



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 10:16 AM JST

PDB ID : 8HP9  
EMDB ID : EMD-34928  
Title : Cryo-EM structure of SARS-CoV-2 Omicron BA.2 S-trimer in complex with  
fab L4.65 and L5.34  
Authors : Gao, G.F.; Liu, S.  
Deposited on : 2022-12-12  
Resolution : 2.75 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

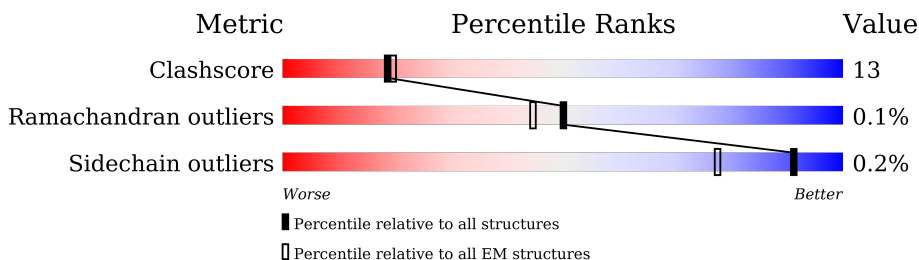
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.75 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1131	72% 21% 6%
1	B	1131	71% 22% 6%
1	C	1131	73% 21% 6%
2	J	215	66% 34%
2	L	215	65% 35%
2	Q	215	73% 27%
3	H	231	66% 34%
3	I	231	68% 32%
3	P	231	68% 32%

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Mol	Chain	Length	Quality of chain
4	E	224	 66%33%
4	K	224	 63%36%.
4	M	224	 60%40%
5	F	216	 68%32%
5	N	216	 68%32%
5	O	216	 63%37%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45516 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike protein S2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8318	5319	1387	1574	38		
1	B	1059	Total	C	N	O	S	0	0
			8311	5320	1385	1568	38		
1	C	1059	Total	C	N	O	S	0	0
			8304	5315	1385	1566	38		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ILE	THR	conflict	UNP P0DTC2
A	43	SER	ALA	variant	UNP P0DTC2
A	158	ASP	GLY	variant	UNP P0DTC2
A	229	GLY	VAL	variant	UNP P0DTC2
A	355	ASP	GLY	variant	UNP P0DTC2
A	387	PHE	SER	variant	UNP P0DTC2
A	389	PRO	SER	variant	UNP P0DTC2
A	391	PHE	SER	variant	UNP P0DTC2
A	392	ALA	THR	variant	UNP P0DTC2
A	421	ASN	ASP	variant	UNP P0DTC2
A	424	SER	ARG	variant	UNP P0DTC2
A	433	ASN	LYS	variant	UNP P0DTC2
A	456	LYS	ASN	variant	UNP P0DTC2
A	493	ASN	SER	variant	UNP P0DTC2
A	494	LYS	THR	variant	UNP P0DTC2
A	500	ALA	GLU	variant	UNP P0DTC2
A	509	ARG	GLN	variant	UNP P0DTC2
A	514	ARG	GLN	variant	UNP P0DTC2
A	517	TYR	ASN	variant	UNP P0DTC2
A	521	HIS	TYR	variant	UNP P0DTC2
A	630	GLY	ASP	variant	UNP P0DTC2
A	671	TYR	HIS	variant	UNP P0DTC2
A	780	LYS	ASN	variant	UNP P0DTC2
A	812	TYR	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	833	PRO	PHE	conflict	UNP P0DTC2
A	908	PRO	ALA	conflict	UNP P0DTC2
A	915	PRO	ALA	conflict	UNP P0DTC2
A	958	PRO	ALA	conflict	UNP P0DTC2
A	970	HIS	GLN	variant	UNP P0DTC2
A	985	LYS	ASN	variant	UNP P0DTC2
A	1002	PRO	LYS	conflict	UNP P0DTC2
A	1003	PRO	VAL	conflict	UNP P0DTC2
B	38	ILE	THR	conflict	UNP P0DTC2
B	43	SER	ALA	variant	UNP P0DTC2
B	158	ASP	GLY	variant	UNP P0DTC2
B	229	GLY	VAL	variant	UNP P0DTC2
B	355	ASP	GLY	variant	UNP P0DTC2
B	387	PHE	SER	variant	UNP P0DTC2
B	389	PRO	SER	variant	UNP P0DTC2
B	391	PHE	SER	variant	UNP P0DTC2
B	392	ALA	THR	variant	UNP P0DTC2
B	421	ASN	ASP	variant	UNP P0DTC2
B	424	SER	ARG	variant	UNP P0DTC2
B	433	ASN	LYS	variant	UNP P0DTC2
B	456	LYS	ASN	variant	UNP P0DTC2
B	493	ASN	SER	variant	UNP P0DTC2
B	494	LYS	THR	variant	UNP P0DTC2
B	500	ALA	GLU	variant	UNP P0DTC2
B	509	ARG	GLN	variant	UNP P0DTC2
B	514	ARG	GLN	variant	UNP P0DTC2
B	517	TYR	ASN	variant	UNP P0DTC2
B	521	HIS	TYR	variant	UNP P0DTC2
B	630	GLY	ASP	variant	UNP P0DTC2
B	671	TYR	HIS	variant	UNP P0DTC2
B	780	LYS	ASN	variant	UNP P0DTC2
B	812	TYR	ASP	variant	UNP P0DTC2
B	833	PRO	PHE	conflict	UNP P0DTC2
B	908	PRO	ALA	conflict	UNP P0DTC2
B	915	PRO	ALA	conflict	UNP P0DTC2
B	958	PRO	ALA	conflict	UNP P0DTC2
B	970	HIS	GLN	variant	UNP P0DTC2
B	985	LYS	ASN	variant	UNP P0DTC2
B	1002	PRO	LYS	conflict	UNP P0DTC2
B	1003	PRO	VAL	conflict	UNP P0DTC2
C	38	ILE	THR	conflict	UNP P0DTC2
C	43	SER	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	158	ASP	GLY	variant	UNP P0DTC2
C	229	GLY	VAL	variant	UNP P0DTC2
C	355	ASP	GLY	variant	UNP P0DTC2
C	387	PHE	SER	variant	UNP P0DTC2
C	389	PRO	SER	variant	UNP P0DTC2
C	391	PHE	SER	variant	UNP P0DTC2
C	392	ALA	THR	variant	UNP P0DTC2
C	421	ASN	ASP	variant	UNP P0DTC2
C	424	SER	ARG	variant	UNP P0DTC2
C	433	ASN	LYS	variant	UNP P0DTC2
C	456	LYS	ASN	variant	UNP P0DTC2
C	493	ASN	SER	variant	UNP P0DTC2
C	494	LYS	THR	variant	UNP P0DTC2
C	500	ALA	GLU	variant	UNP P0DTC2
C	509	ARG	GLN	variant	UNP P0DTC2
C	514	ARG	GLN	variant	UNP P0DTC2
C	517	TYR	ASN	variant	UNP P0DTC2
C	521	HIS	TYR	variant	UNP P0DTC2
C	630	GLY	ASP	variant	UNP P0DTC2
C	671	TYR	HIS	variant	UNP P0DTC2
C	780	LYS	ASN	variant	UNP P0DTC2
C	812	TYR	ASP	variant	UNP P0DTC2
C	833	PRO	PHE	conflict	UNP P0DTC2
C	908	PRO	ALA	conflict	UNP P0DTC2
C	915	PRO	ALA	conflict	UNP P0DTC2
C	958	PRO	ALA	conflict	UNP P0DTC2
C	970	HIS	GLN	variant	UNP P0DTC2
C	985	LYS	ASN	variant	UNP P0DTC2
C	1002	PRO	LYS	conflict	UNP P0DTC2
C	1003	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
2	Q	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
2	J	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		

- Molecule 3 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
3	P	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
3	I	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		

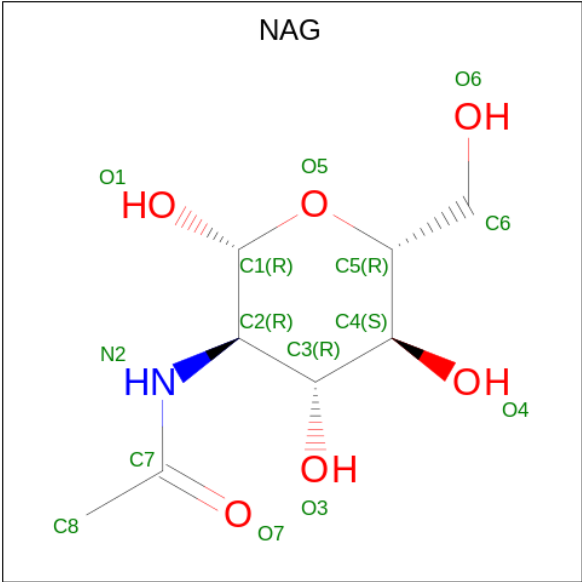
- Molecule 4 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		
4	E	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		
4	K	224	Total	C	N	O	S	0	0
			1656	1040	279	329	8		

- Molecule 5 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		
5	F	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		
5	O	216	Total	C	N	O	S	0	0
			1641	1020	280	335	6		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

