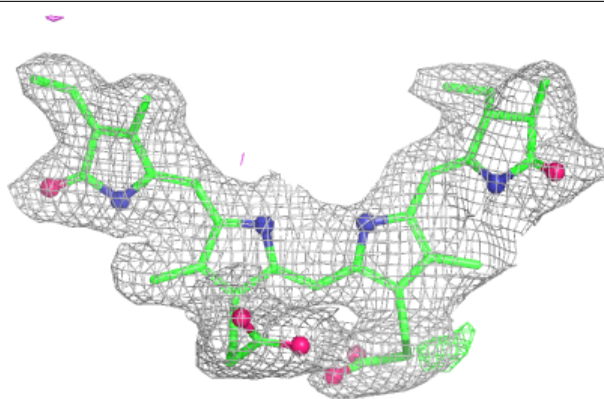
Electron density around A1JTN KKK 202:

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and green (positive)

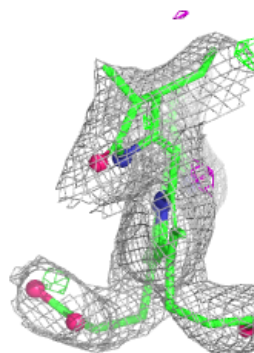
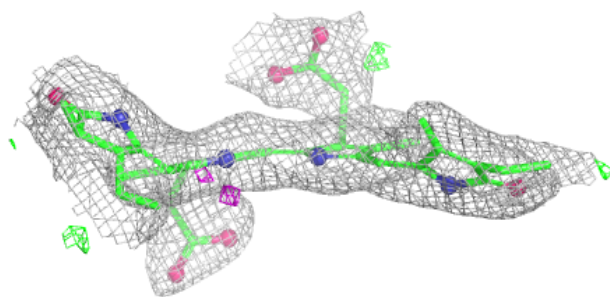
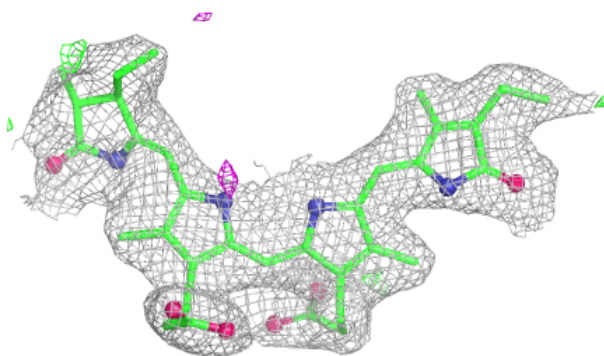


Electron density around CYC BBB 203:

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and green (positive)

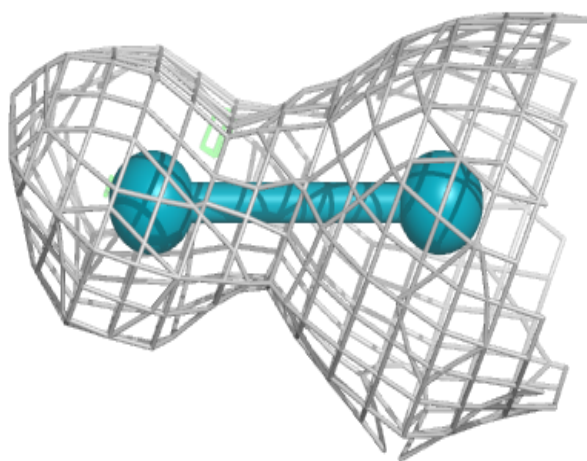
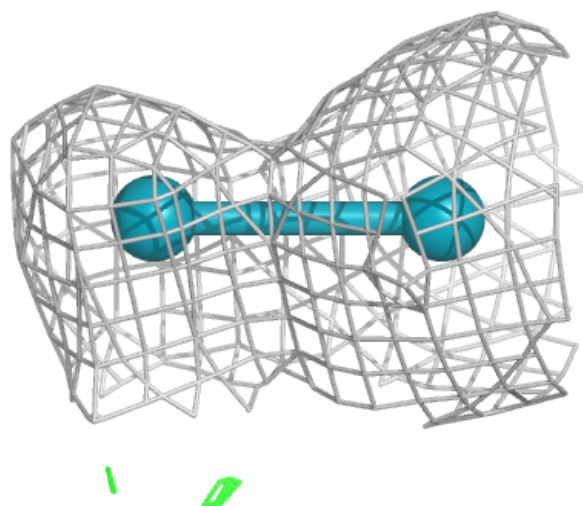
**Electron density around CYC FFF 504:**

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and green (positive)



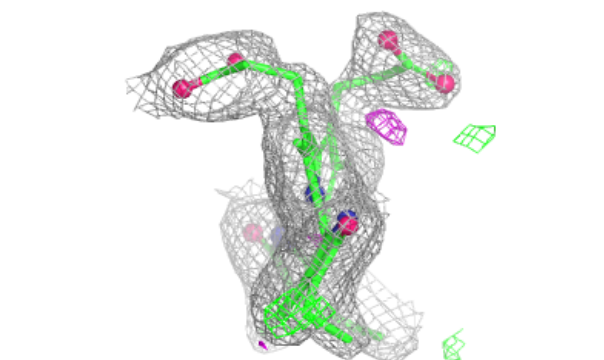
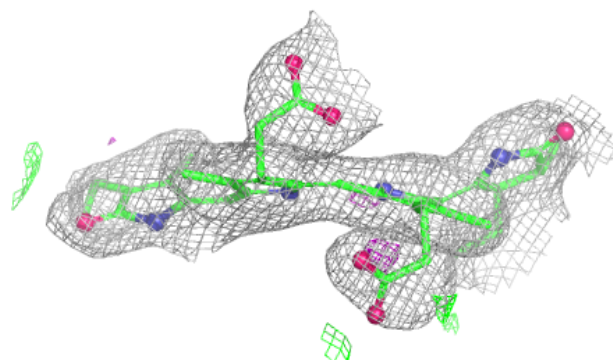
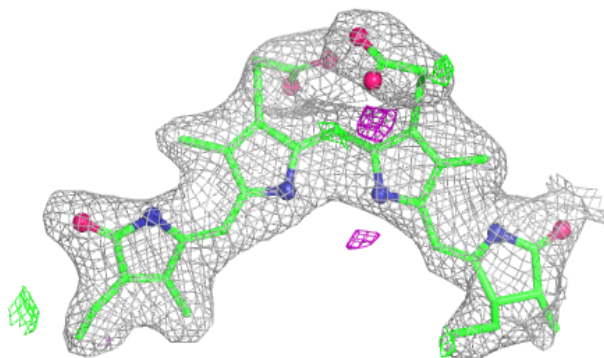
Electron density around A1JTN EEE 203:

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and green (positive)

