



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 01:40 PM EST

PDB ID : 1B33
Title : STRUCTURE OF LIGHT HARVESTING COMPLEX OF ALLOPHYCOCYANIN ALPHA AND BETA CHAINS/CORE-LINKER COMPLEX AP*LC7.8
Authors : Reuter, W.; Wiegand, G.; Huber, R.; Than, M.E.
Deposited on : 1998-12-15
Resolution : 2.30 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

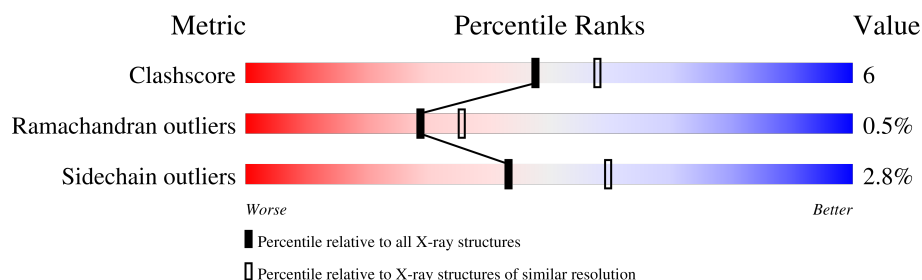
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)


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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	160	
1	C	160	
1	E	160	
1	H	160	
1	J	160	
1	L	160	
2	B	161	
2	D	161	

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Mol	Chain	Length	Quality of chain
2	F	161	 91% 9% .
2	I	161	 92% 7% .
2	K	161	 83% 17% .
2	M	161	 90% 9% .
3	N	67	 73% 22% .
3	O	67	 66% 31% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CYC	C	203	X	-	-	-
5	CYC	D	204	X	-	-	-
5	CYC	E	205	X	-	-	-
5	CYC	F	206	X	-	-	-
5	CYC	H	207	X	-	-	-
5	CYC	I	208	X	-	-	-
5	CYC	J	209	X	-	-	-
5	CYC	K	210	X	-	-	-
5	CYC	L	211	X	-	-	-
5	CYC	M	212	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17502 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 ALLOPHYCOCYANIN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	22	0	0
			1203	754	206	239	4			
1	C	160	Total	C	N	O	S	19	0	0
			1203	754	206	239	4			
1	E	160	Total	C	N	O	S	12	0	0
			1203	754	206	239	4			
1	H	160	Total	C	N	O	S	13	0	0
			1203	754	206	239	4			
1	J	160	Total	C	N	O	S	18	0	0
			1203	754	206	239	4			
1	L	160	Total	C	N	O	S	11	0	0
			1203	754	206	239	4			

- Molecule 2 is a protein called ALLOPHYCOCYANIN, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	21	0	0
			1219	769	202	241	7			
2	D	161	Total	C	N	O	S	6	0	0
			1219	769	202	241	7			
2	F	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	I	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	K	161	Total	C	N	O	S	10	0	0
			1219	769	202	241	7			
2	M	161	Total	C	N	O	S	13	0	0
			1219	769	202	241	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	MEN	ASN	modified residue	UNP P00318

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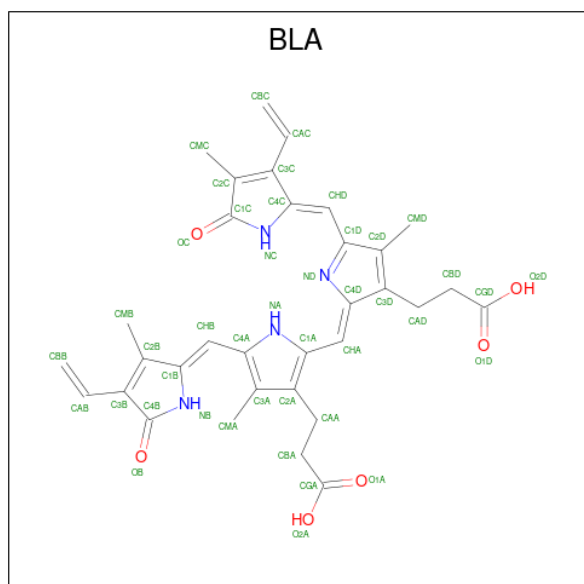
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Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MEN	ASN	modified residue	UNP P00318
F	71	MEN	ASN	modified residue	UNP P00318
I	71	MEN	ASN	modified residue	UNP P00318
K	71	MEN	ASN	modified residue	UNP P00318
M	71	MEN	ASN	modified residue	UNP P00318

- Molecule 3 is a protein called PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE.

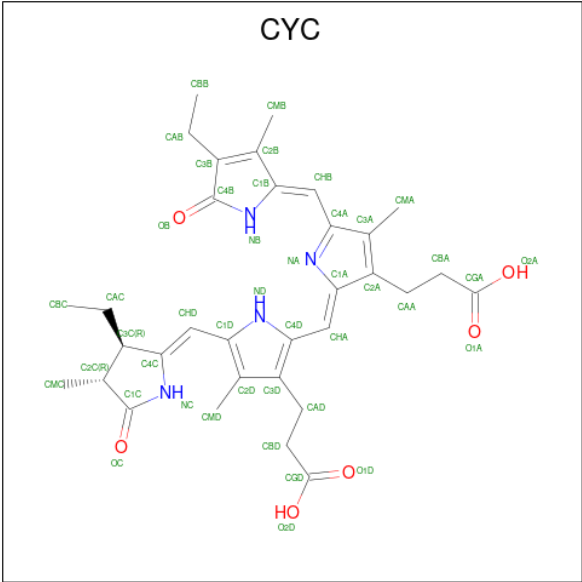
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	67	Total	C	N	O	S	13	0	0
			545	345	102	96	2			
3	O	67	Total	C	N	O	S	28	0	0
			545	345	102	96	2			

- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



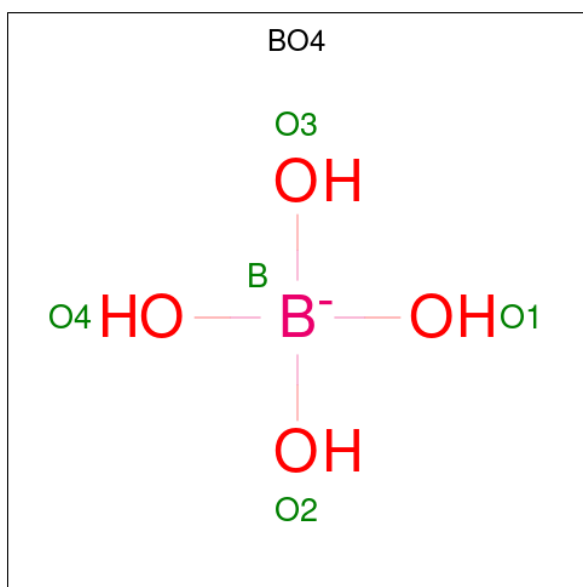
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	4	6		
4	B	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			43	33	4	6		
5	D	1	Total	C	N	O	0	0
			43	33	4	6		
5	E	1	Total	C	N	O	0	0
			43	33	4	6		
5	F	1	Total	C	N	O	0	0
			43	33	4	6		
5	H	1	Total	C	N	O	0	0
			43	33	4	6		
5	I	1	Total	C	N	O	0	0
			43	33	4	6		
5	J	1	Total	C	N	O	0	0
			43	33	4	6		
5	K	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		
5	M	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 6 is BORATE ION (three-letter code: BO4) (formula: BH₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total B O 5 1 4	0	0
6	E	1	Total B O 5 1 4	0	0
6	J	1	Total B O 5 1 4	0	0
6	L	1	Total B O 5 1 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	81	Total O 81 81	0	0
7	C	82	Total O 82 82	0	0
7	D	145	Total O 145 145	0	0
7	E	101	Total O 101 101	0	0
7	F	127	Total O 127 127	0	0
7	N	31	Total O 31 31	0	0
7	H	99	Total O 99 99	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	113	Total 113	O 113	0	0
7	J	109	Total 109	O 109	0	0
7	K	117	Total 117	O 117	0	0
7	L	126	Total 126	O 126	0	0
7	M	136	Total 136	O 136	0	0
7	O	15	Total 15	O 15	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. 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. 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.