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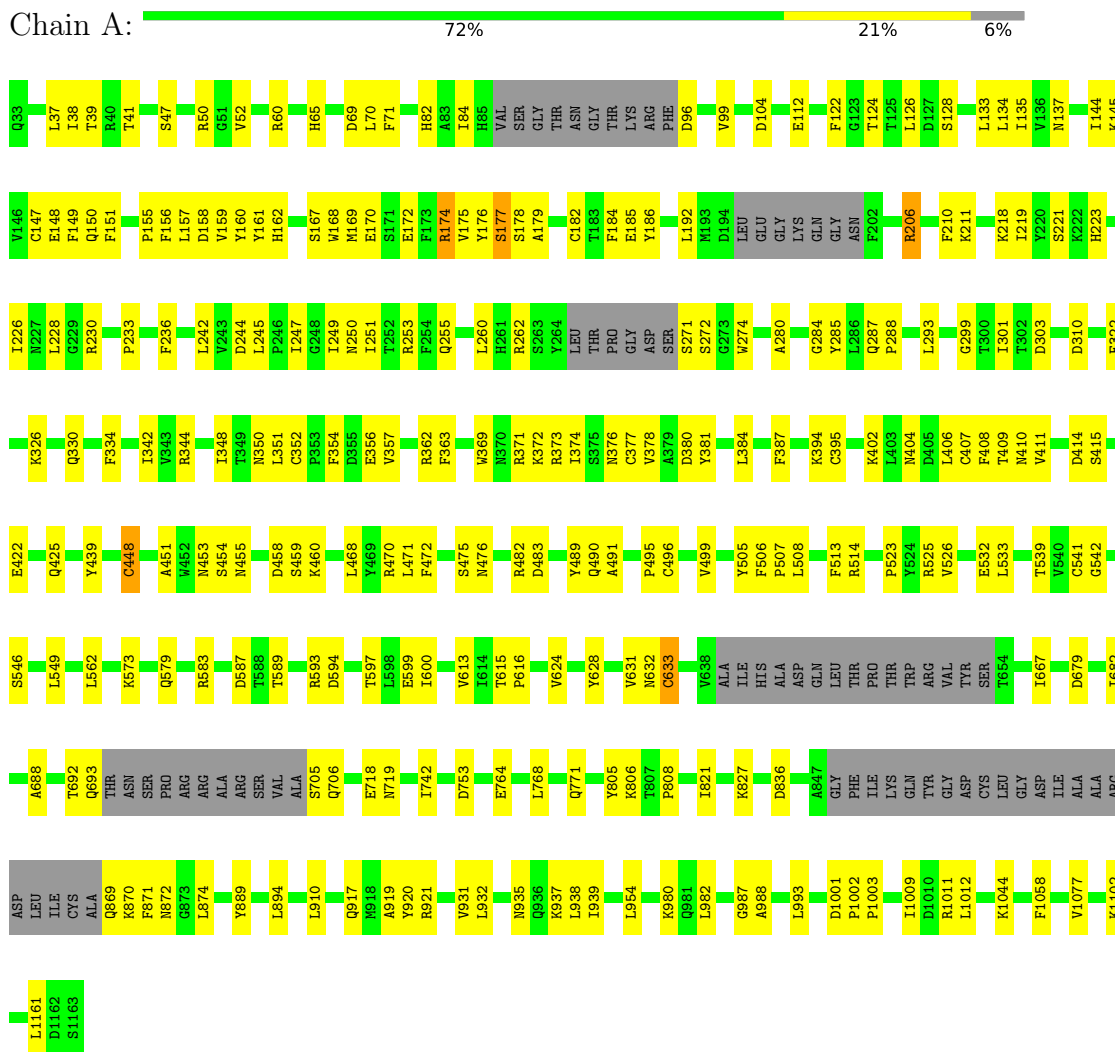
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

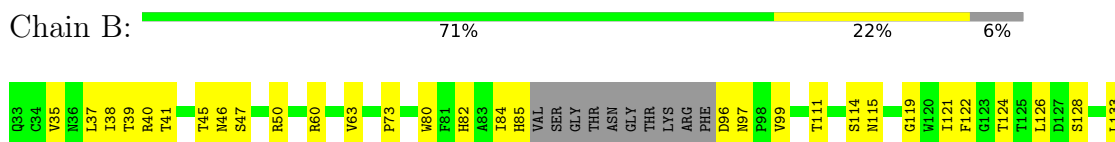
### 3 Residue-property plots

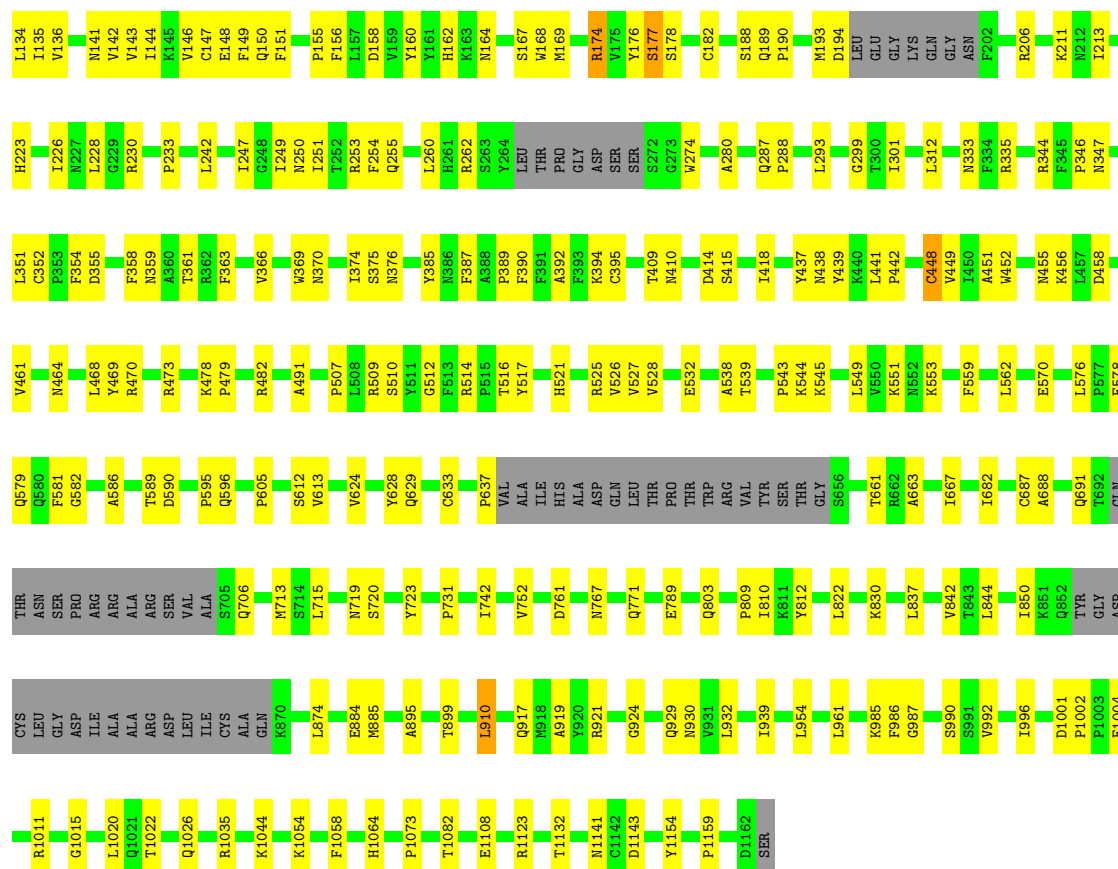
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

- Molecule 1: Spike protein S2'



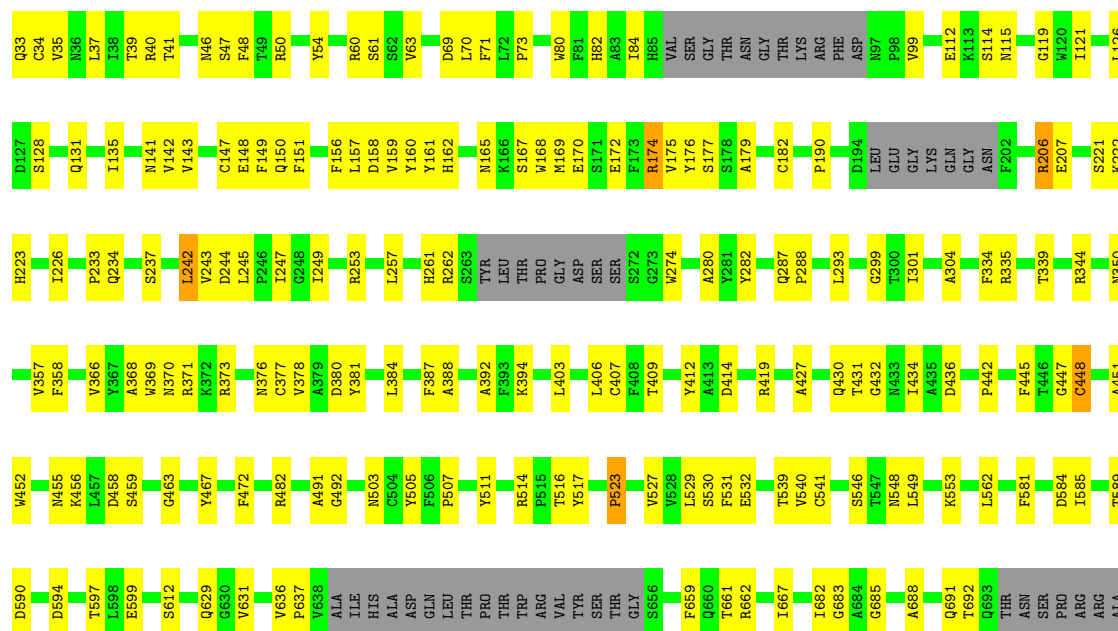
- Molecule 1: Spike protein S2'