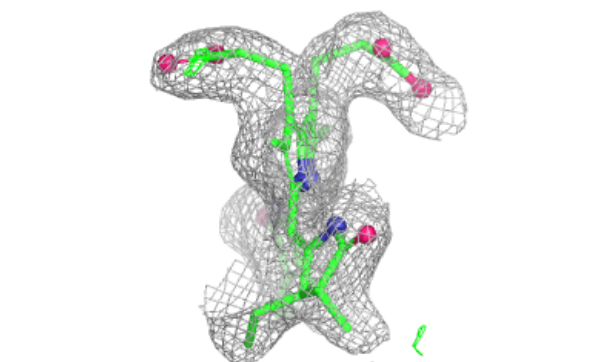
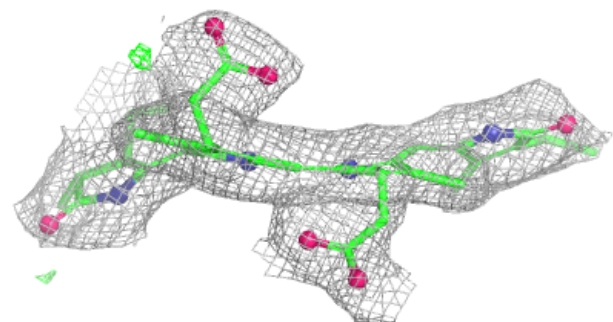
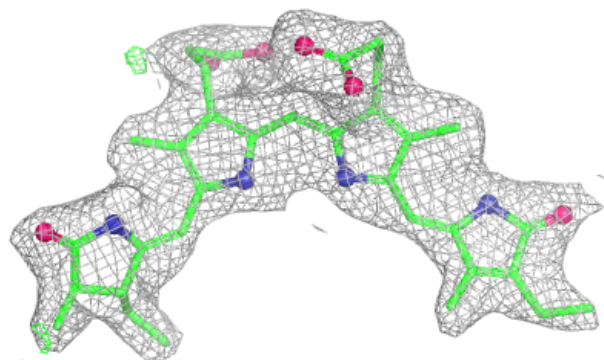


Electron density around CYC HHH 203:

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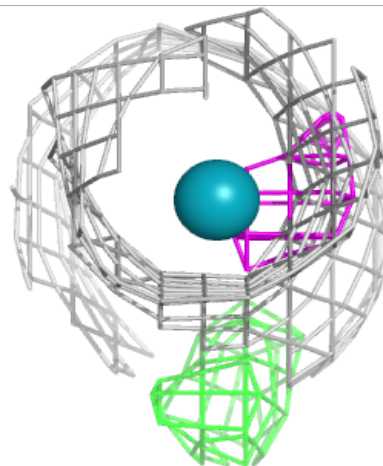
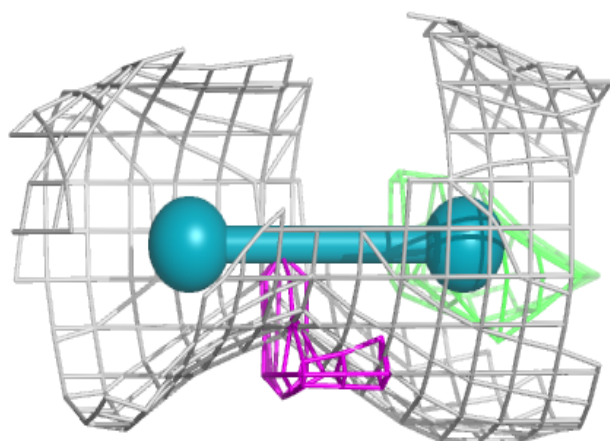
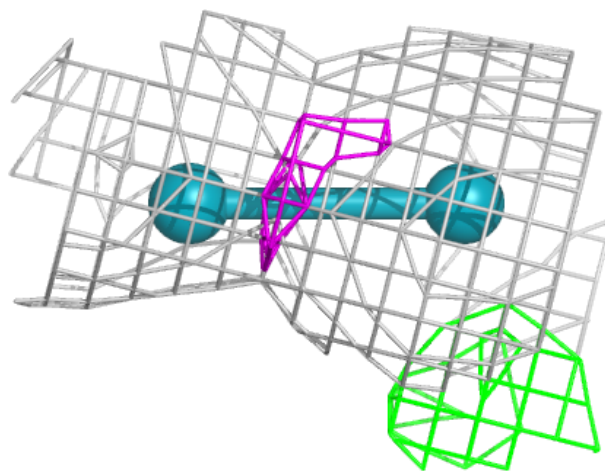
**Electron density around CYC JJJ 203:**

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and green (positive)



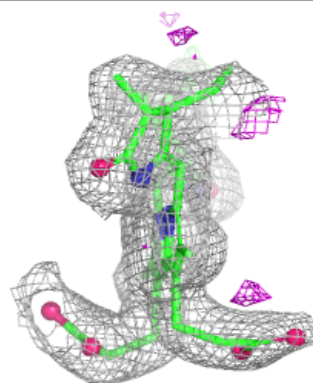
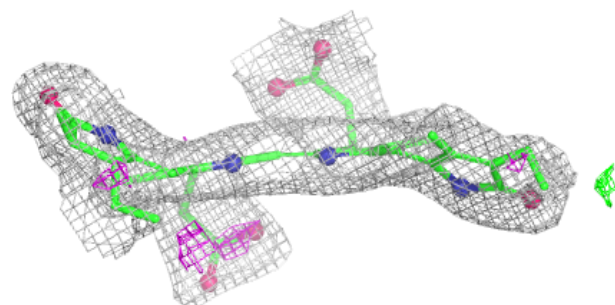
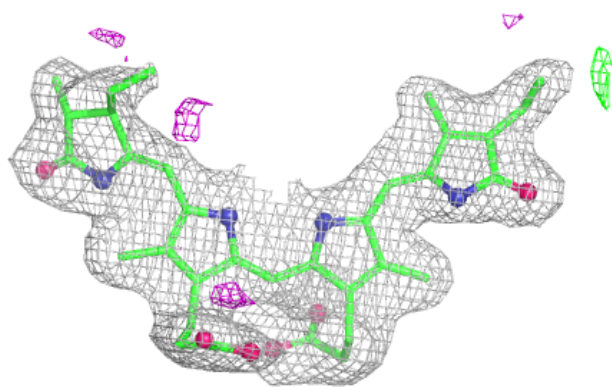
Electron density around A1JTN AAA 202:

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and green (positive)



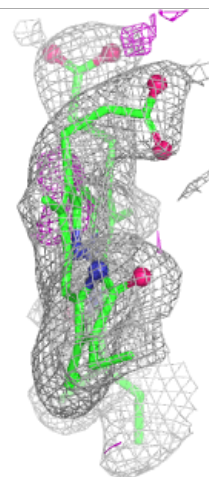
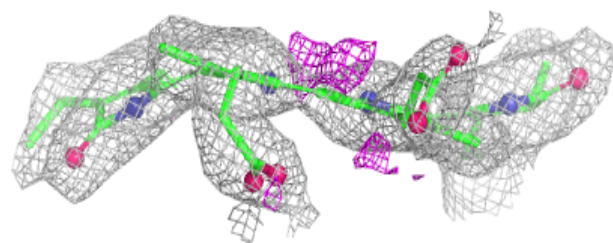
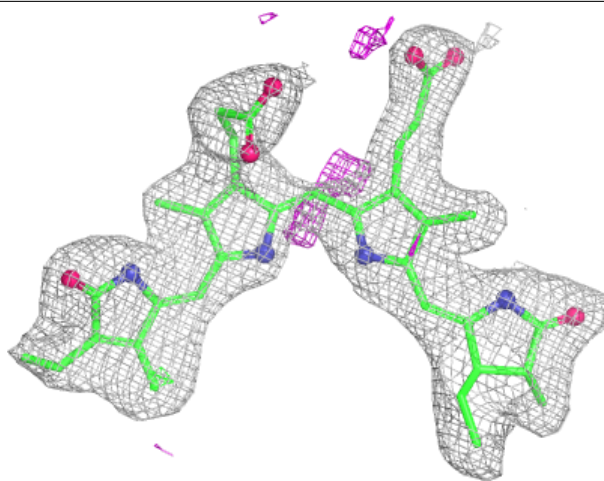
Electron density around CYC DDD 203:

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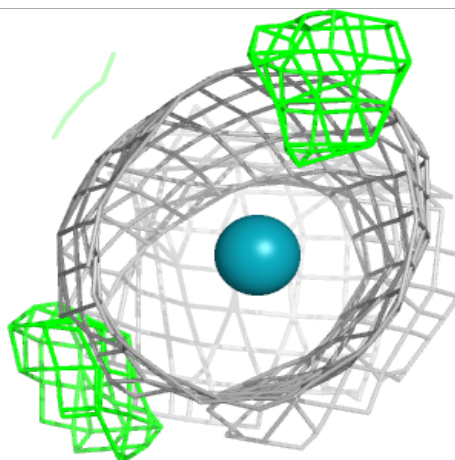
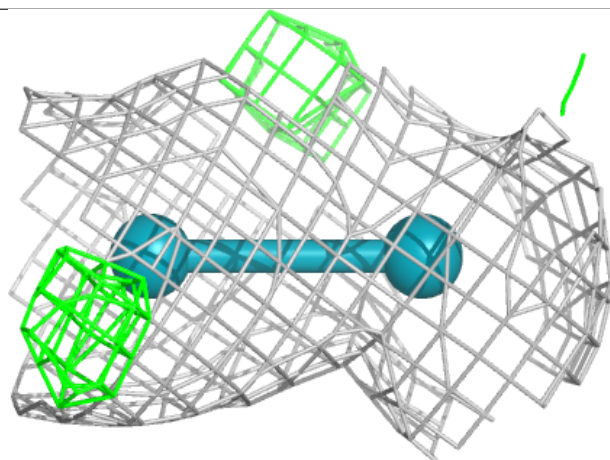
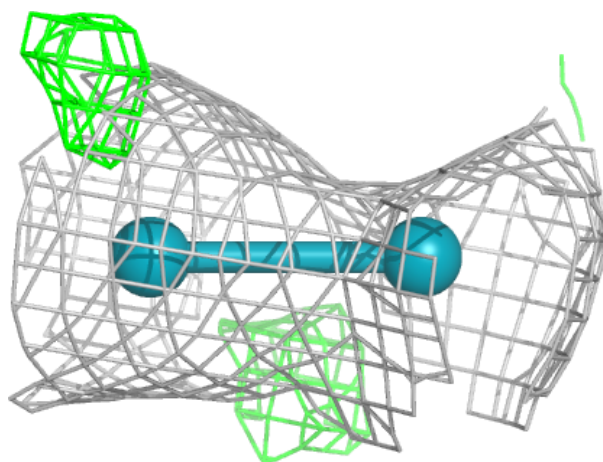
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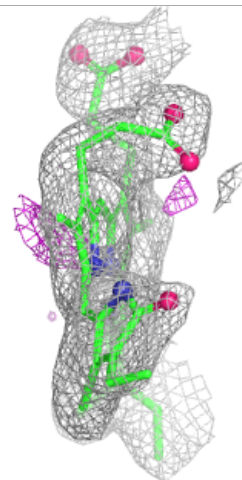
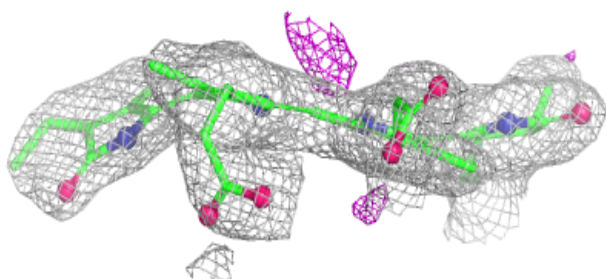
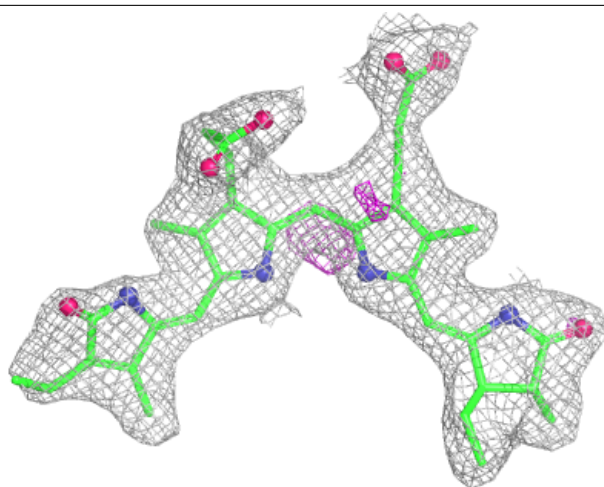
Electron density around A1JTN GGG 203:

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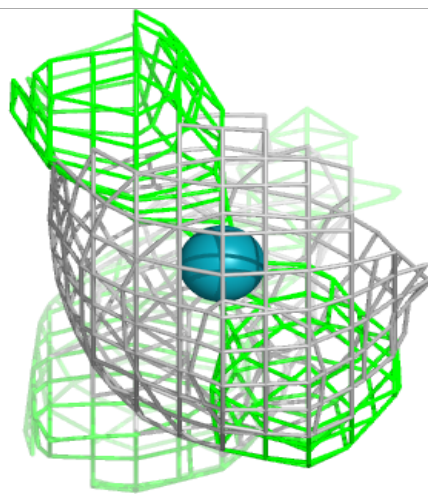
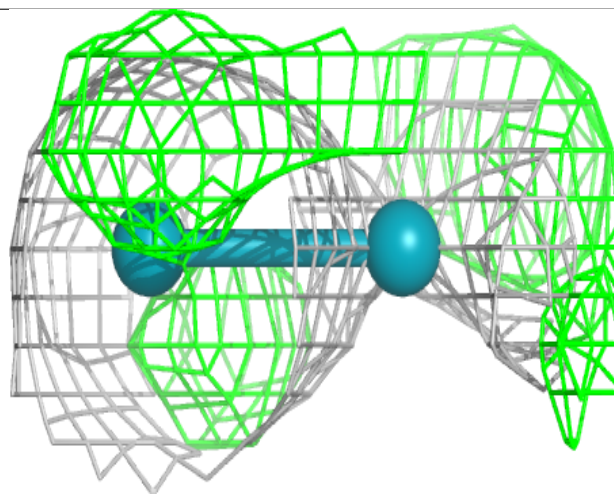
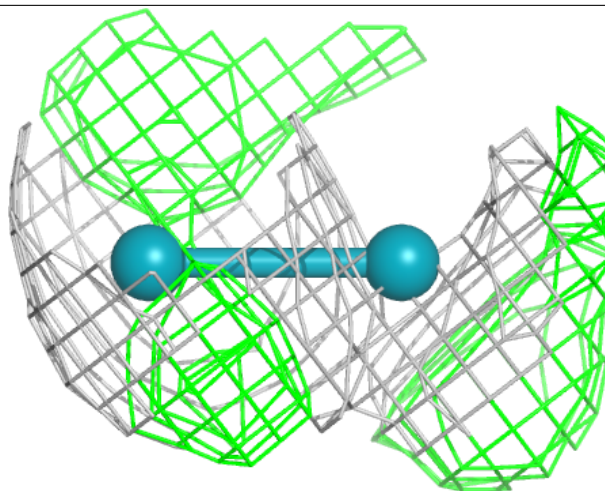
Electron density around CYC FFF 503:

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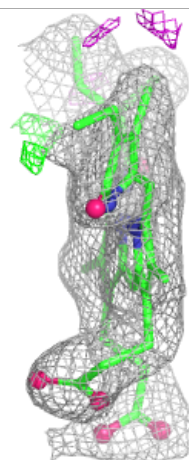
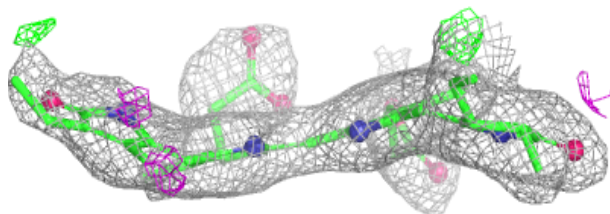
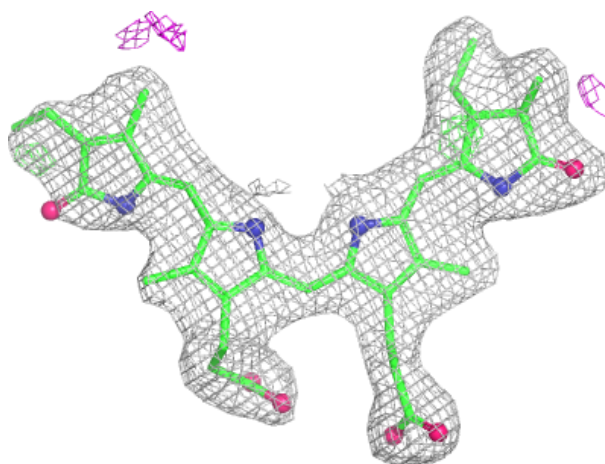
Electron density around A1JTN III 202:

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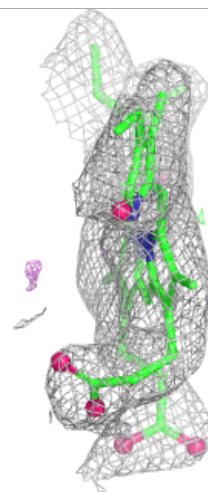
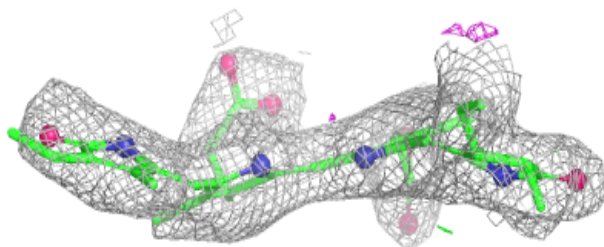
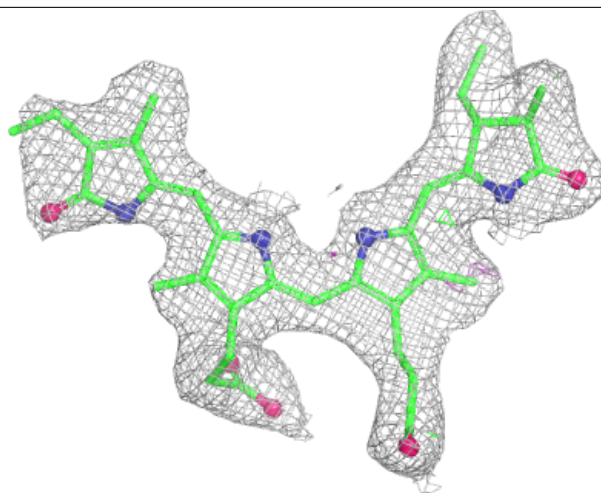
Electron density around CYC BBB 202:

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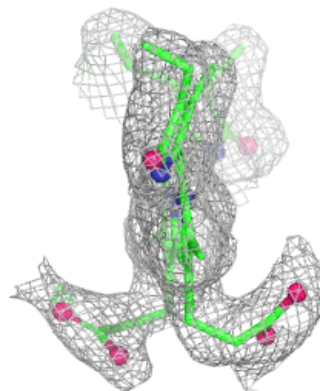
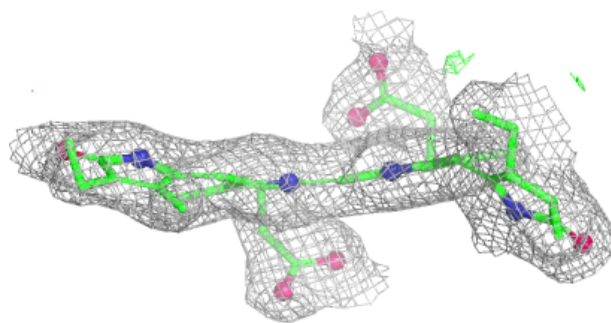
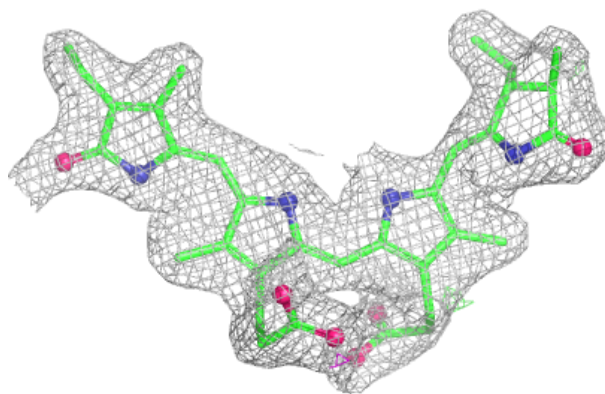
Electron density around CYC HHH 202:

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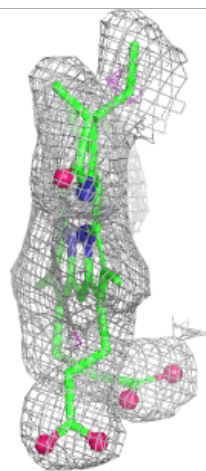
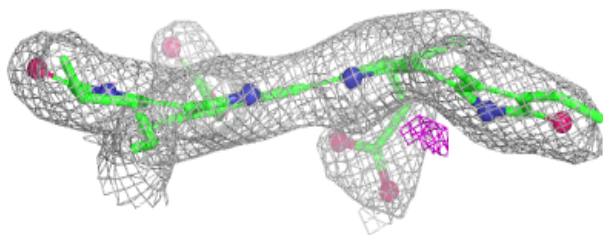
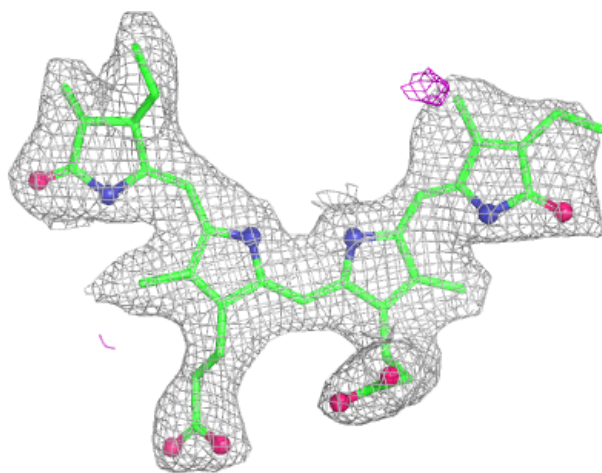
Electron density around CYC LLL 203:

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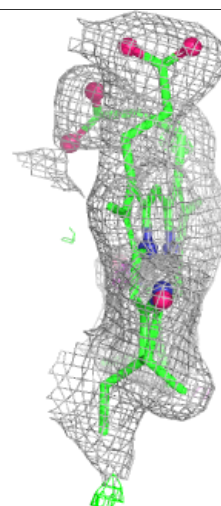
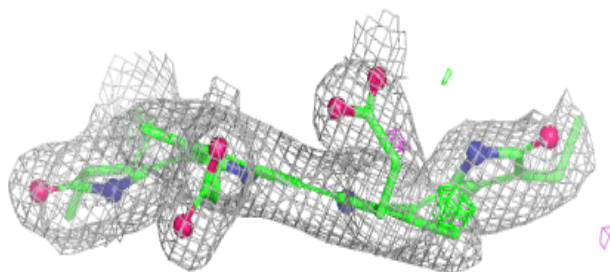
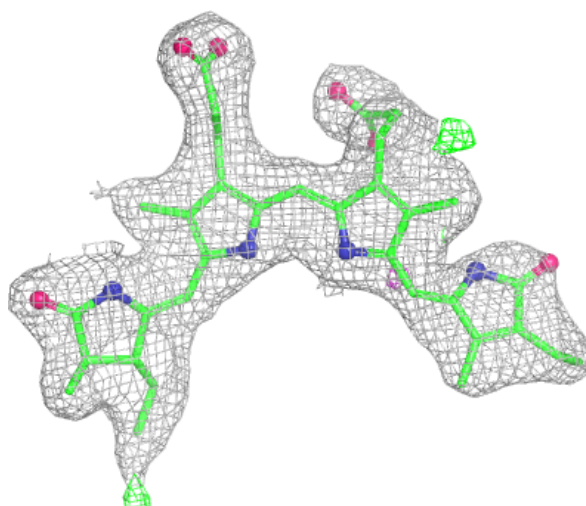
Electron density around CYC JJJ 202:

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and green (positive)



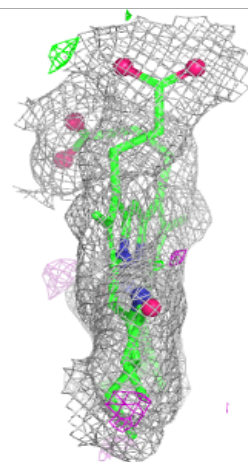
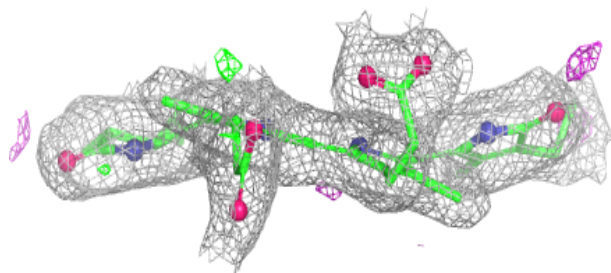
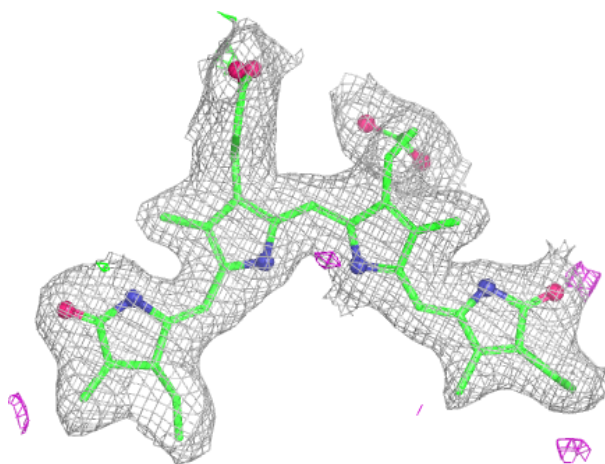
Electron density around CYC LLL 202:

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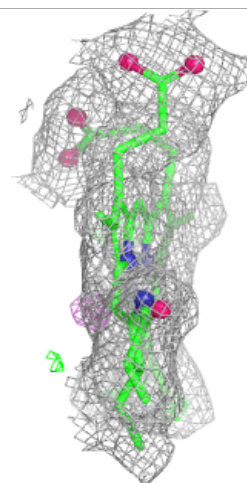
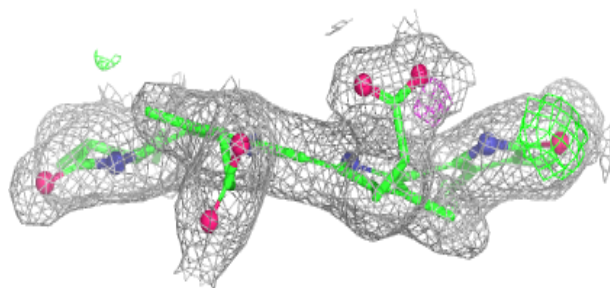
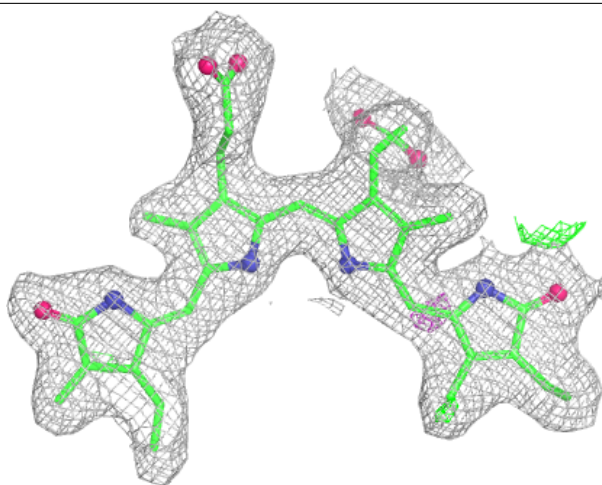
Electron density around CYC III 201:

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



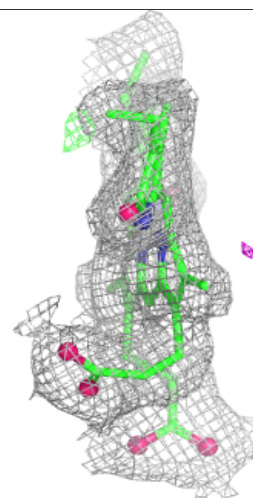
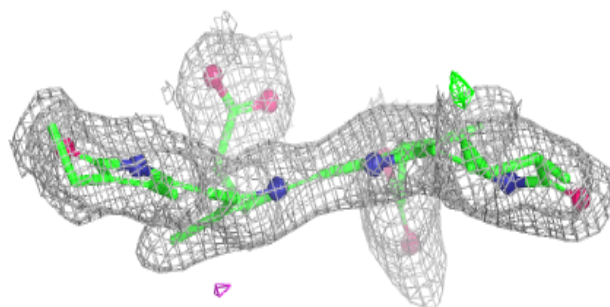
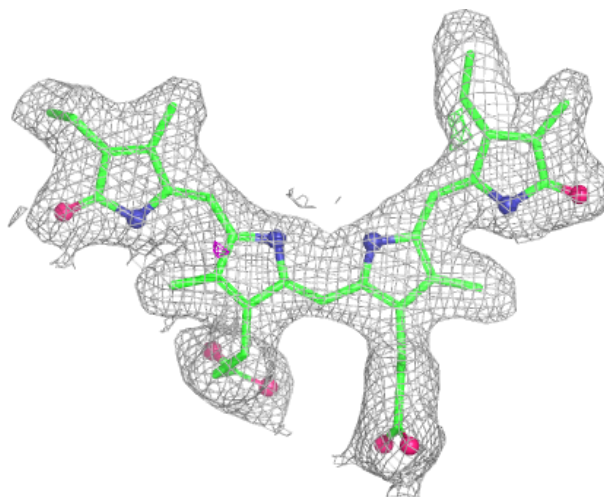
Electron density around CYC GGG 201:

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



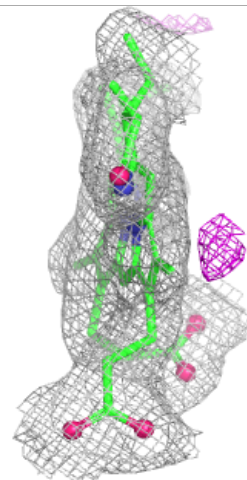
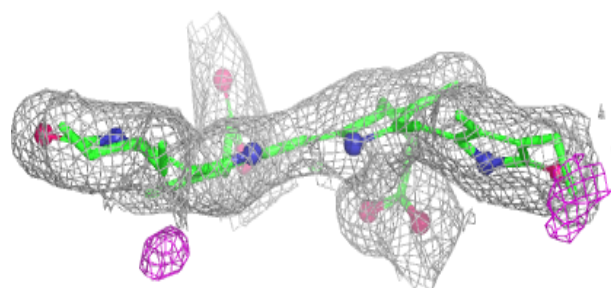
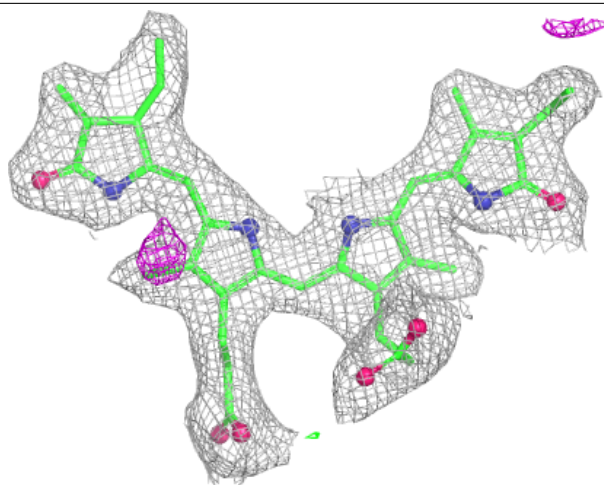
Electron density around CYC CCC 201:

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



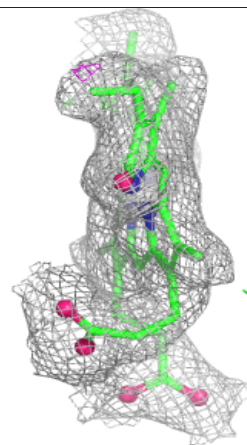
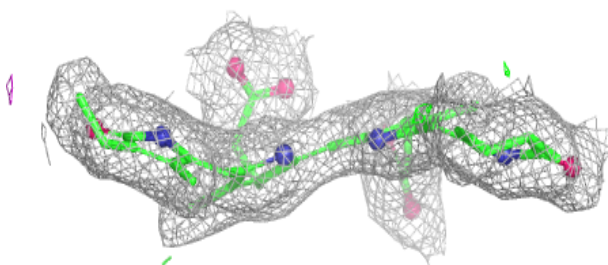
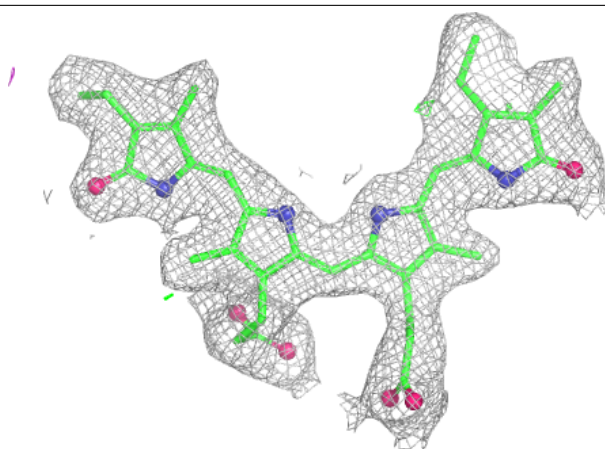
Electron density around CYC KKK 201:

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



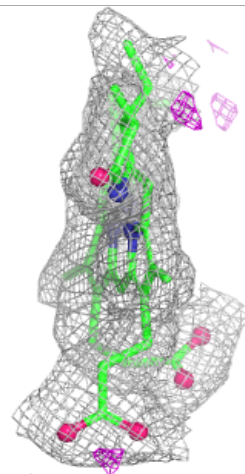
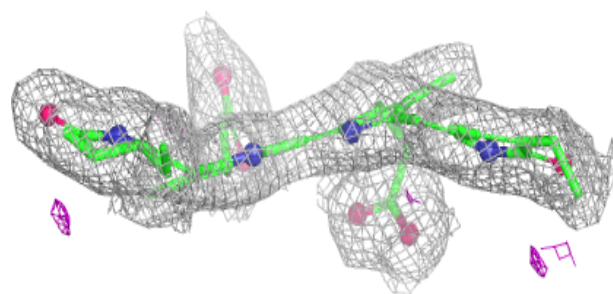
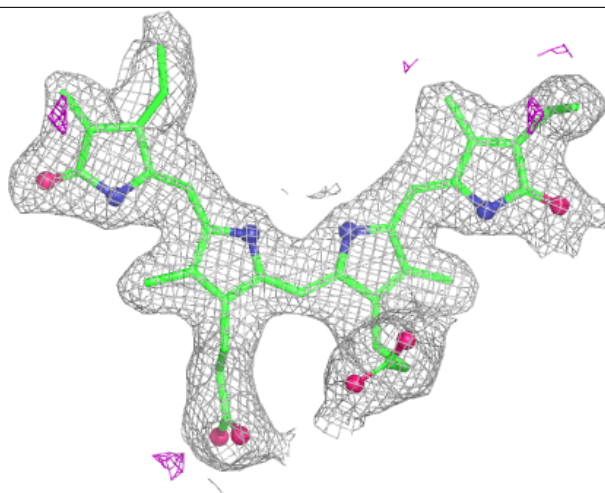
Electron density around CYC EEE 201:

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



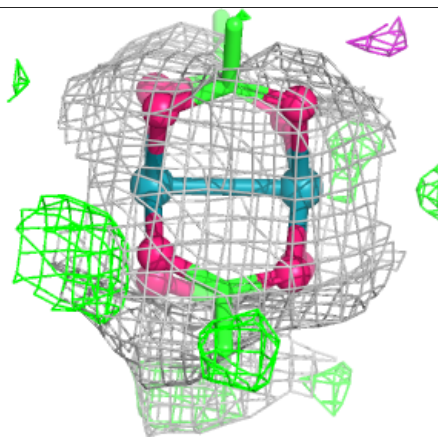
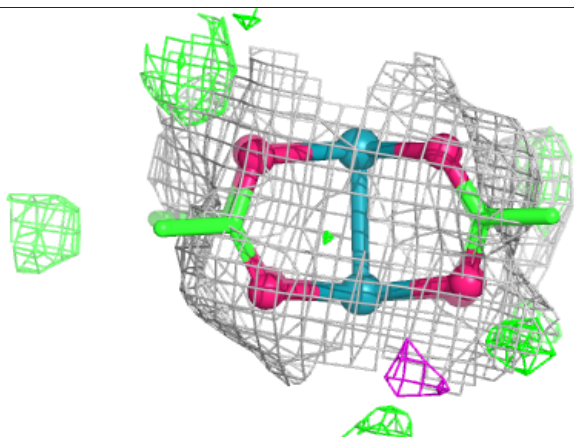
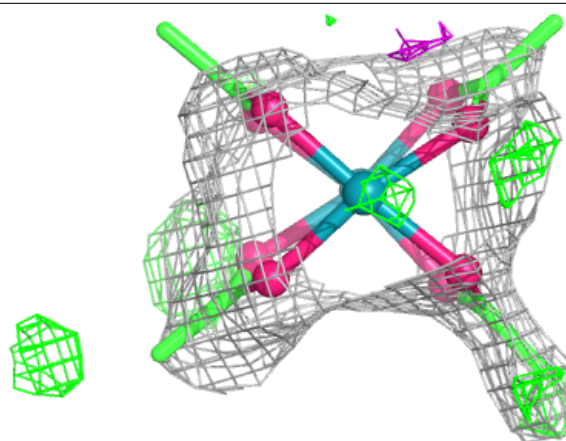
Electron density around CYC AAA 201:

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



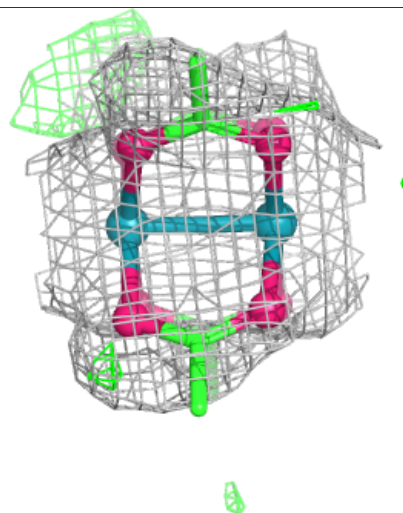
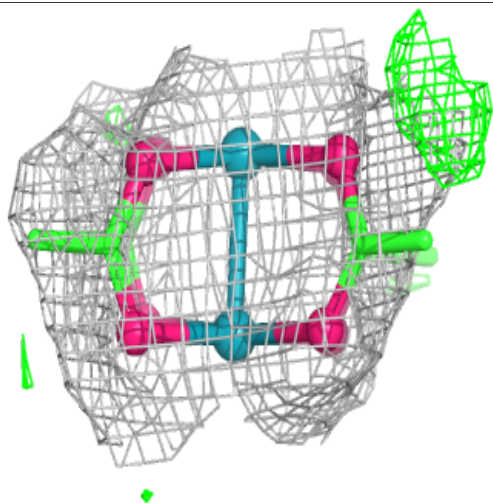
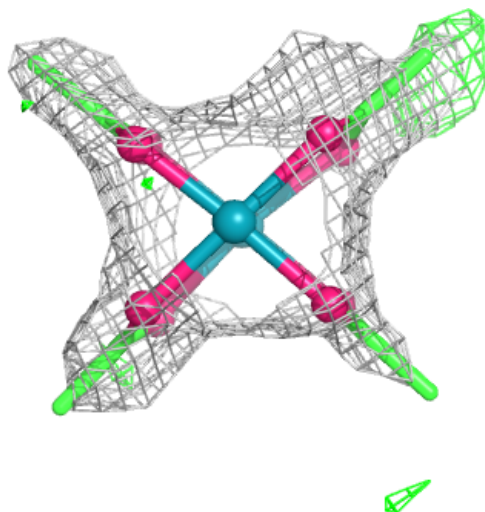
Electron density around A1JTN FFF 502:

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



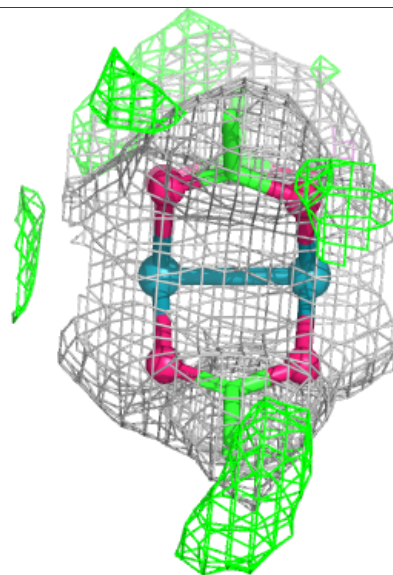
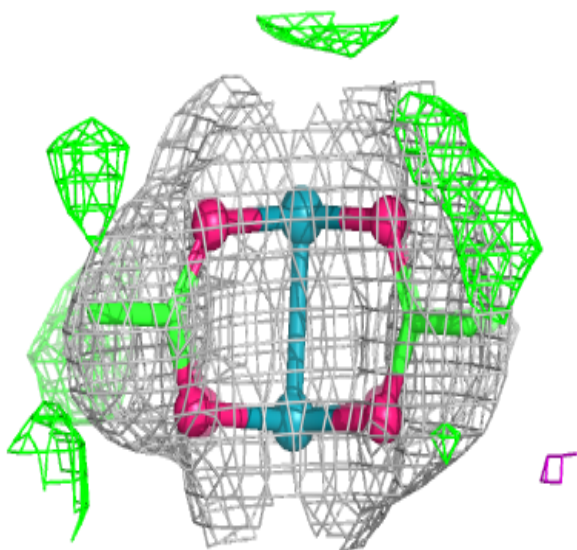
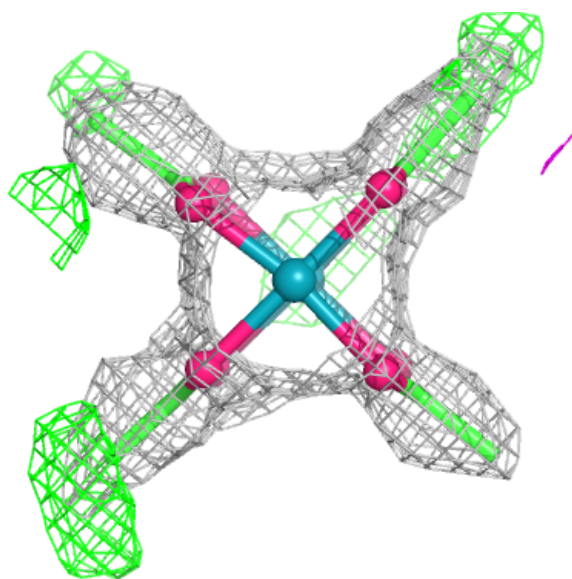
Electron density around A1JTN HHH 201:

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



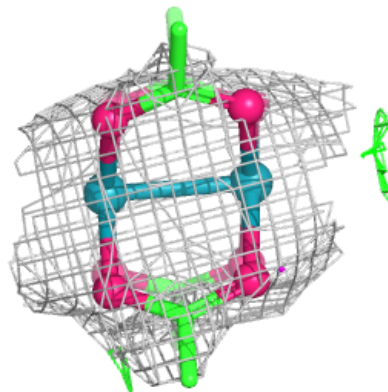
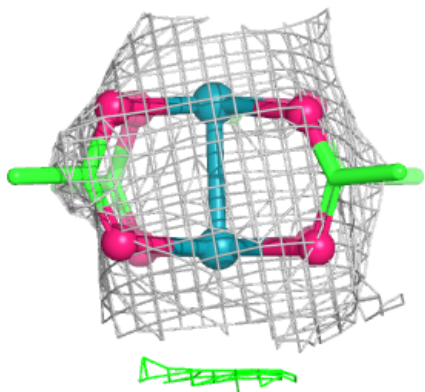
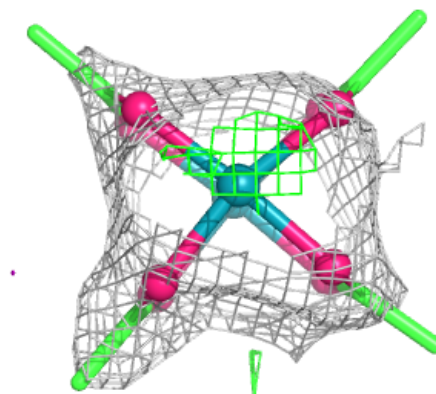
Electron density around A1JTN JJJ 201:

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



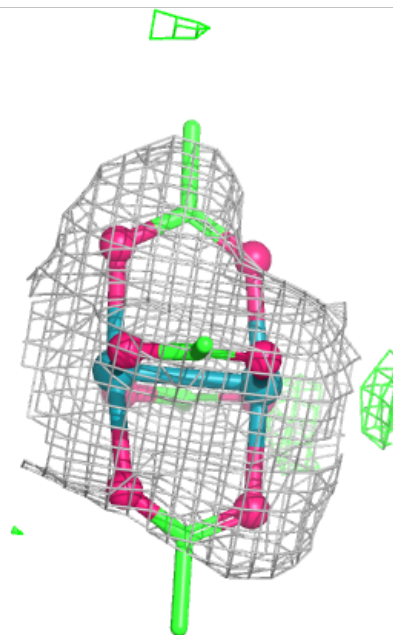
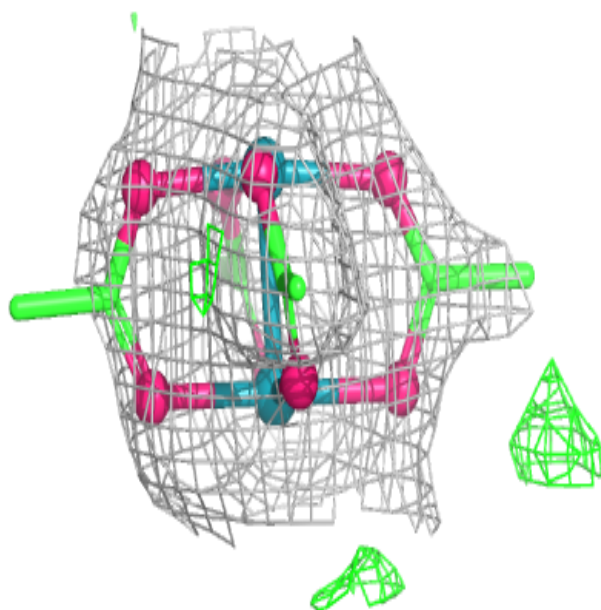
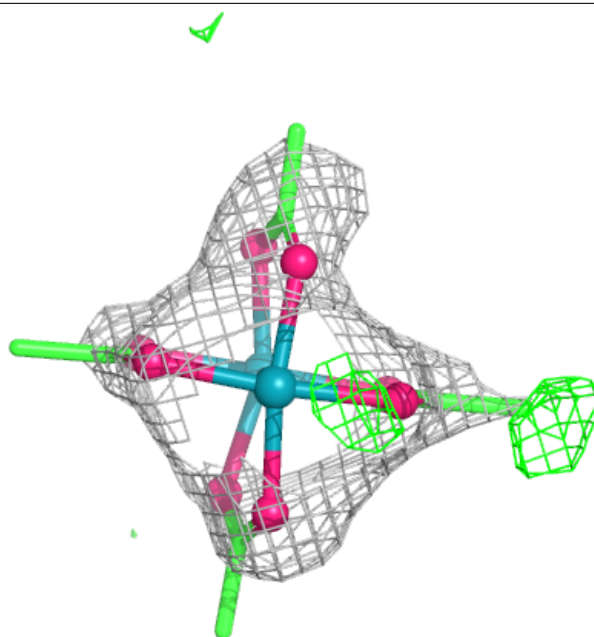
Electron density around A1JTN BBB 201:

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



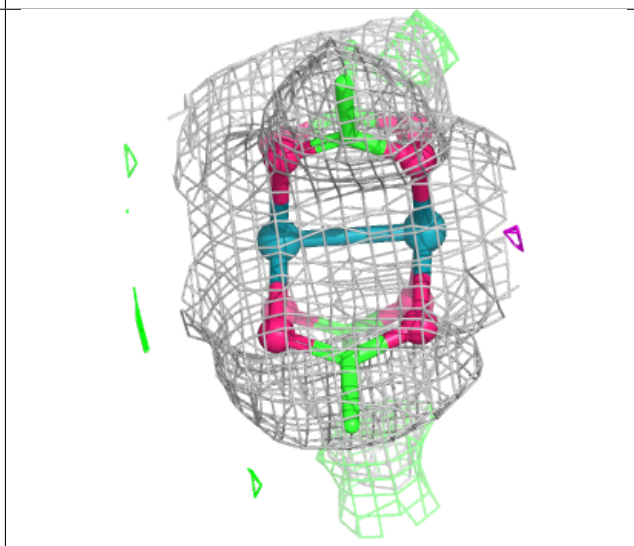
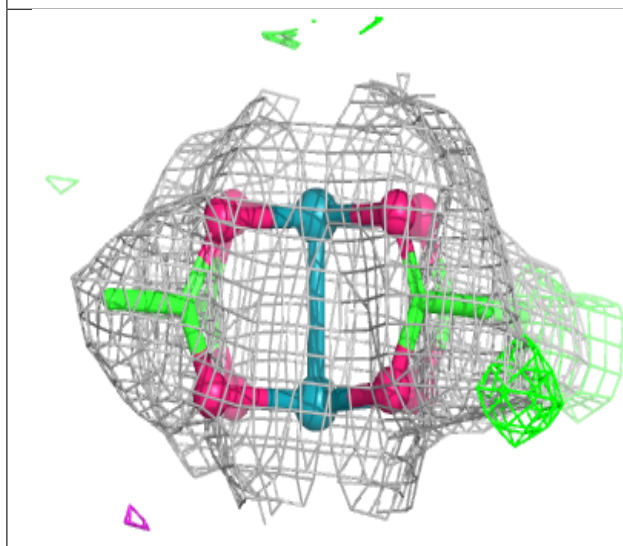
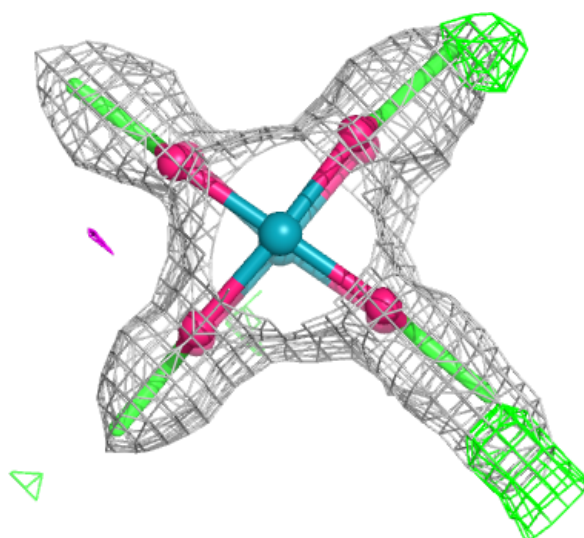
Electron density around A1JTN DDD 201:

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



Electron density around A1JTN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.