Note EDS was not executed.

- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain A:  91% 9%




- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain C:  88% 12%




- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain E:  82% 16%




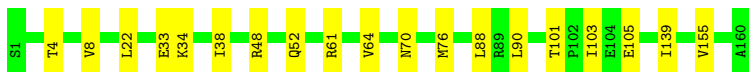
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain H:  89% 11%




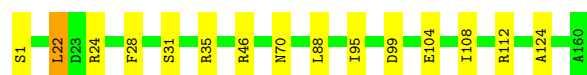
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain J:  88% 12%




- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain L:  91% 9% .




• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain B:  89% 10% .




• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain D:  89% 10% .




• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain F:  91% 9% .




• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain I:  92% 7% .




• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain K:  83% 17% .



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain M:  90% 9% .



• Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain N:

73%

22%



● Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain O:

66%

31%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.12Å 151.90Å 137.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (25.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17502	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: BO4, CYC, BLA, MEN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.37	0/1218	0.56	0/1647
1	C	0.39	0/1218	0.56	0/1647
1	E	0.38	0/1218	0.56	0/1647
1	H	0.41	0/1218	0.57	0/1647
1	J	0.40	0/1218	0.58	0/1647
1	L	0.40	0/1218	0.59	1/1647 (0.1%)
2	B	0.41	0/1226	0.61	0/1659
2	D	0.42	0/1226	0.64	0/1659
2	F	0.41	0/1226	0.65	0/1659
2	I	0.44	0/1226	0.65	0/1659
2	K	0.42	0/1226	0.62	0/1659
2	M	0.43	0/1226	0.66	0/1659
3	N	0.47	0/553	0.69	0/740
3	O	0.49	0/553	0.74	0/740
All	All	0.41	0/15770	0.61	1/21316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	22	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1203	0	1213	11	0
1	C	1203	0	1213	10	0
1	E	1203	0	1213	17	0
1	H	1203	0	1213	10	0
1	J	1203	0	1213	12	0
1	L	1203	0	1213	9	0
2	B	1219	0	1229	13	0
2	D	1219	0	1229	8	0
2	F	1219	0	1229	11	0
2	I	1219	0	1229	8	0
2	K	1219	0	1229	16	0
2	M	1219	0	1229	11	0
3	N	545	0	572	17	0
3	O	545	0	572	14	0
4	A	43	0	31	6	0
4	B	43	0	31	8	0
5	C	43	0	35	4	0
5	D	43	0	35	3	0
5	E	43	0	35	5	0
5	F	43	0	35	3	0
5	H	43	0	35	6	0
5	I	43	0	35	3	0
5	J	43	0	35	7	0
5	K	43	0	35	3	0
5	L	43	0	35	5	0
5	M	43	0	35	3	0
6	C	5	0	4	0	0
6	E	5	0	4	0	0
6	J	5	0	4	0	0
6	L	5	0	4	0	0
7	A	62	0	0	1	0
7	B	81	0	0	2	0
7	C	82	0	0	2	0
7	D	145	0	0	0	0
7	E	101	0	0	3	0
7	F	127	0	0	1	0
7	H	99	0	0	2	0
7	I	113	0	0	4	0
7	J	109	0	0	1	0
7	K	117	0	0	2	0
7	L	126	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	136	0	0	0	0
7	N	31	0	0	1	0
7	O	15	0	0	3	0
All	All	17502	0	16224	193	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 6.

The worst 5 of 193 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)
5:E:205:CYC:HMA1	5:E:205:CYC:HB	1.31	0.96
5:H:207:CYC:HMA1	5:H:207:CYC:HB	1.32	0.93
2:F:110:ASN:HD21	3:N:56:ALA:HB1	1.33	0.91
5:C:203:CYC:HMA1	5:C:203:CYC:HB	1.38	0.89
1:J:48:ARG:HH21	1:J:139:ILE:HD11	1.38	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
1	C	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
1	E	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
1	H	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
1	J	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
1	L	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
2	B	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	25	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	12	12
2	F	158/161 (98%)	152 (96%)	4 (2%)	2 (1%)	12	12
2	I	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	12	12
2	K	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	25	31
2	M	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	12	12
3	N	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
3	O	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
All	All	2026/2060 (98%)	1975 (98%)	41 (2%)	10 (0%)	29	35

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	110	ASN
2	D	110	ASN
2	F	110	ASN
2	I	110	ASN
2	F	74	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/125 (100%)	123 (98%)	2 (2%)	62	78
1	C	125/125 (100%)	123 (98%)	2 (2%)	62	78
1	E	125/125 (100%)	121 (97%)	4 (3%)	39	54
1	H	125/125 (100%)	122 (98%)	3 (2%)	49	66
1	J	125/125 (100%)	121 (97%)	4 (3%)	39	54
1	L	125/125 (100%)	122 (98%)	3 (2%)	49	66
2	B	126/126 (100%)	121 (96%)	5 (4%)	31	44
2	D	126/126 (100%)	122 (97%)	4 (3%)	39	54
2	F	126/126 (100%)	124 (98%)	2 (2%)	62	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	126/126 (100%)	124 (98%)	2 (2%)	62	78
2	K	126/126 (100%)	123 (98%)	3 (2%)	49	66
2	M	126/126 (100%)	124 (98%)	2 (2%)	62	78
3	N	58/58 (100%)	53 (91%)	5 (9%)	10	12
3	O	58/58 (100%)	54 (93%)	4 (7%)	15	20
All	All	1622/1622 (100%)	1577 (97%)	45 (3%)	43	60

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	144	ASP
2	K	160	LEU
1	J	33	GLU
1	J	90	LEU
1	L	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	9	ASN
2	K	117	ASN
1	J	56	GLN
2	K	2	GLN
1	L	40	GLN

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	D	71	2	7,8,9	0.55	0	6,9,11	0.48	0
2	MEN	B	71	2	7,8,9	0.52	0	6,9,11	0.33	0
2	MEN	F	71	2	7,8,9	0.58	0	6,9,11	0.55	0
2	MEN	I	71	2	7,8,9	0.54	0	6,9,11	0.42	0
2	MEN	K	71	2	7,8,9	0.50	0	6,9,11	0.30	0
2	MEN	M	71	2	7,8,9	0.40	0	6,9,11	0.33	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	D	71	2	-	2/7/8/10	-
2	MEN	B	71	2	-	2/7/8/10	-
2	MEN	F	71	2	-	2/7/8/10	-
2	MEN	I	71	2	-	2/7/8/10	-
2	MEN	K	71	2	-	2/7/8/10	-
2	MEN	M	71	2	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	71	MEN	CA-CB-CG-OD1
2	F	71	MEN	CA-CB-CG-OD1
2	I	71	MEN	CA-CB-CG-OD1
2	K	71	MEN	CA-CB-CG-OD1
2	M	71	MEN	CA-CB-CG-OD1