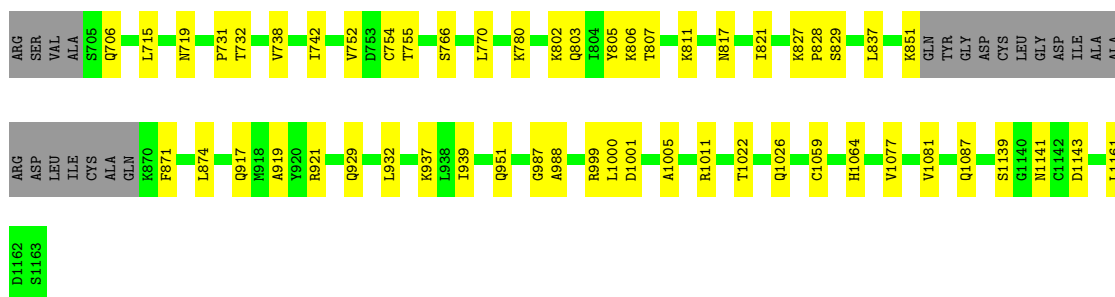




### • Molecule 1: Spike protein S2'

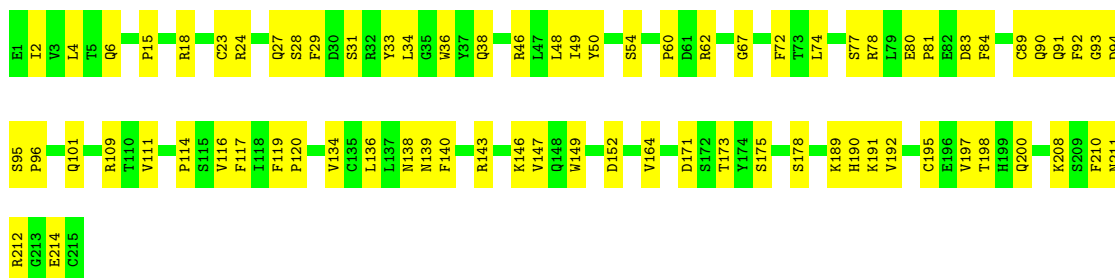
Chain C: 73% 21% 6%





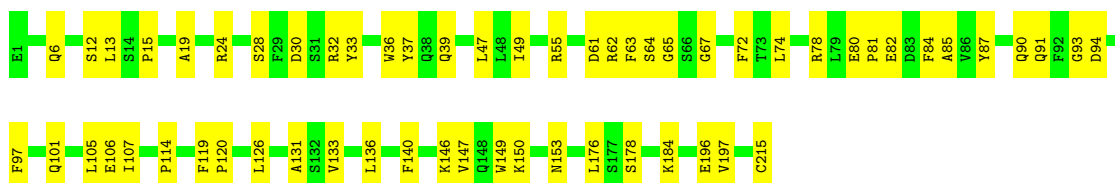
- Molecule 2: fab L4.65

Chain L: 65% 35%



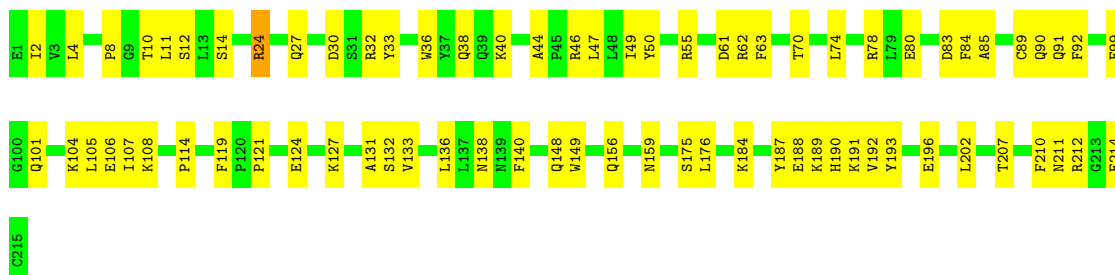
- Molecule 2: fab L4.65

Chain Q: 73% 27%



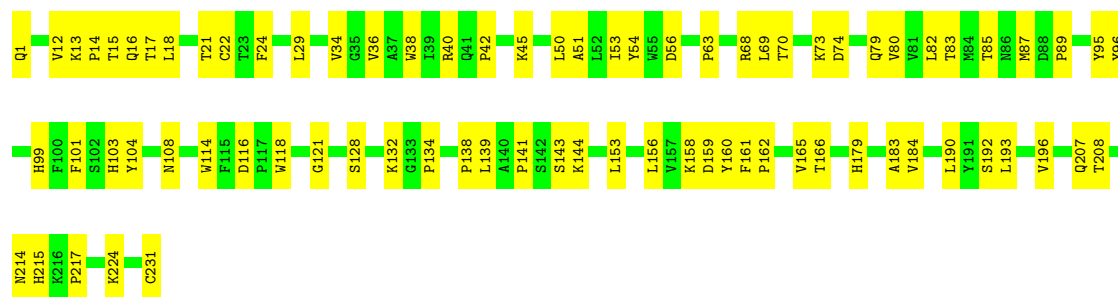
- Molecule 2: fab L4.65

Chain J: 66% 34%



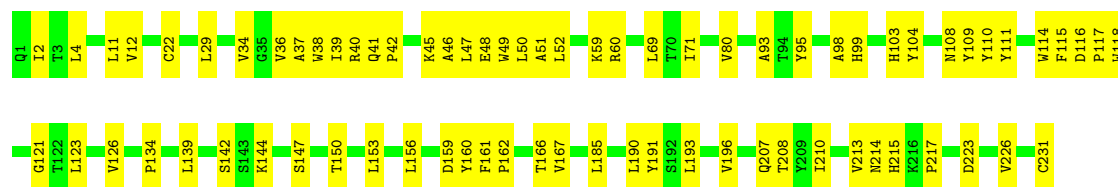
- Molecule 3: fab L4.65

Chain H: 66% 34%



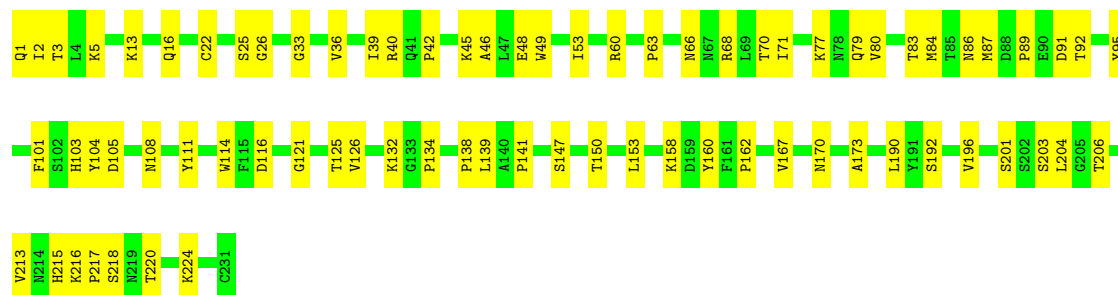
- Molecule 3: fab L4.65

Chain P: 68% 32%



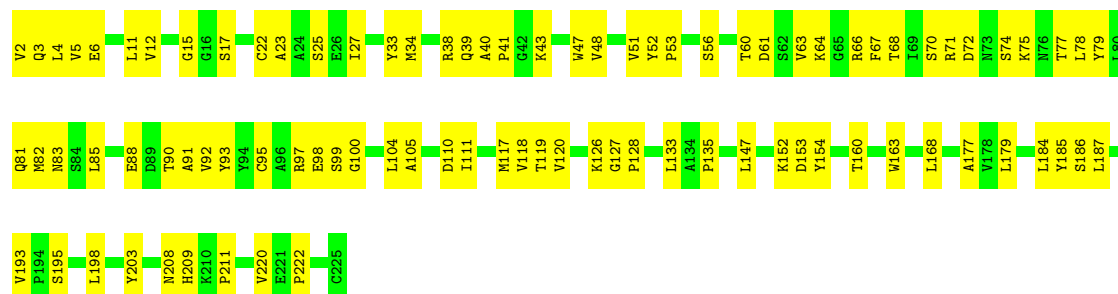
- Molecule 3: fab L4.65

Chain I: 68% 32%



- Molecule 4: fab L5.34

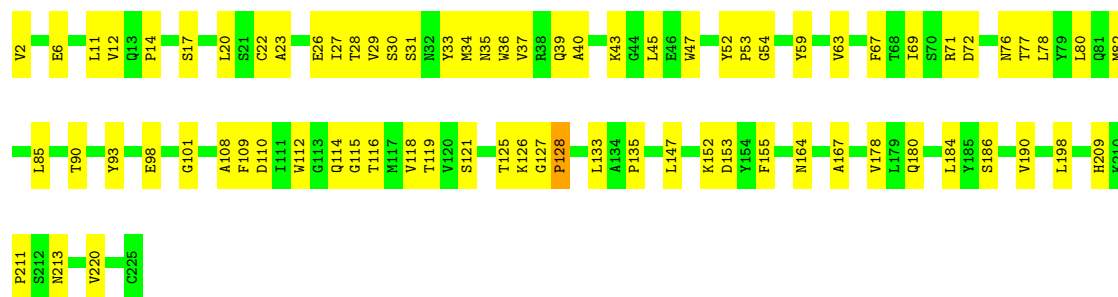
Chain M: 60% 40%



- Molecule 4: fab L5.34

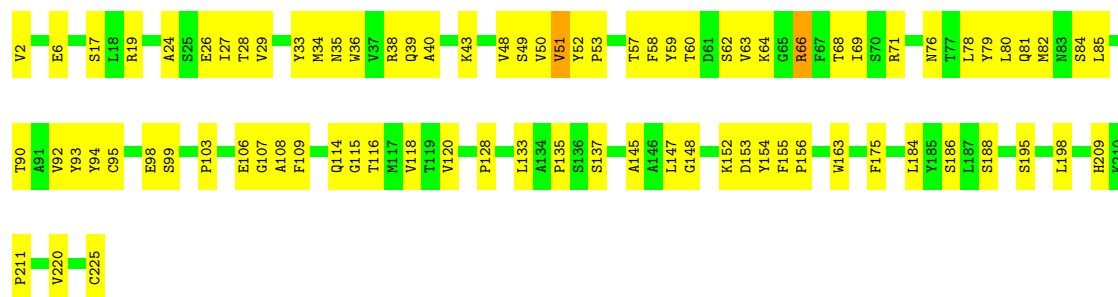
Chain E: 66% 33%





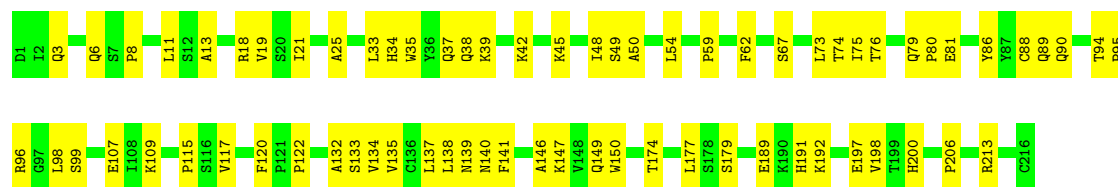
- Molecule 4: fab L5.34

Chain K: 63% 36%



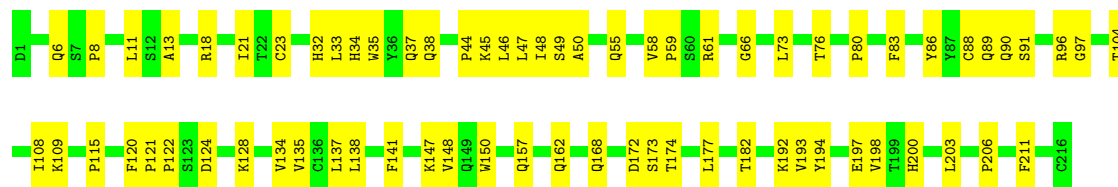
- Molecule 5: fab L5.34

Chain N: 68% 32%



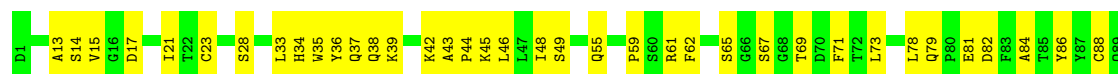
- Molecule 5: fab L5.34

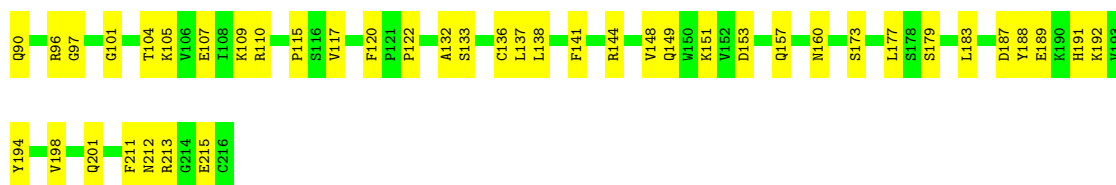
Chain F: 68% 32%



- Molecule 5: fab L5.34

Chain O: 63% 37%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	588002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.39	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor



## 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: NAG

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	0.51	0/8517	0.57	1/11591 (0.0%)
1	B	0.51	0/8511	0.58	4/11581 (0.0%)
1	C	0.53	2/8502 (0.0%)	0.62	7/11567 (0.1%)
2	J	0.26	0/1694	0.54	0/2294
2	L	0.26	0/1694	0.52	0/2294
2	Q	0.26	0/1694	0.53	0/2294
3	H	0.27	0/1805	0.52	0/2471
3	I	0.26	0/1805	0.52	0/2471
3	P	0.26	0/1805	0.50	0/2471
4	E	0.39	1/1694 (0.1%)	0.63	3/2308 (0.1%)
4	K	0.28	0/1694	0.56	1/2308 (0.0%)
4	M	0.28	0/1694	0.53	0/2308
5	F	0.26	0/1676	0.51	0/2272
5	N	0.27	0/1676	0.50	0/2272
5	O	0.26	0/1675	0.48	0/2272
All	All	0.43	3/46136 (0.0%)	0.56	16/62774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	637	PRO	CG-CD	-14.35	1.03	1.50
4	E	128	PRO	CG-CD	-11.27	1.13	1.50
1	C	821	ILE	C-N	-6.66	1.18	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	637	PRO	N-CD-CG	-17.88	76.38	103.20
4	E	128	PRO	N-CD-CG	-13.69	82.66	103.20
1	C	637	PRO	CA-CB-CG	-10.25	84.52	104.00
1	C	448	CYS	CA-CB-SG	7.83	128.09	114.00
1	A	448	CYS	CA-CB-SG	7.46	127.42	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	615	THR	Peptide
1	A	633	CYS	Peptide
1	B	633	CYS	Peptide
1	C	165	ASN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8318	0	8107	189	0
1	B	8311	0	8105	201	0
1	C	8304	0	8104	178	0
2	J	1658	0	1599	55	0
2	L	1658	0	1599	59	0
2	Q	1658	0	1599	48	0
3	H	1756	0	1713	58	0
3	I	1756	0	1713	52	0
3	P	1756	0	1713	54	0
4	E	1656	0	1620	58	0
4	K	1656	0	1620	62	0
4	M	1656	0	1620	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1642	0	1599	46	0
5	N	1642	0	1599	55	0
5	O	1641	0	1599	52	0
6	A	140	0	130	2	0
6	B	154	0	143	4	0
6	C	154	0	143	3	0
All	All	45516	0	44325	1138	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 13.

The worst 5 of 1138 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)
4:K:93:TYR:O	4:K:115:GLY:HA2	1.51	1.08
1:A:395:CYS:HA	1:A:448:CYS:HB3	1.40	1.03
4:E:90:THR:HA	4:E:118:VAL:O	1.62	0.99
4:E:93:TYR:O	4:E:115:GLY:HA2	1.62	0.99
1:B:149:PHE:HB3	1:B:176:TYR:HB2	1.44	0.97

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 PDB entries followed by that with respect to all EM entries.

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	1047/1131 (93%)	962 (92%)	84 (8%)	1 (0%)	48	70
1	B	1045/1131 (92%)	964 (92%)	80 (8%)	1 (0%)	48	70
1	C	1043/1131 (92%)	948 (91%)	94 (9%)	1 (0%)	48	70
2	J	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	L	213/215 (99%)	204 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
3	H	229/231 (99%)	216 (94%)	13 (6%)	0	100	100
3	I	229/231 (99%)	211 (92%)	18 (8%)	0	100	100
3	P	229/231 (99%)	215 (94%)	14 (6%)	0	100	100
4	E	222/224 (99%)	207 (93%)	15 (7%)	0	100	100
4	K	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
4	M	222/224 (99%)	205 (92%)	17 (8%)	0	100	100
5	F	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
5	N	214/216 (99%)	200 (94%)	14 (6%)	0	100	100
5	O	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
All	All	5769/6051 (95%)	5356 (93%)	410 (7%)	3 (0%)	50	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	SER
1	B	177	SER
1	C	177	SER

### 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 PDB entries followed by that with respect to all EM entries.

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	929/984 (94%)	927 (100%)	2 (0%)	92	96
1	B	927/984 (94%)	926 (100%)	1 (0%)	92	97
1	C	927/984 (94%)	925 (100%)	2 (0%)	92	96
2	J	186/186 (100%)	185 (100%)	1 (0%)	86	92
2	L	186/186 (100%)	184 (99%)	2 (1%)	70	83
2	Q	186/186 (100%)	185 (100%)	1 (0%)	86	92
3	H	204/204 (100%)	203 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	204/204 (100%)	204 (100%)	0	100	100
3	P	204/204 (100%)	204 (100%)	0	100	100
4	E	187/187 (100%)	187 (100%)	0	100	100
4	K	187/187 (100%)	186 (100%)	1 (0%)	86	92
4	M	187/187 (100%)	187 (100%)	0	100	100
5	F	189/189 (100%)	189 (100%)	0	100	100
5	N	189/189 (100%)	189 (100%)	0	100	100
5	O	189/189 (100%)	189 (100%)	0	100	100
All	All	5081/5250 (97%)	5070 (100%)	11 (0%)	91	96

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	174	ARG
1	C	206	ARG
4	K	66	ARG
2	J	24	ARG
3	H	1	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	90	GLN
5	O	149	GLN
5	N	37	GLN
2	Q	90	GLN
5	F	37	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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	$\# Z  > 2$
6	NAG	A	1203	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	B	2205	1	14,14,15	0.34	0	17,19,21	0.48	0
6	NAG	A	1208	1	14,14,15	0.38	0	17,19,21	0.49	0
6	NAG	C	1210	1	14,14,15	0.40	0	17,19,21	0.49	0
6	NAG	B	2211	1	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	C	1209	1	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	A	1206	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
6	NAG	C	1204	1	14,14,15	0.32	0	17,19,21	0.43	0
6	NAG	A	1210	1	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	C	1208	1	14,14,15	0.35	0	17,19,21	0.49	0
6	NAG	A	1209	1	14,14,15	0.29	0	17,19,21	0.49	0
6	NAG	C	1206	1	14,14,15	0.34	0	17,19,21	0.59	0
6	NAG	A	1202	1	14,14,15	0.18	0	17,19,21	0.59	0
6	NAG	B	2203	1	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
6	NAG	B	2204	1	14,14,15	0.30	0	17,19,21	0.37	0
6	NAG	C	1202	1	14,14,15	0.17	0	17,19,21	0.62	1 (5%)
6	NAG	B	2210	1	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
6	NAG	B	2206	1	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	C	1203	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)
6	NAG	B	2209	1	14,14,15	0.35	0	17,19,21	0.59	0
6	NAG	A	1204	1	14,14,15	0.15	0	17,19,21	0.64	1 (5%)
6	NAG	A	1201	1	14,14,15	0.23	0	17,19,21	0.34	0
6	NAG	A	1205	1	14,14,15	0.29	0	17,19,21	0.53	0
6	NAG	B	2208	1	14,14,15	0.38	0	17,19,21	0.63	1 (5%)
6	NAG	C	1211	1	14,14,15	0.18	0	17,19,21	0.46	0
6	NAG	C	1201	1	14,14,15	0.38	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	1205	1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
6	NAG	B	2201	1	14,14,15	0.41	0	17,19,21	0.38	0
6	NAG	B	2202	1	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	C	1207	1	14,14,15	0.37	0	17,19,21	0.51	0
6	NAG	B	2207	1	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
6	NAG	A	1207	1	14,14,15	0.26	0	17,19,21	0.62	1 (5%)

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
6	NAG	A	1203	1	-	1/6/23/26	0/1/1/1
6	NAG	B	2205	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1210	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2211	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1206	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1210	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1208	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1202	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2203	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2204	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	B	2210	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2206	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2209	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1205	1	-	1/6/23/26	0/1/1/1
6	NAG	B	2208	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1211	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
6	NAG	B	2201	1	-	1/6/23/26	0/1/1/1
6	NAG	B	2202	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2207	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1207	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2203	NAG	C1-O5-C5	2.65	115.78	112.19
6	C	1203	NAG	C1-O5-C5	2.30	115.31	112.19
6	A	1206	NAG	C1-O5-C5	2.16	115.12	112.19
6	B	2207	NAG	C1-O5-C5	2.15	115.10	112.19
6	C	1205	NAG	C1-O5-C5	2.09	115.03	112.19

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1209	NAG	O5-C5-C6-O6
6	B	2203	NAG	O5-C5-C6-O6
6	A	1210	NAG	O5-C5-C6-O6
6	C	1205	NAG	O5-C5-C6-O6
6	C	1211	NAG	O5-C5-C6-O6

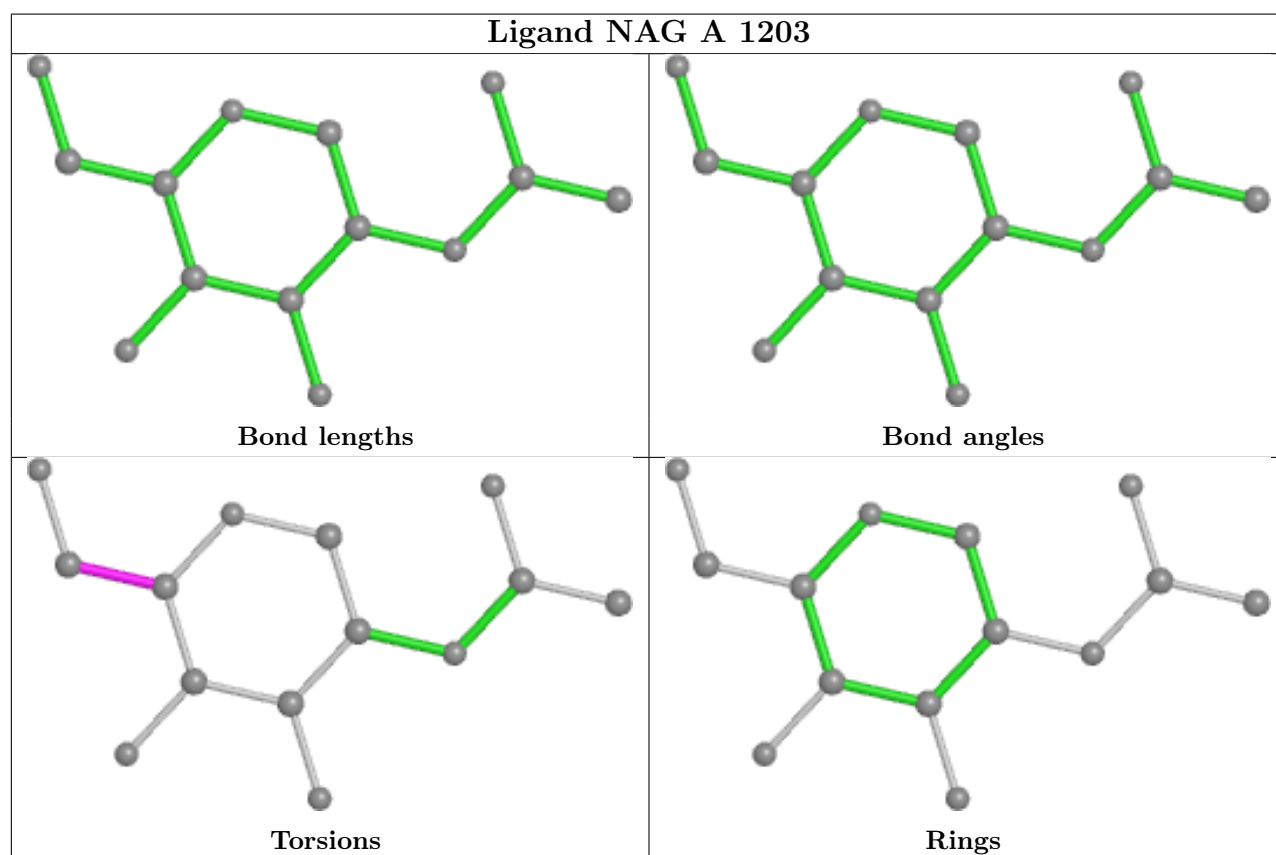
There are no ring outliers.