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	71	MEN	1	0
2	F	71	MEN	1	0
2	I	71	MEN	1	0
2	K	71	MEN	1	0
2	M	71	MEN	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
5	CYC	L	211	1	42,46,46	2.63	6 (14%)	50,67,67	2.66	20 (40%)
5	CYC	J	209	1	42,46,46	2.50	8 (19%)	50,67,67	2.36	16 (32%)
4	BLA	B	202	2	42,46,46	1.92	8 (19%)	53,67,67	1.84	10 (18%)
6	BO4	J	2002	-	4,4,4	0.76	0	6,6,6	0.61	0
6	BO4	L	2001	-	4,4,4	1.07	0	6,6,6	1.03	1 (16%)
4	BLA	A	201	1	42,46,46	1.83	7 (16%)	53,67,67	1.87	10 (18%)
5	CYC	F	206	2	42,46,46	2.26	7 (16%)	50,67,67	2.85	19 (38%)
5	CYC	I	208	2	42,46,46	2.69	7 (16%)	50,67,67	2.68	18 (36%)
5	CYC	C	203	1	42,46,46	2.58	7 (16%)	50,67,67	2.39	17 (34%)
5	CYC	K	210	2	42,46,46	2.80	8 (19%)	50,67,67	2.49	20 (40%)
5	CYC	M	212	2	42,46,46	2.65	8 (19%)	50,67,67	2.72	18 (36%)
6	BO4	C	2003	-	4,4,4	0.82	0	6,6,6	0.85	0
5	CYC	H	207	1	42,46,46	2.29	9 (21%)	50,67,67	2.20	13 (26%)
5	CYC	D	204	2	42,46,46	2.27	9 (21%)	50,67,67	2.41	20 (40%)
6	BO4	E	2004	-	4,4,4	0.71	0	6,6,6	0.58	0
5	CYC	E	205	1	42,46,46	2.19	8 (19%)	50,67,67	2.51	15 (30%)

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
5	CYC	L	211	1	2/2/14/19	9/25/74/74	0/4/4/4
5	CYC	J	209	1	1/1/14/19	9/25/74/74	0/4/4/4
4	BLA	B	202	2	-	8/26/74/74	0/4/4/4
4	BLA	A	201	1	-	10/26/74/74	0/4/4/4
5	CYC	F	206	2	2/2/14/19	13/25/74/74	0/4/4/4
5	CYC	I	208	2	1/1/14/19	11/25/74/74	0/4/4/4
5	CYC	C	203	1	2/2/14/19	7/25/74/74	0/4/4/4
5	CYC	K	210	2	1/1/14/19	11/25/74/74	0/4/4/4
5	CYC	M	212	2	2/2/14/19	11/25/74/74	0/4/4/4
5	CYC	H	207	1	2/2/14/19	9/25/74/74	0/4/4/4
5	CYC	D	204	2	1/1/14/19	8/25/74/74	0/4/4/4
5	CYC	E	205	1	2/2/14/19	9/25/74/74	0/4/4/4

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	210	CYC	C2C-C1C	-12.22	1.41	1.52
5	I	208	CYC	C2C-C1C	-12.05	1.41	1.52
5	M	212	CYC	C2C-C1C	-11.91	1.41	1.52
5	C	203	CYC	C2C-C1C	-10.95	1.42	1.52
5	L	211	CYC	CHA-C1A	9.66	1.43	1.35

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	205	CYC	CAC-C3C-C2C	8.79	136.21	114.26
5	C	203	CYC	CAC-C3C-C2C	8.39	135.21	114.26
5	H	207	CYC	CAC-C3C-C2C	8.04	134.35	114.26
5	J	209	CYC	CAC-C3C-C2C	7.70	133.51	114.26
5	L	211	CYC	CAC-C3C-C2C	7.64	133.34	114.26

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	203	CYC	C3C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
5	C	203	CYC	C2C
5	D	204	CYC	C2C
5	E	205	CYC	C3C
5	E	205	CYC	C2C

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	BLA	NA-C4A-CHB-C1B
4	A	201	BLA	C3A-C4A-CHB-C1B
4	A	201	BLA	C2B-C3B-CAB-CBB
4	A	201	BLA	C4B-C3B-CAB-CBB
4	A	201	BLA	ND-C1D-CHD-C4C

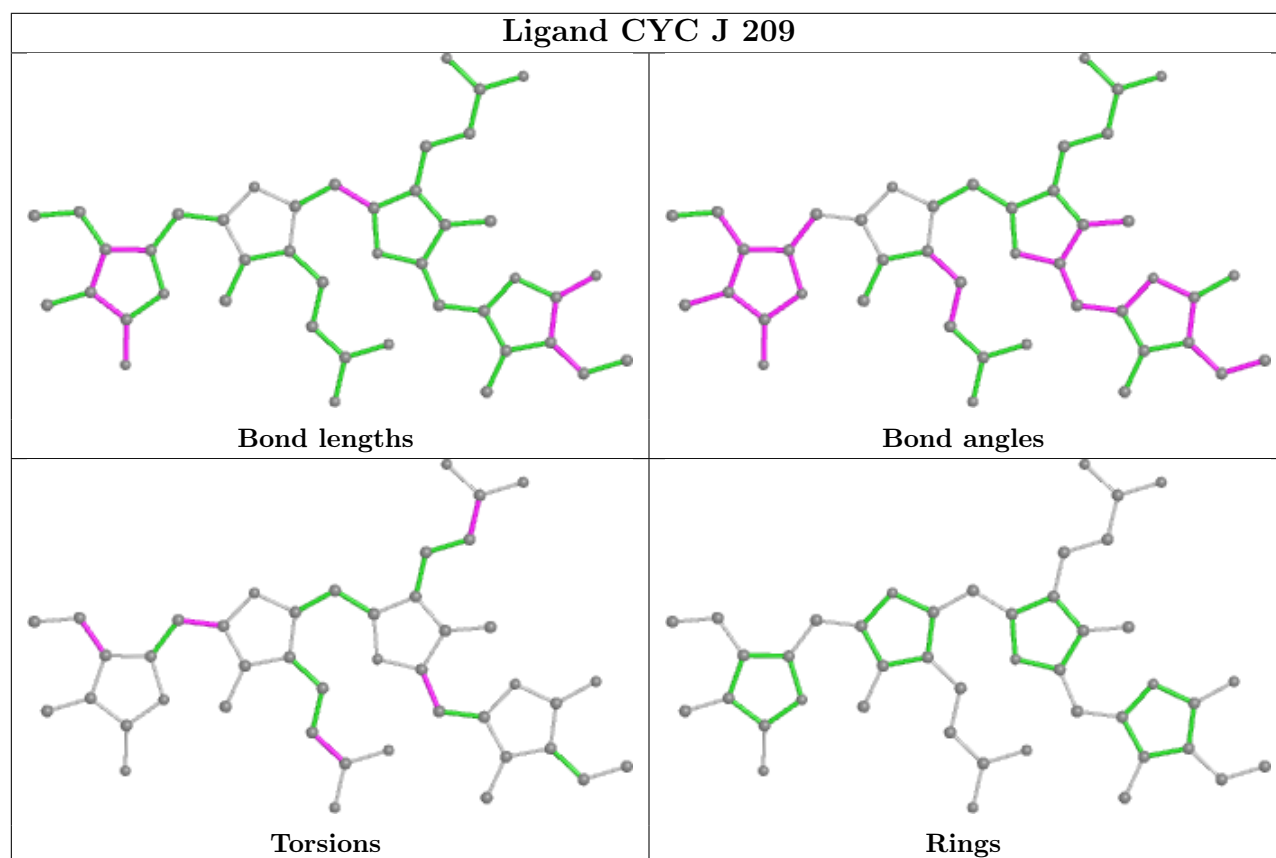
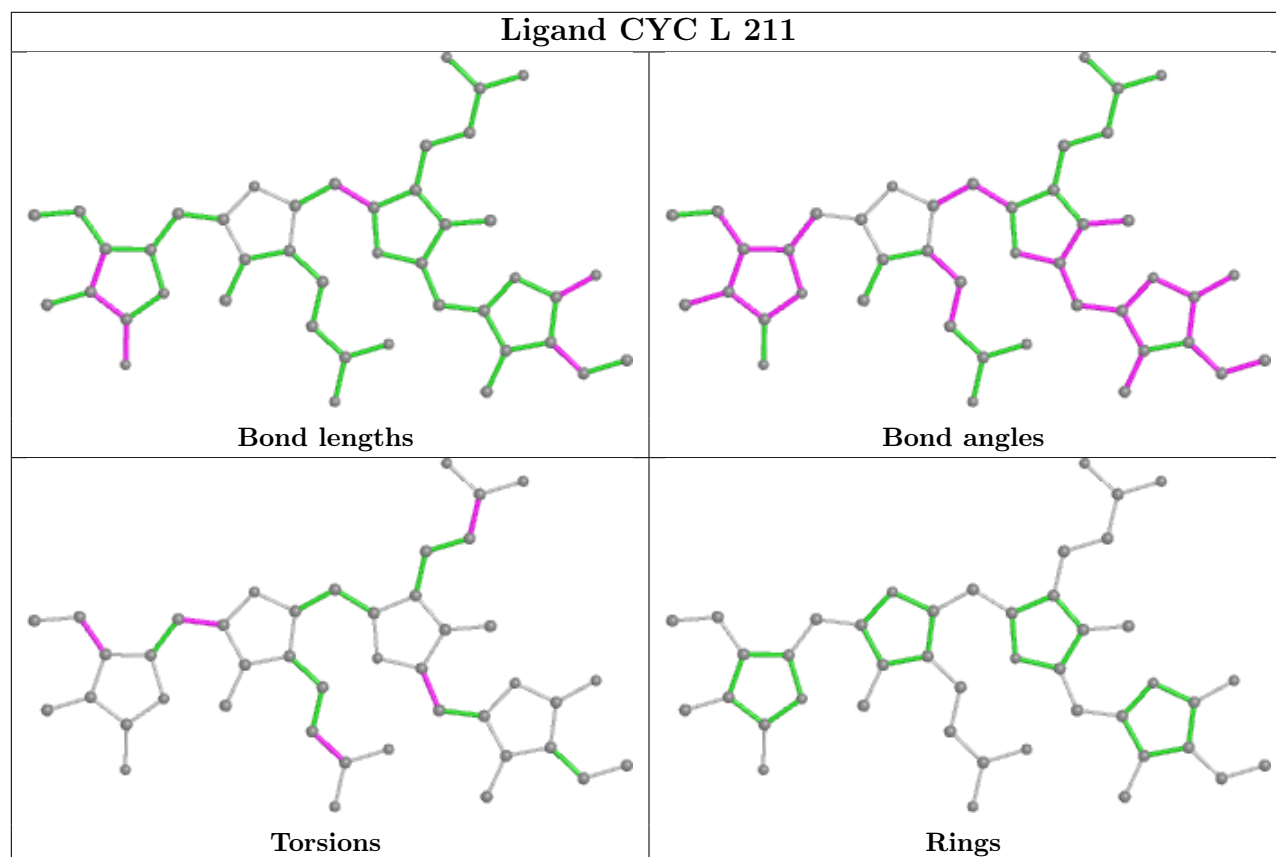
There are no ring outliers.

12 monomers are involved in 56 short contacts:

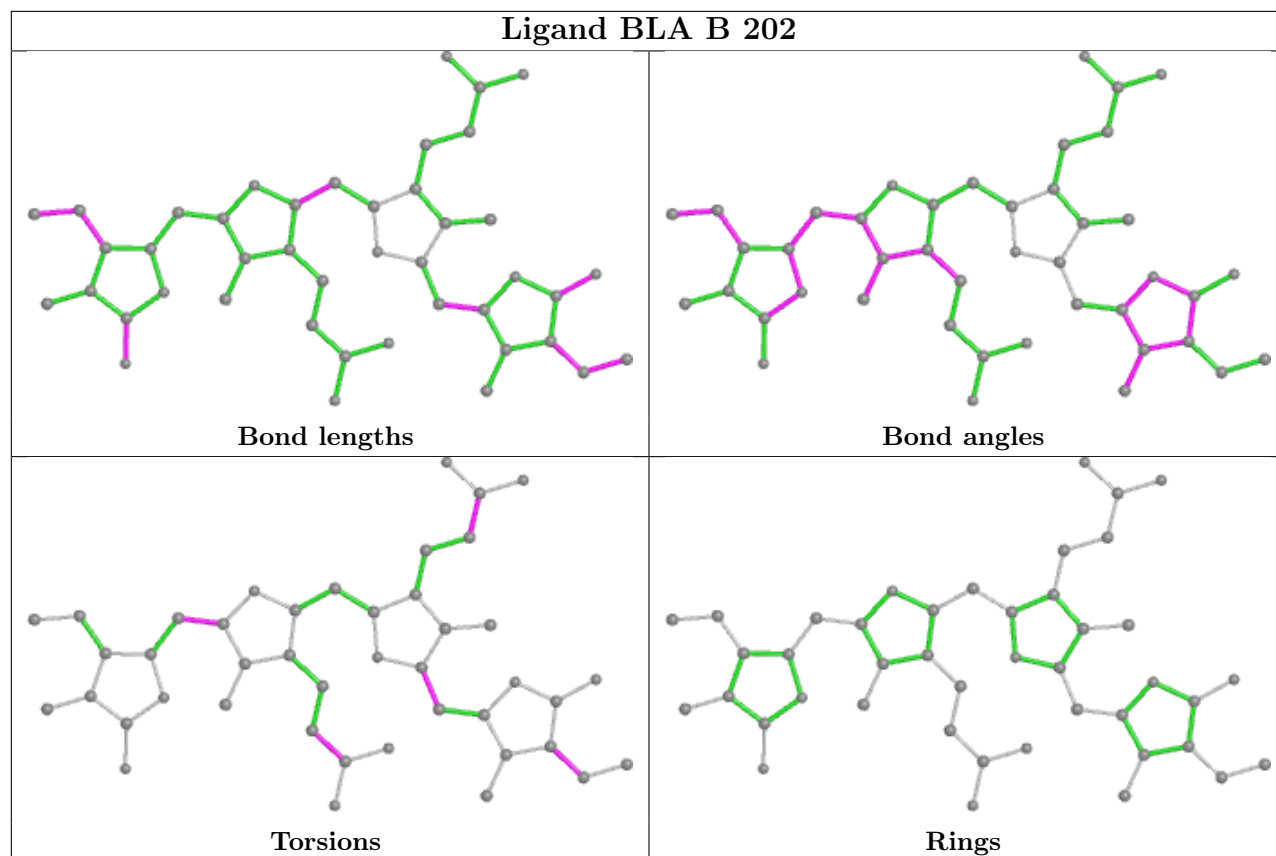
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	211	CYC	5	0
5	J	209	CYC	7	0
4	B	202	BLA	8	0
4	A	201	BLA	6	0
5	F	206	CYC	3	0
5	I	208	CYC	3	0
5	C	203	CYC	4	0
5	K	210	CYC	3	0
5	M	212	CYC	3	0
5	H	207	CYC	6	0
5	D	204	CYC	3	0
5	E	205	CYC	5	0