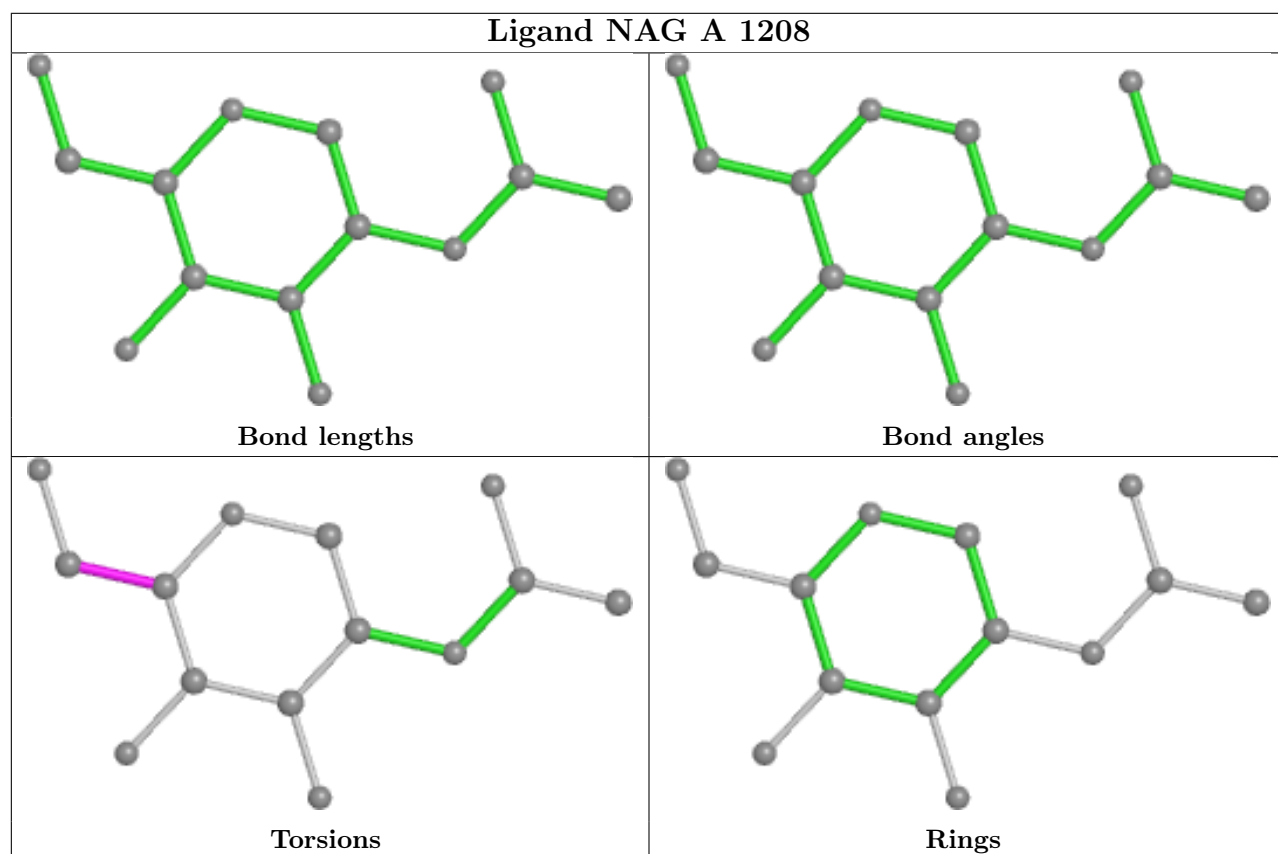
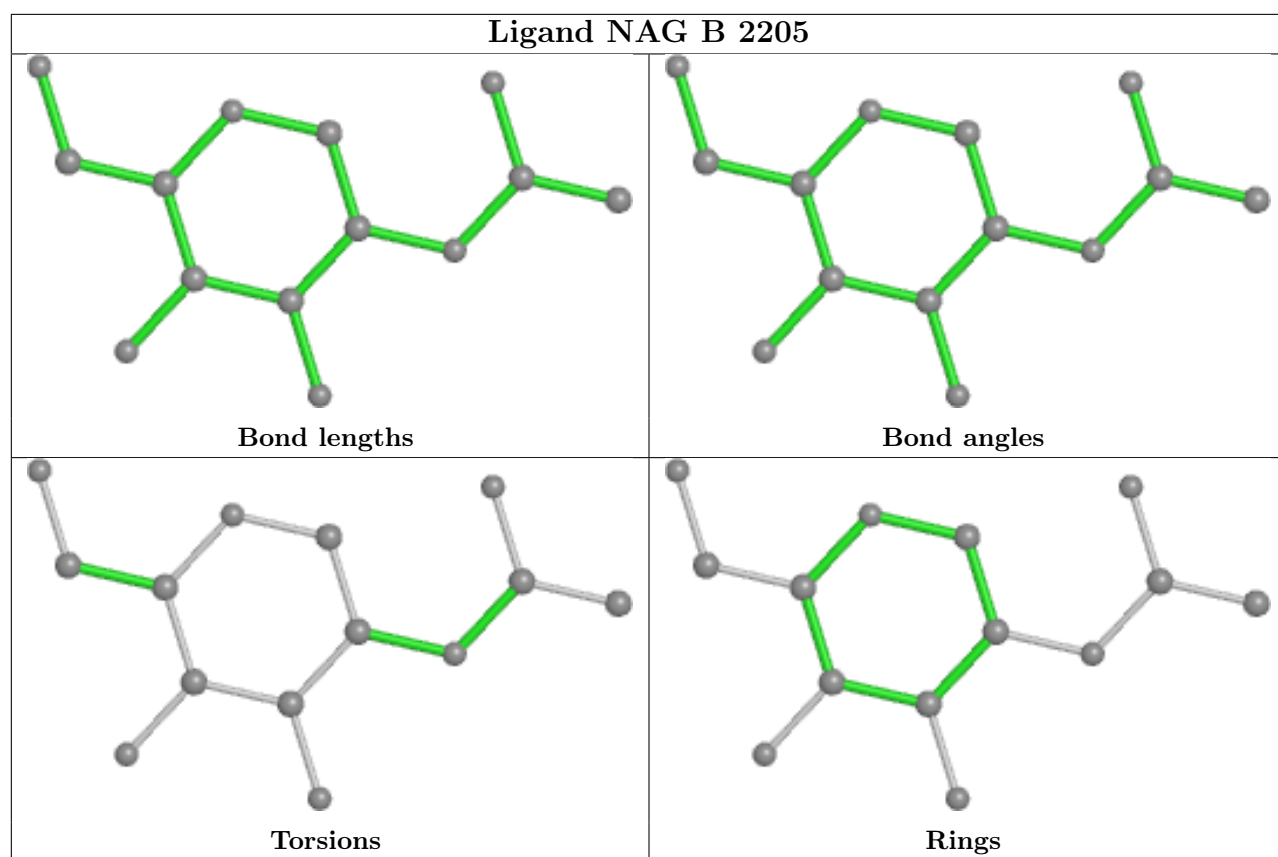
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2205	NAG	1	0
6	A	1206	NAG	1	0
6	C	1208	NAG	1	0
6	C	1206	NAG	1	0
6	B	2203	NAG	1	0
6	C	1202	NAG	1	0
6	A	1201	NAG	1	0
6	B	2202	NAG	2	0