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

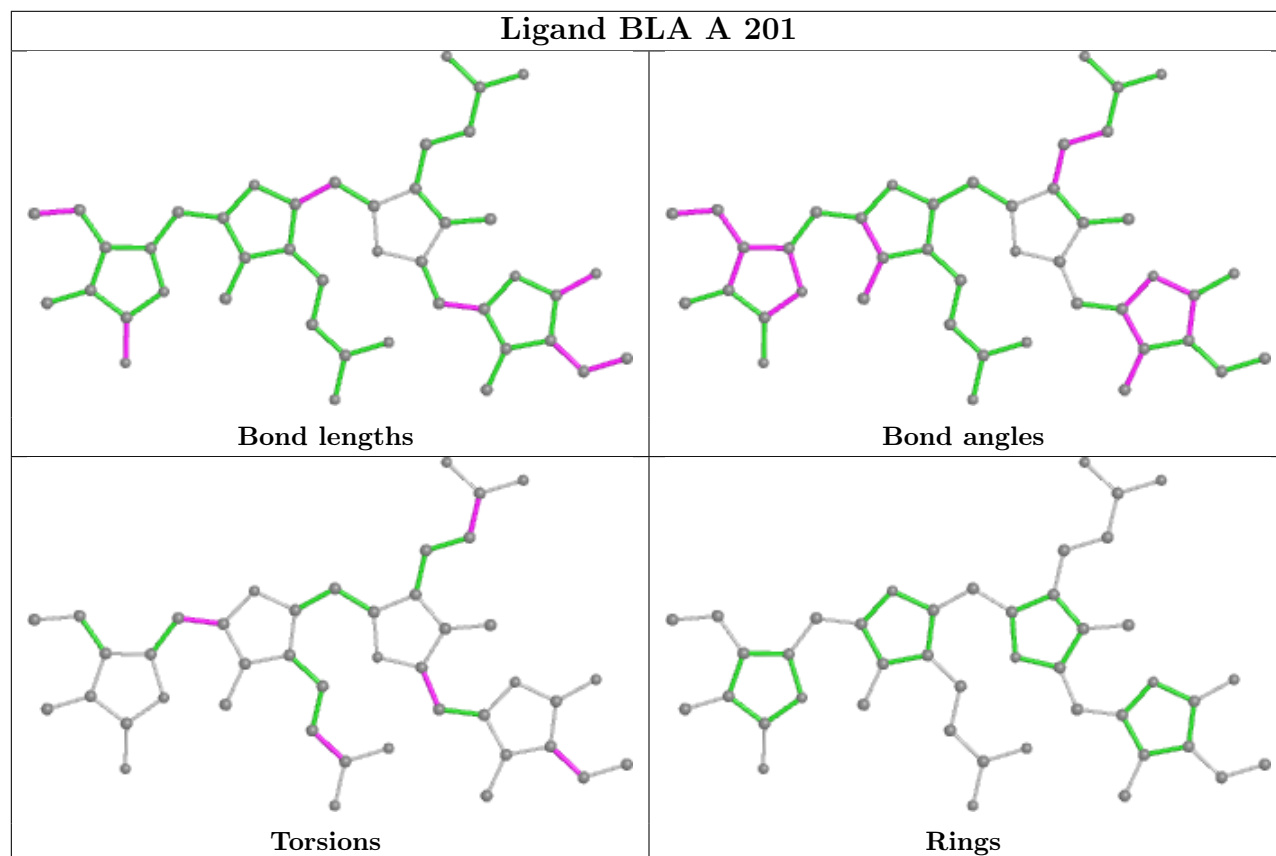
equivalents in the CSD to analyse the geometry.



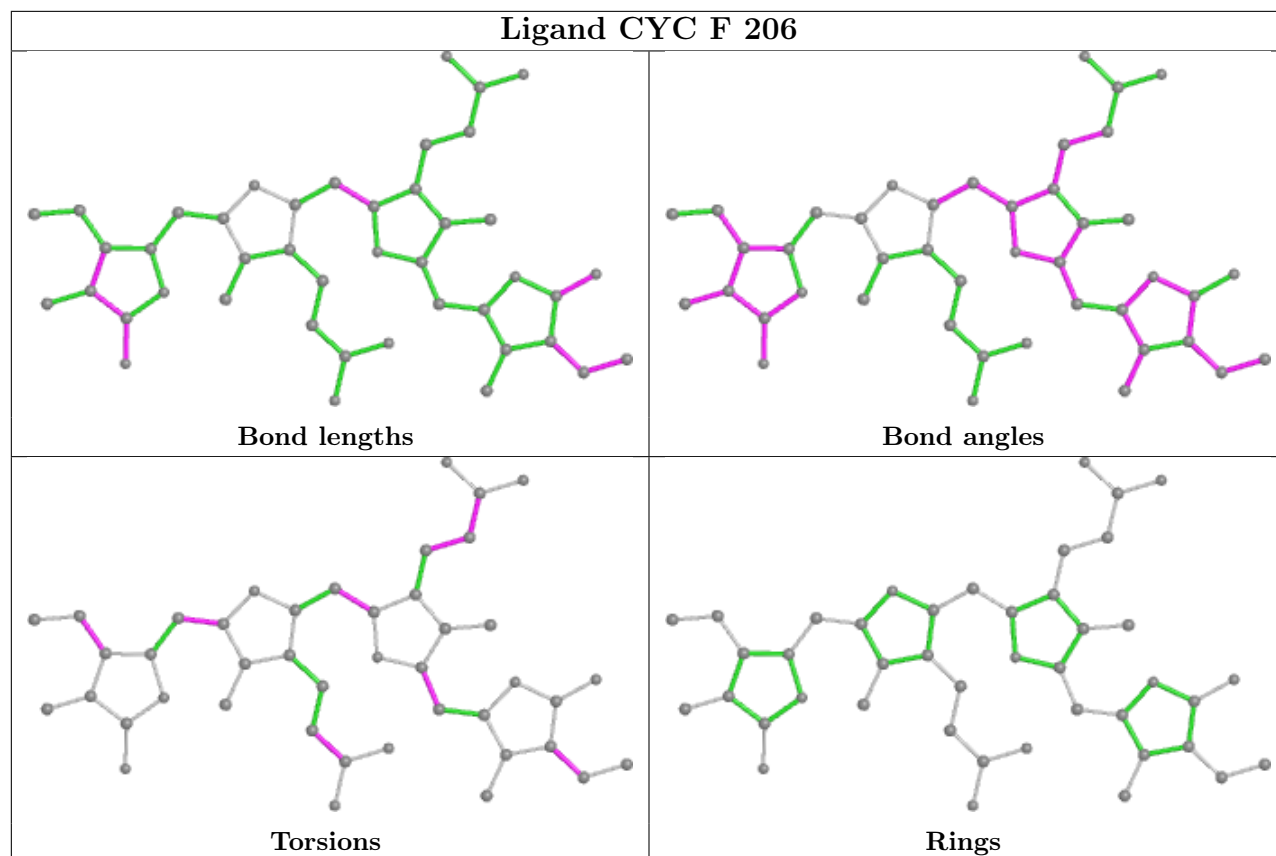
Ligand BLA B 202



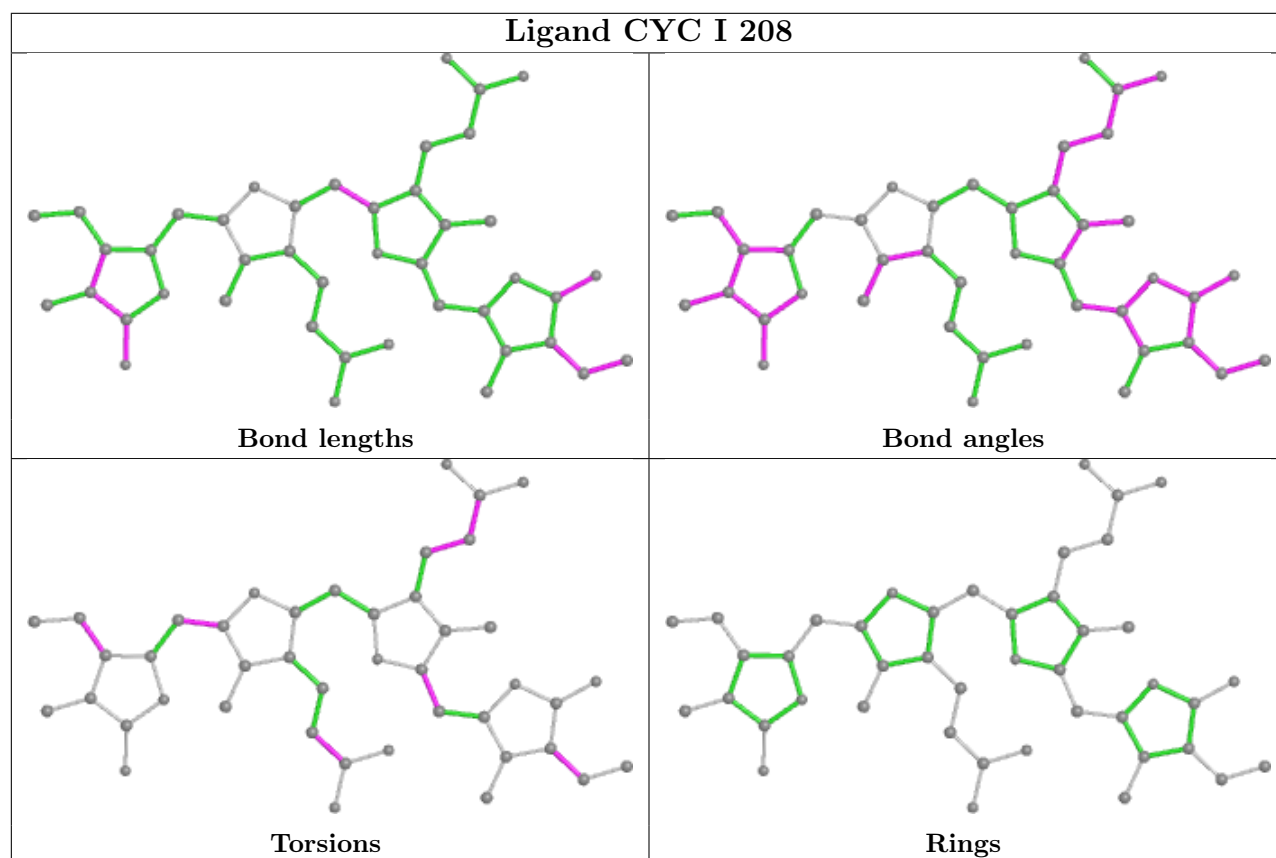
Ligand BLA A 201

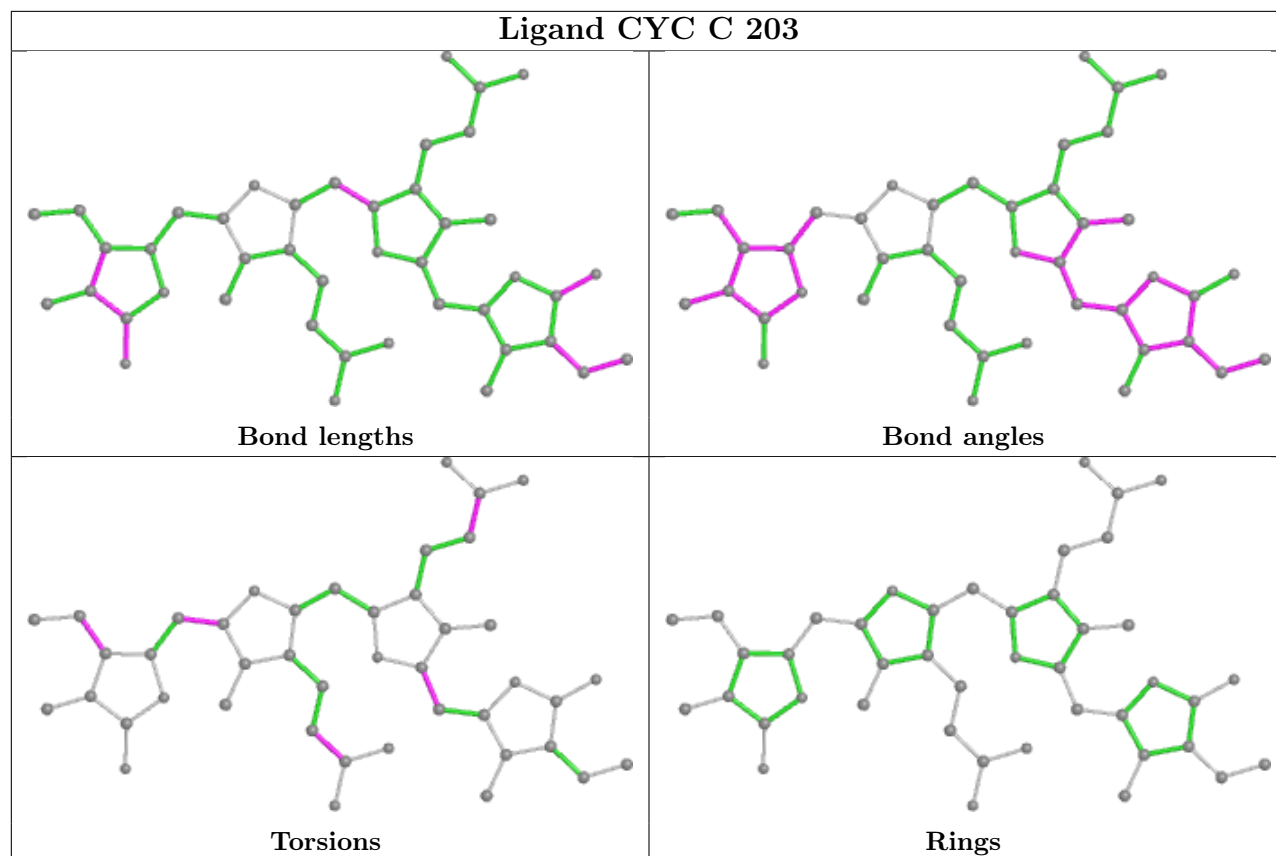
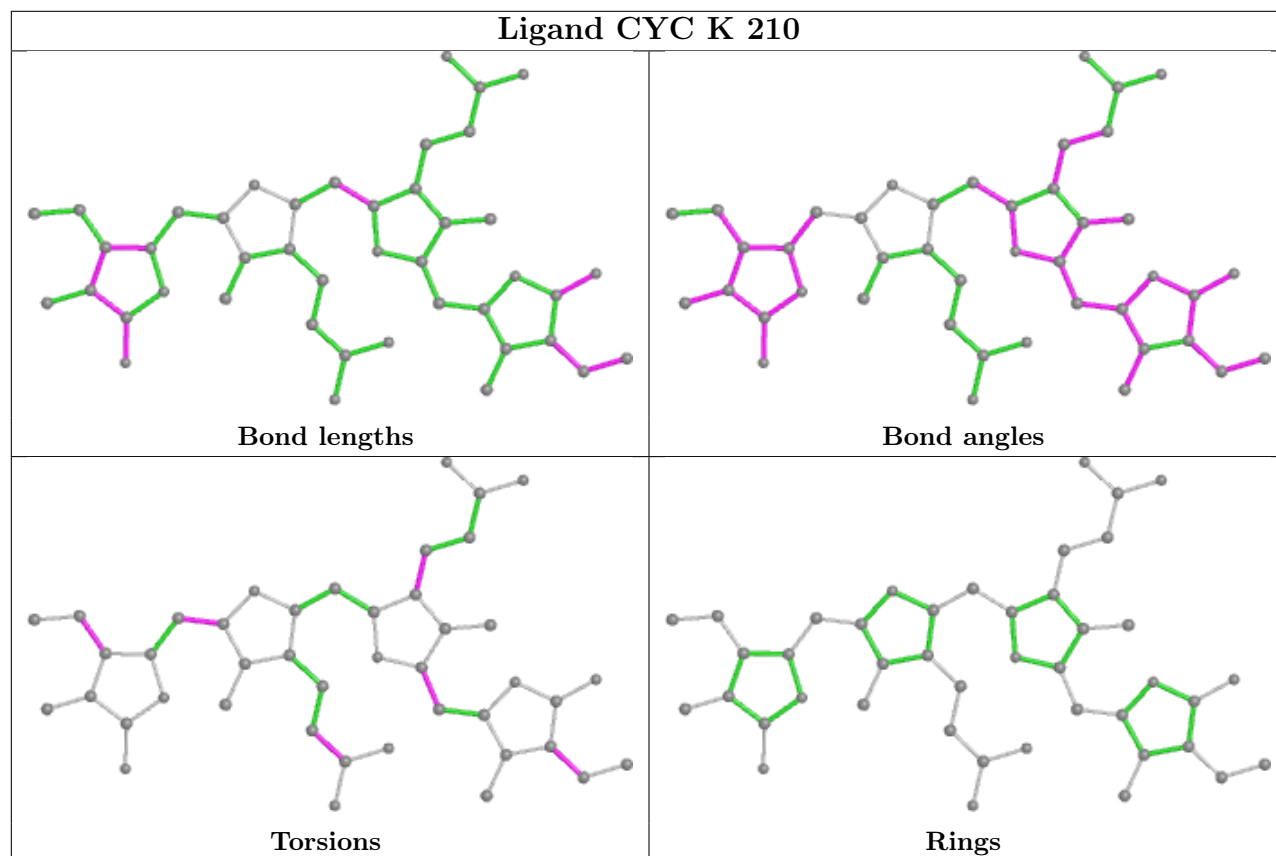