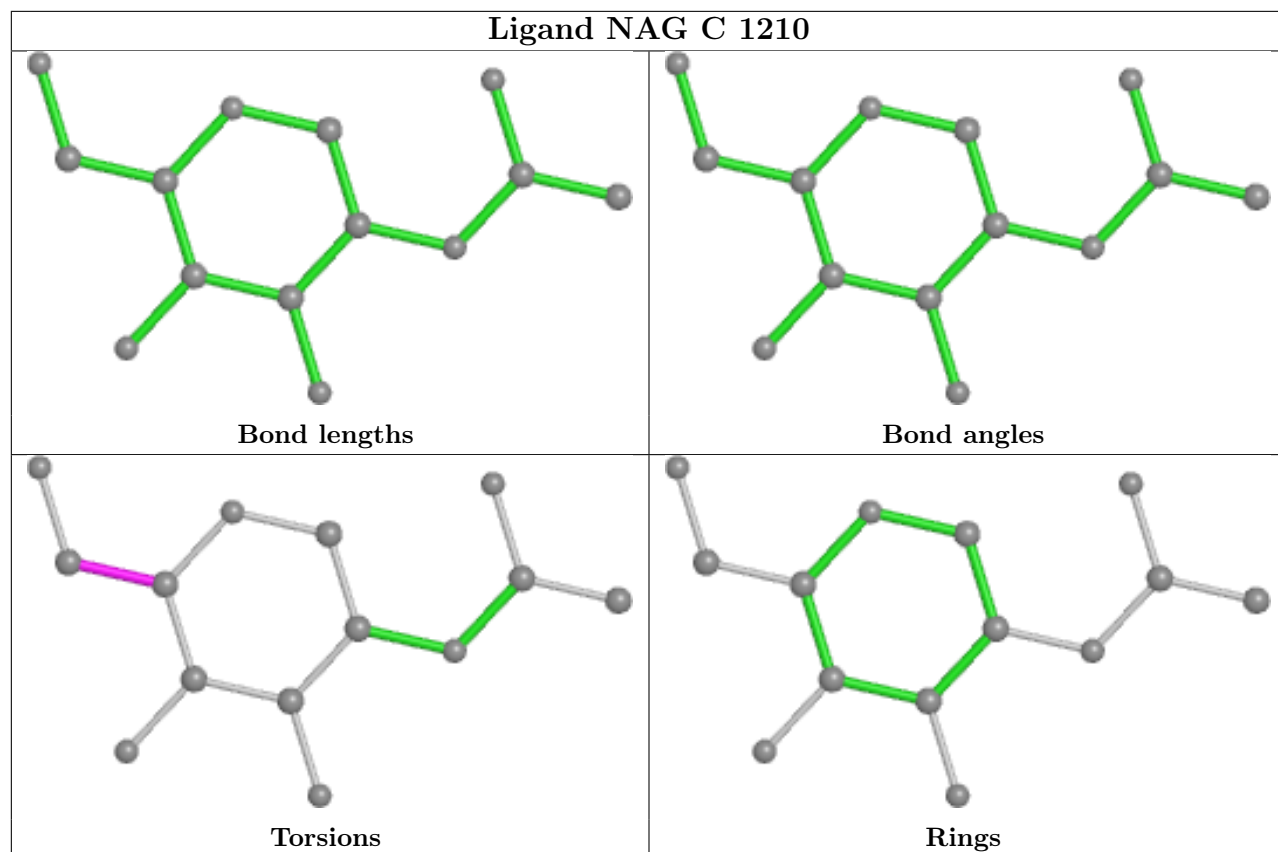


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

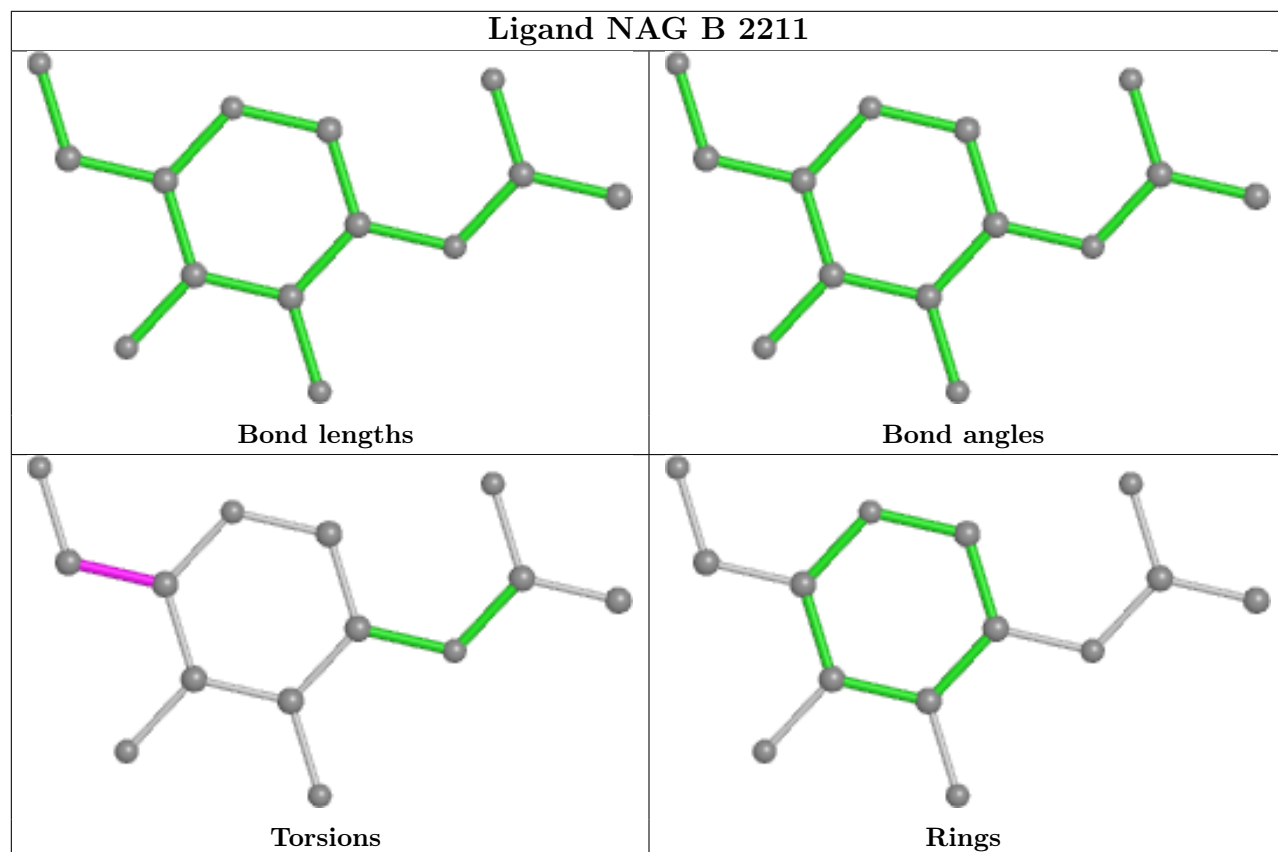


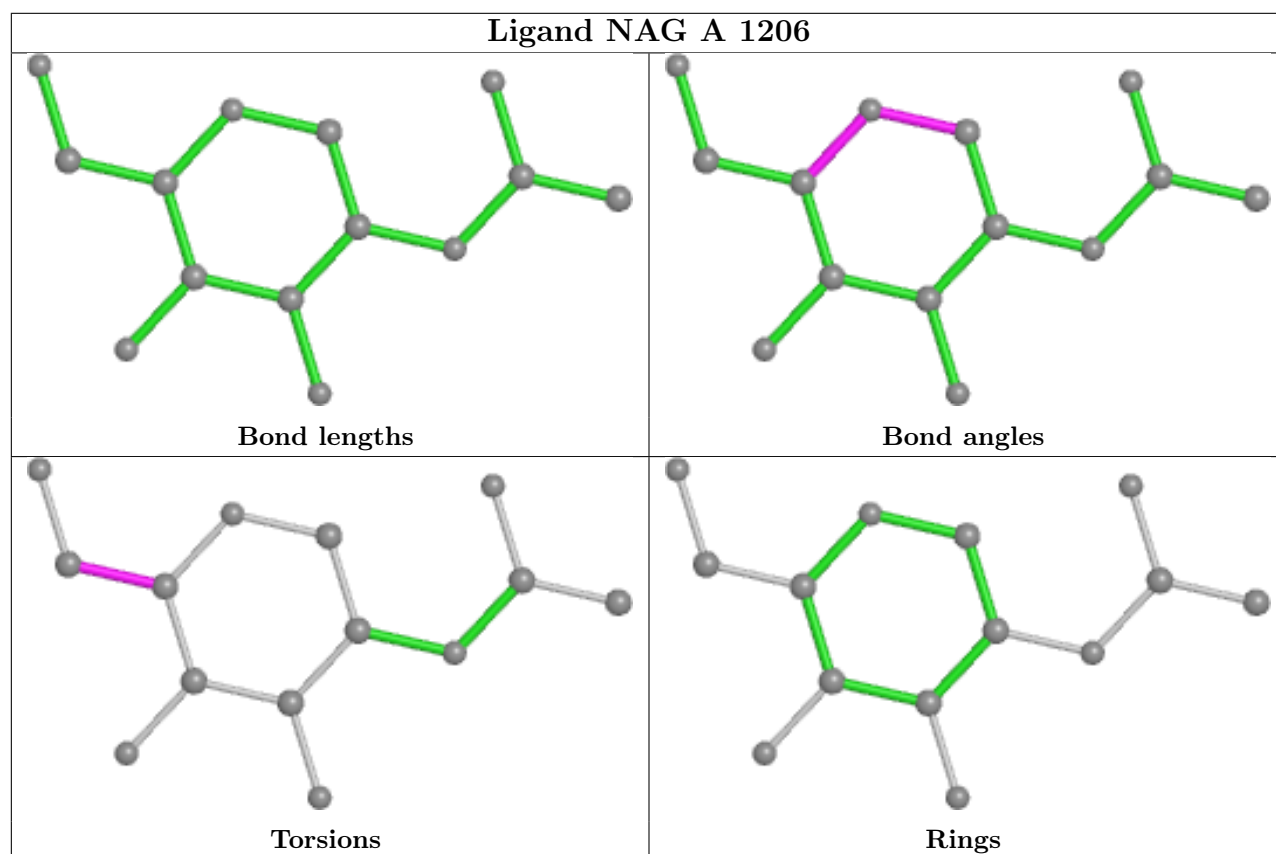
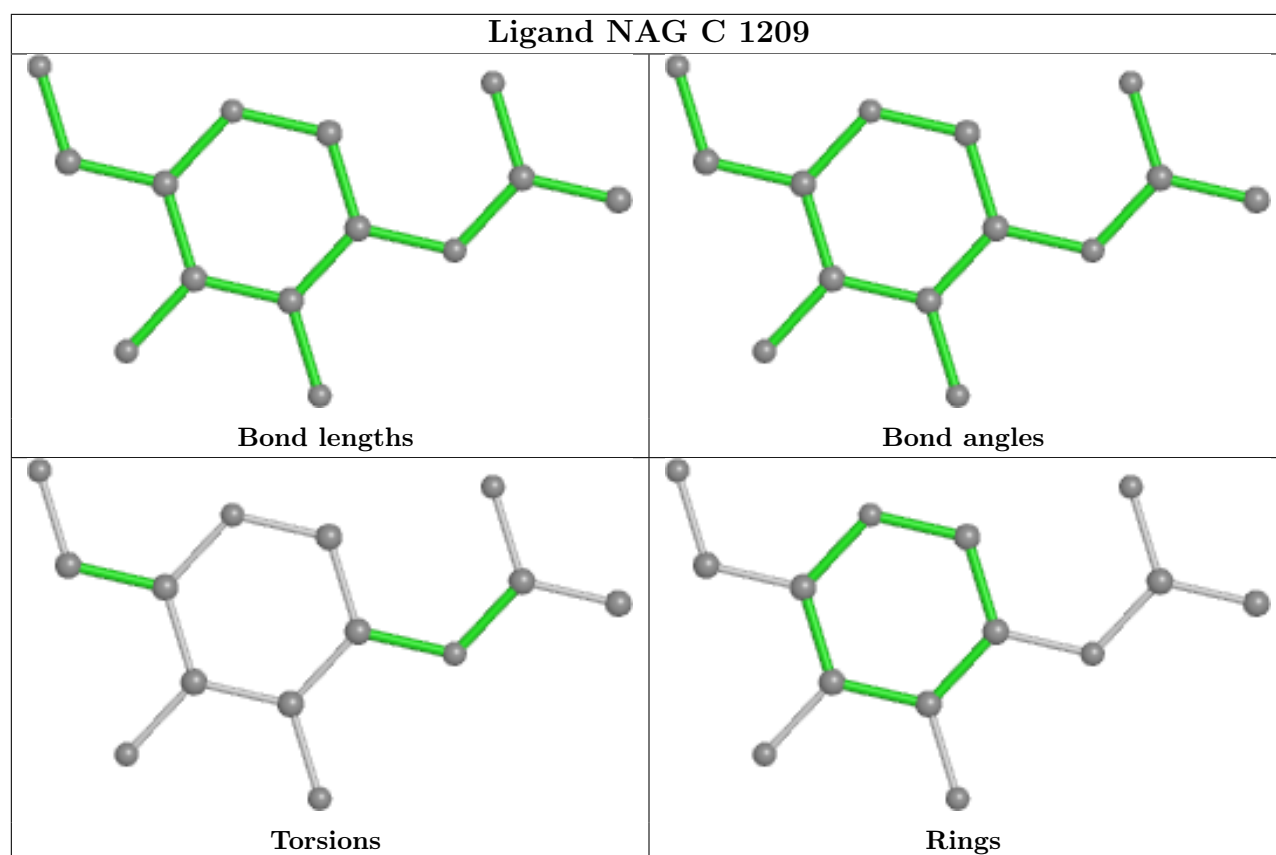