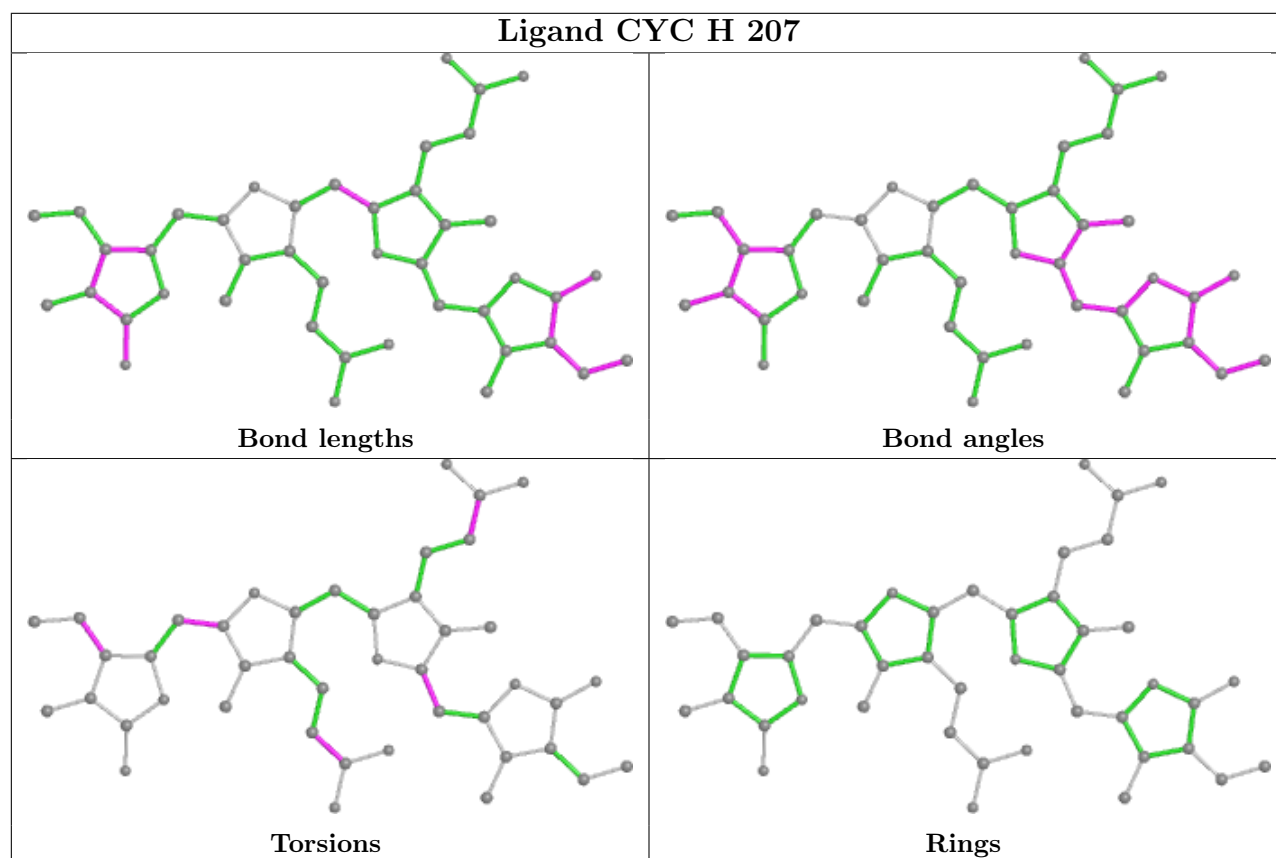
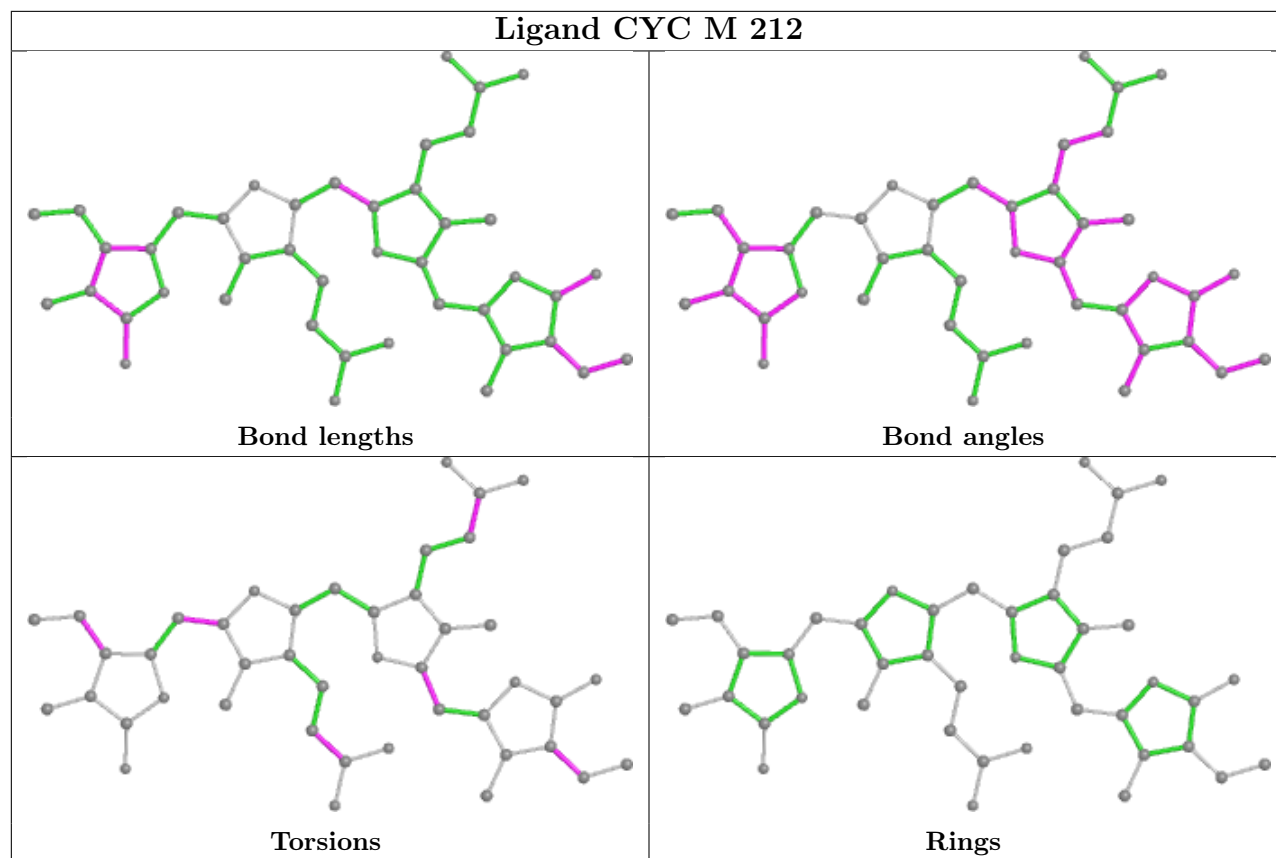
Ligand CYC F 206