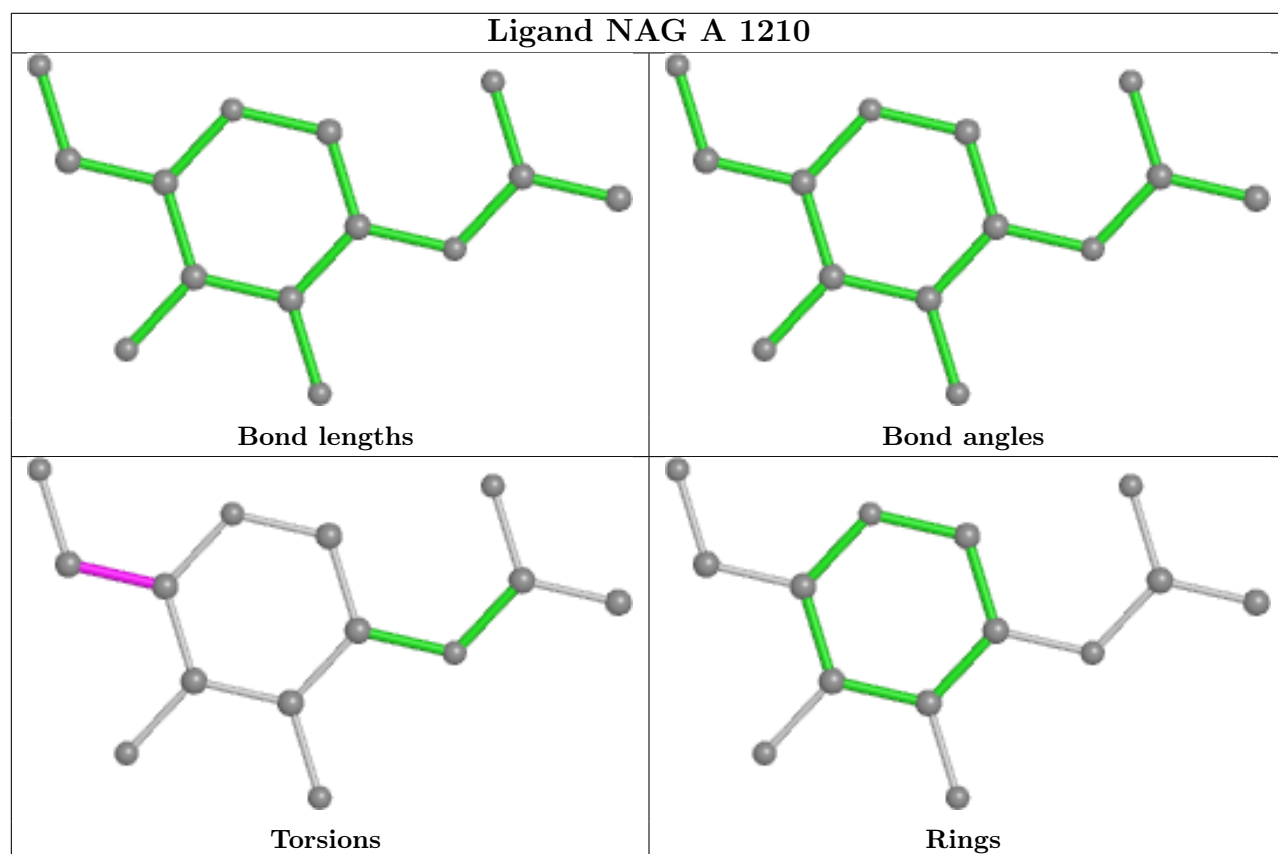
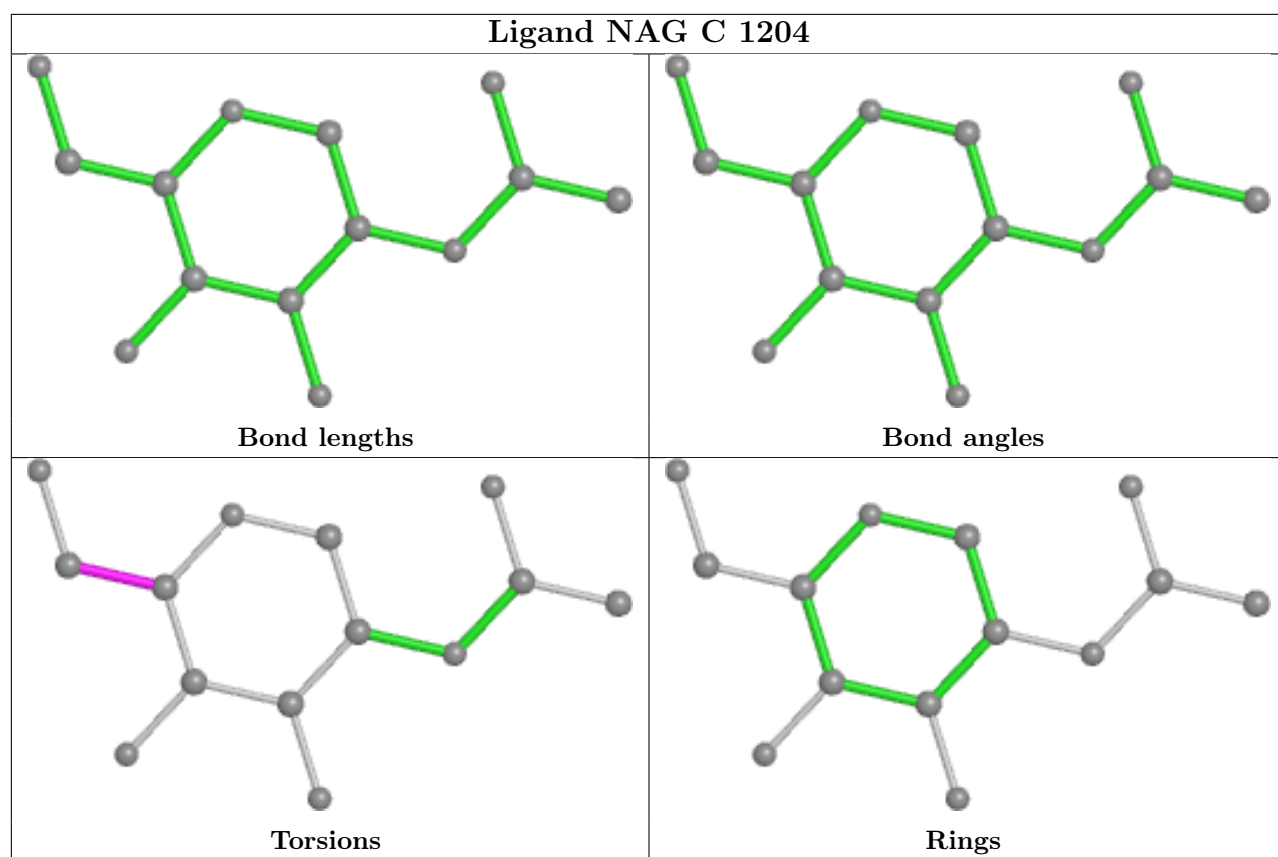
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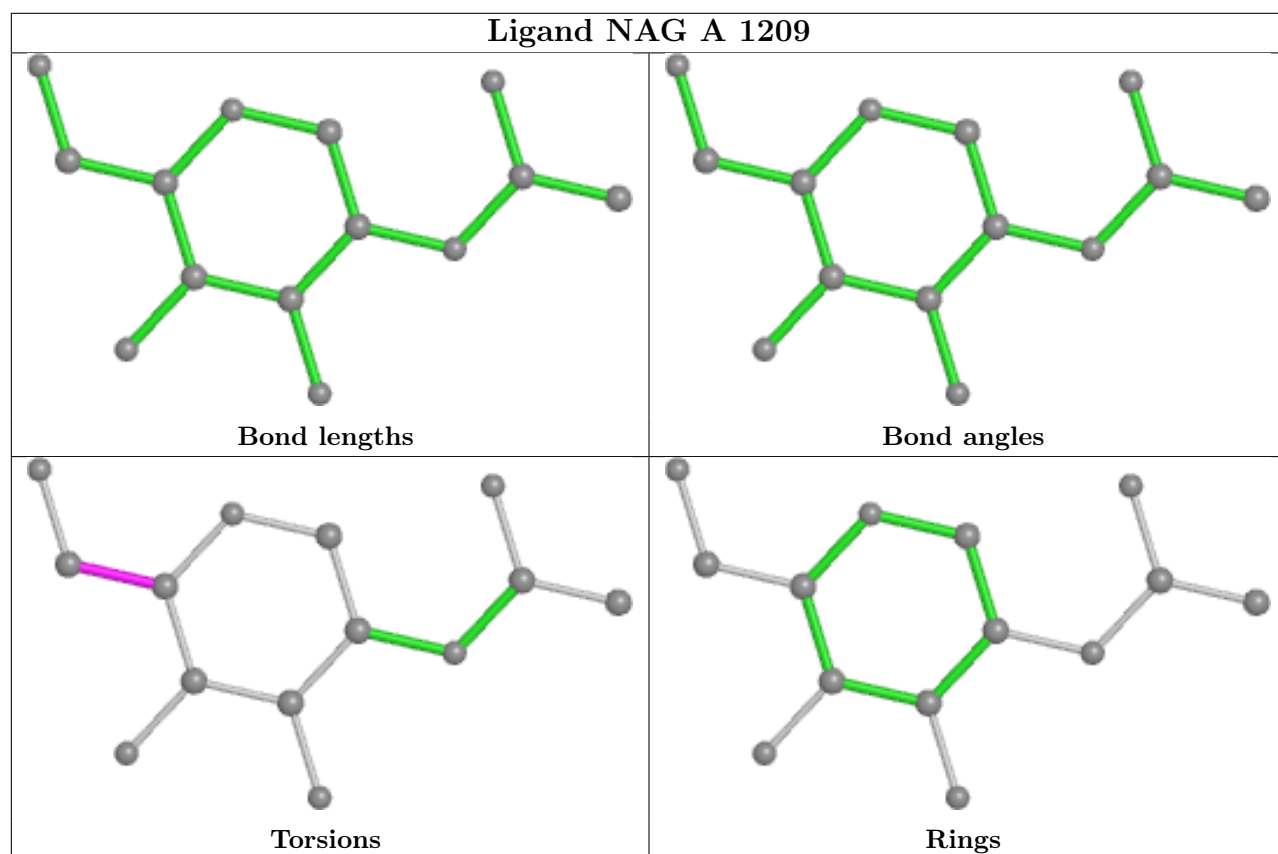
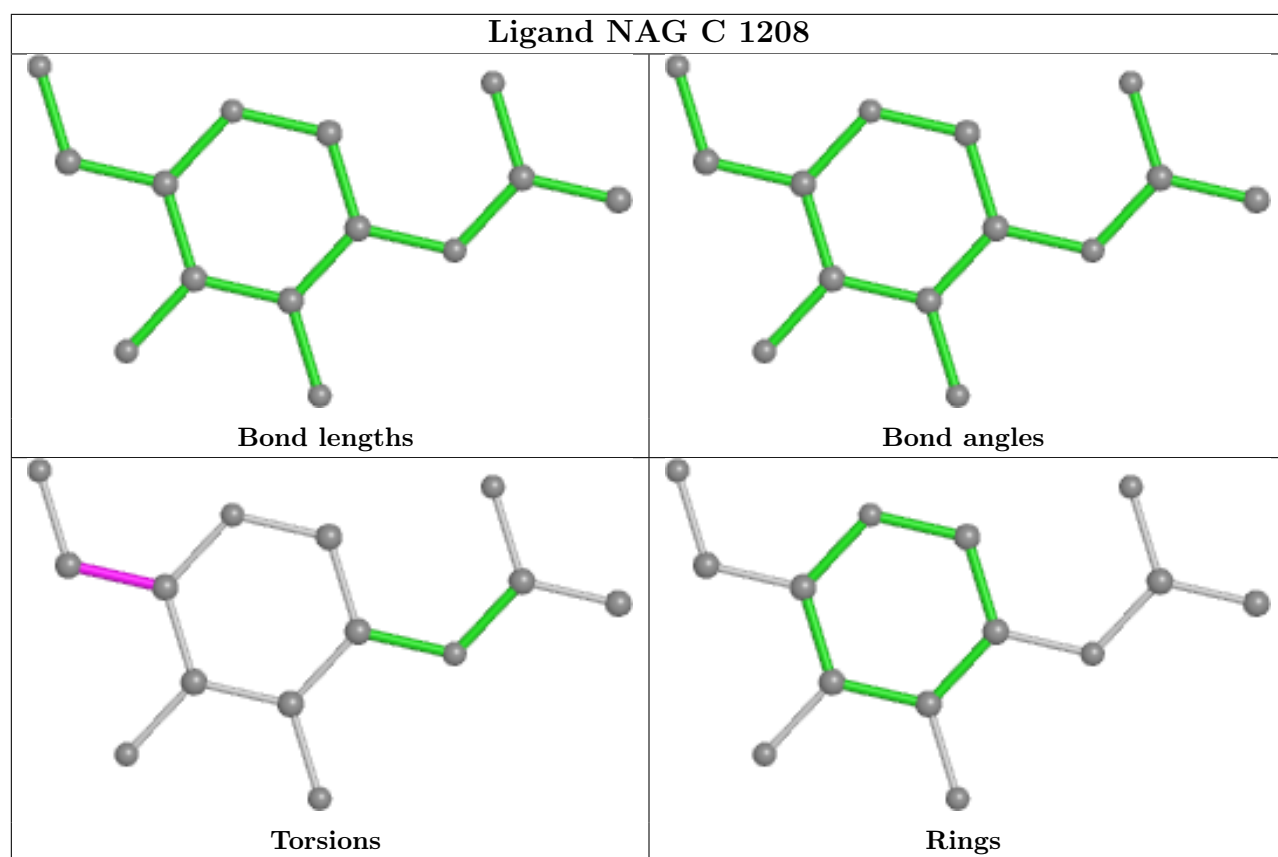