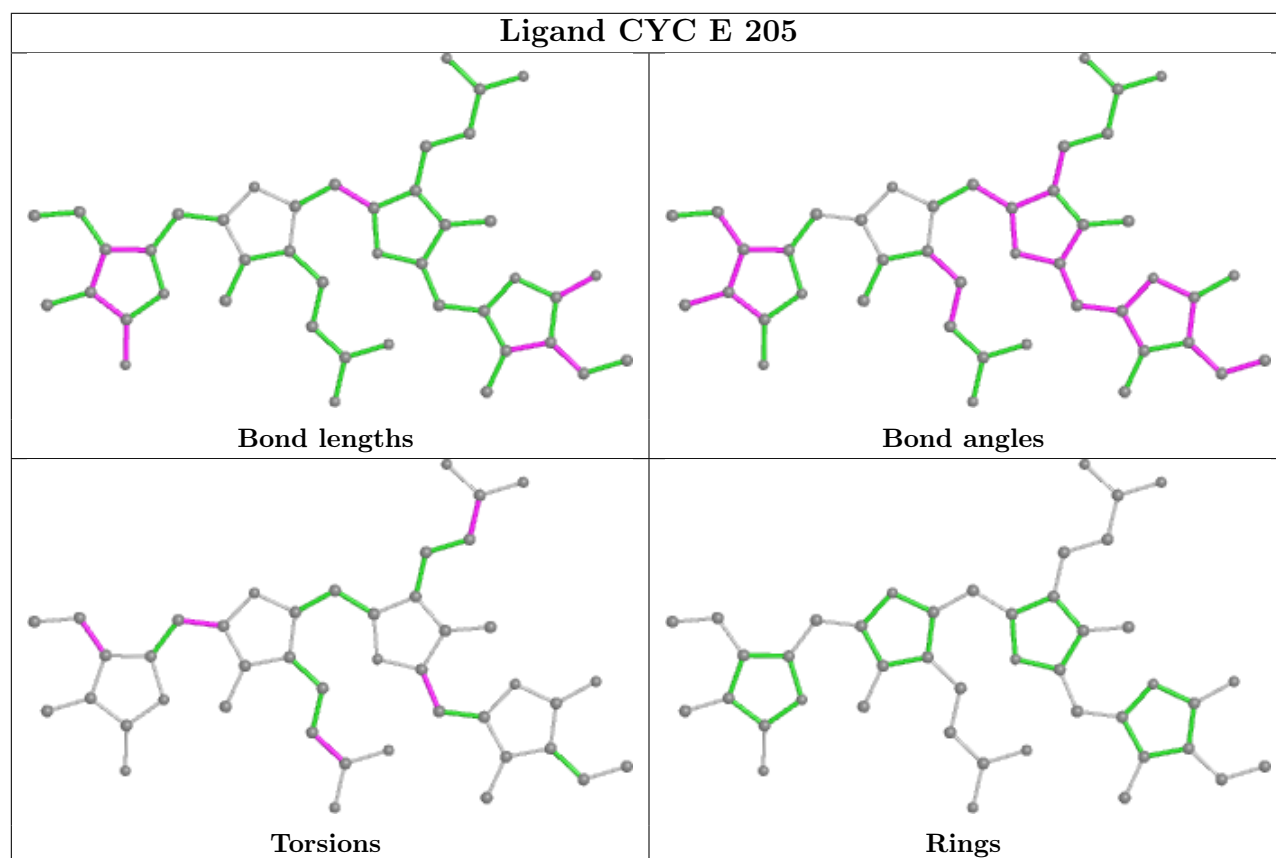
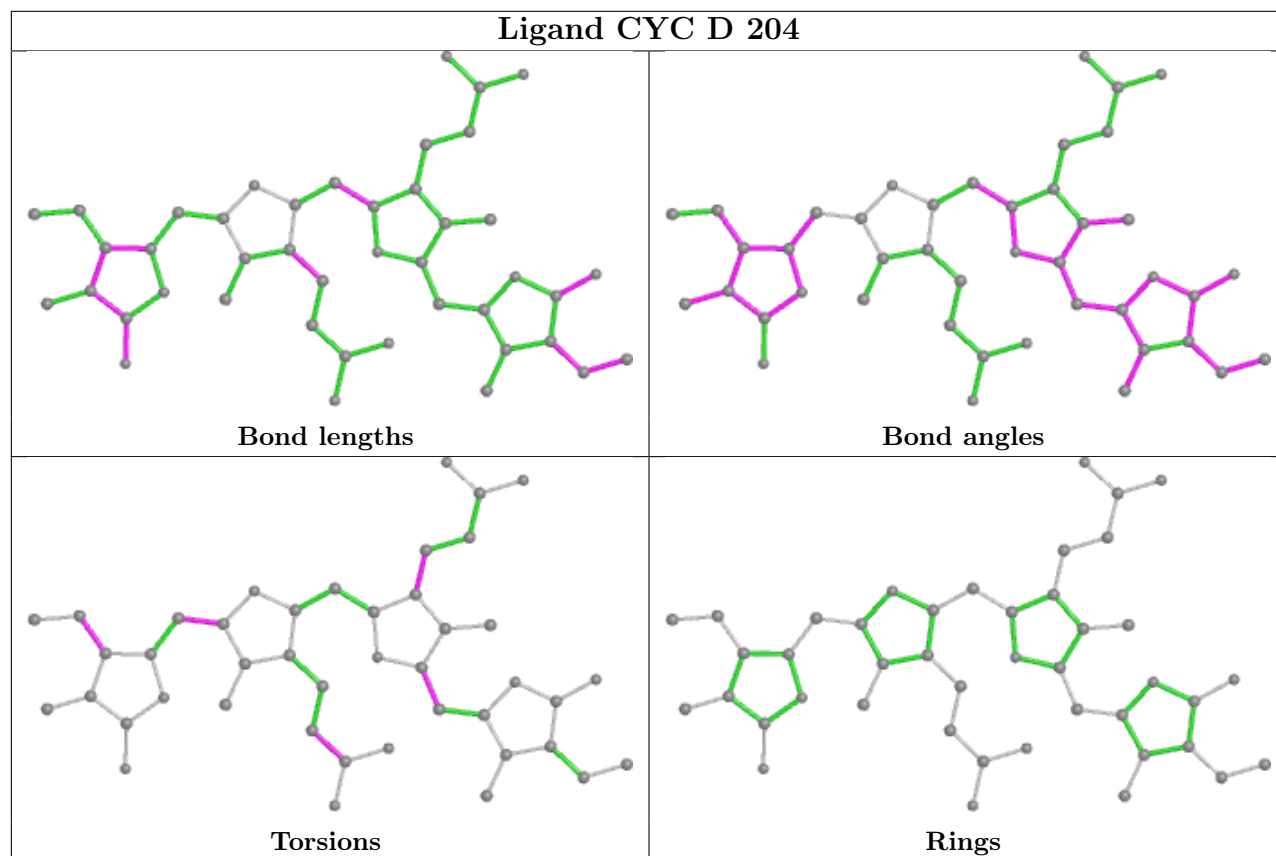


Ligand CYC I 208



Ligand CYC C 203**Ligand CYC K 210**





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.