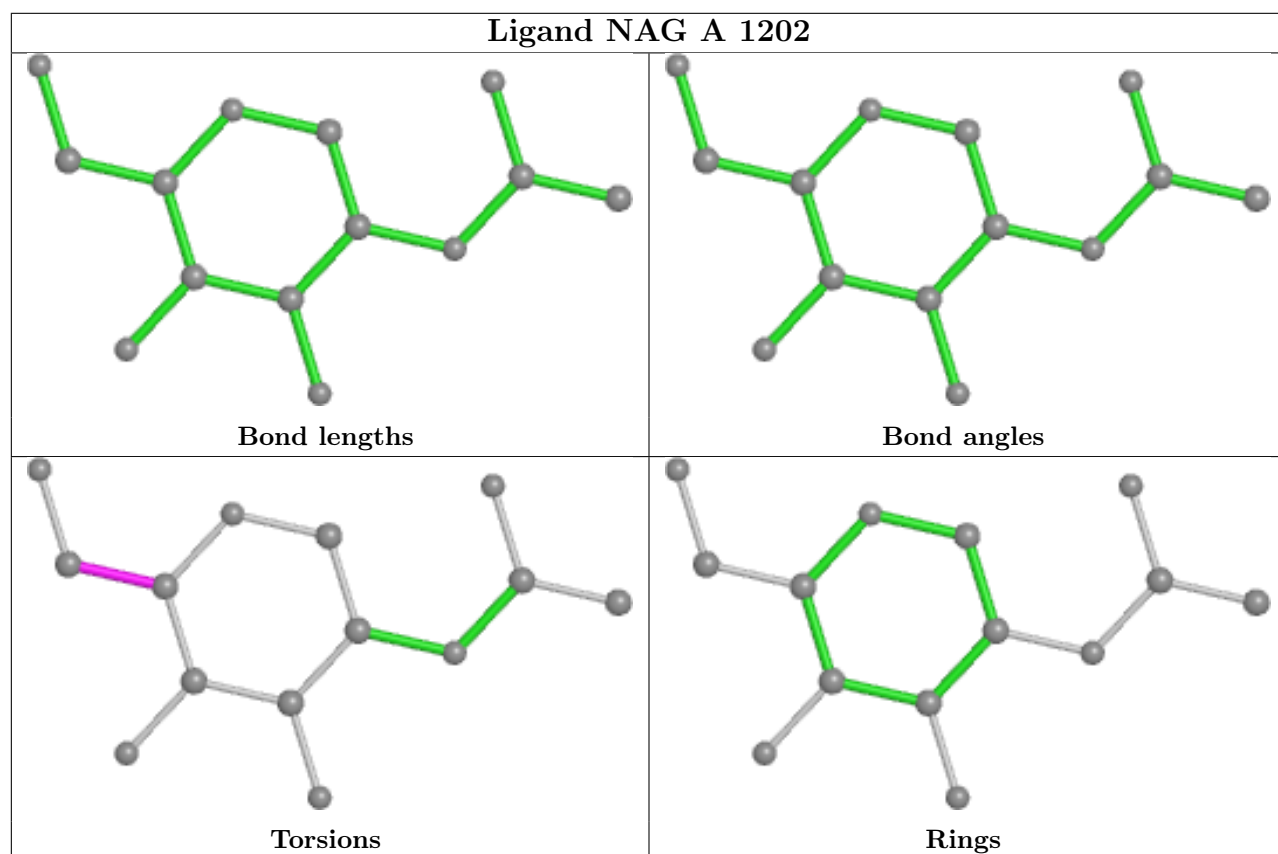
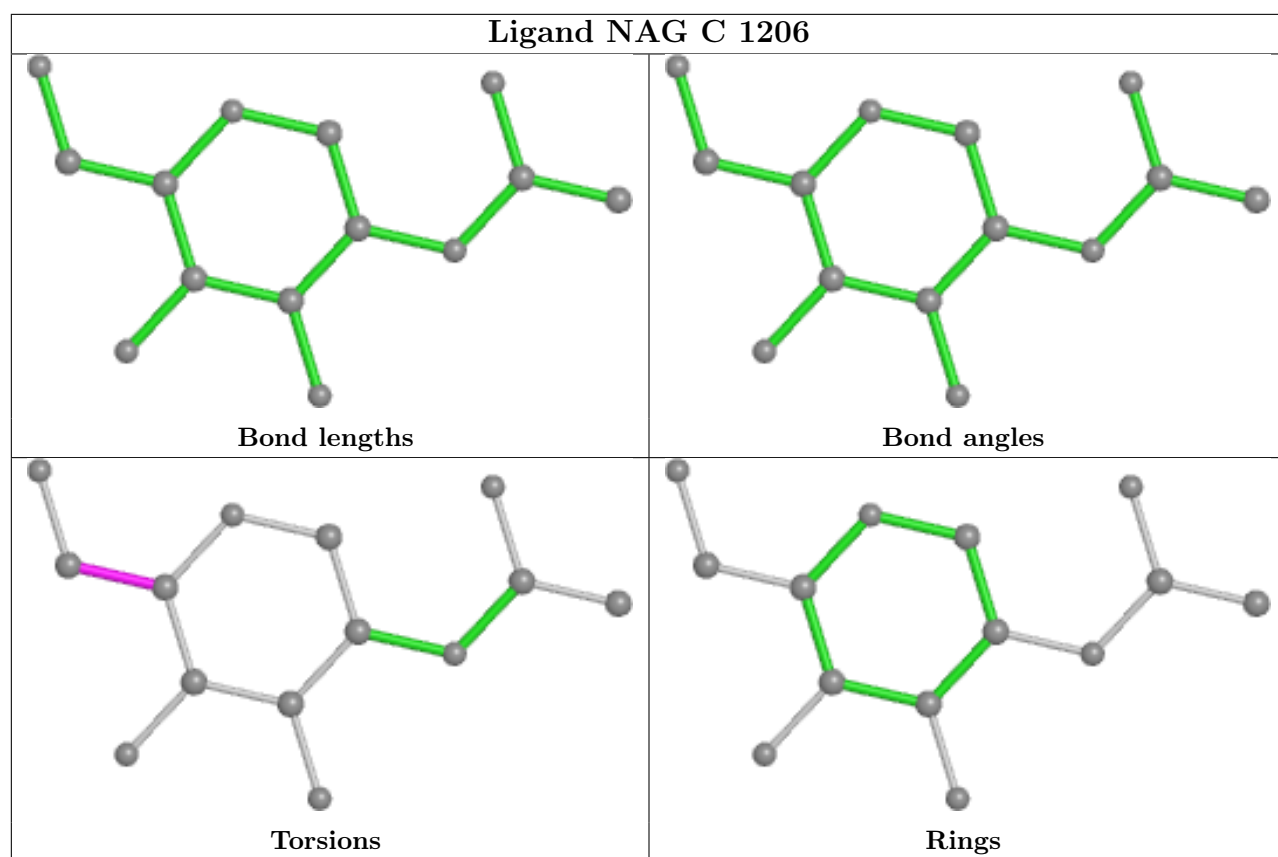
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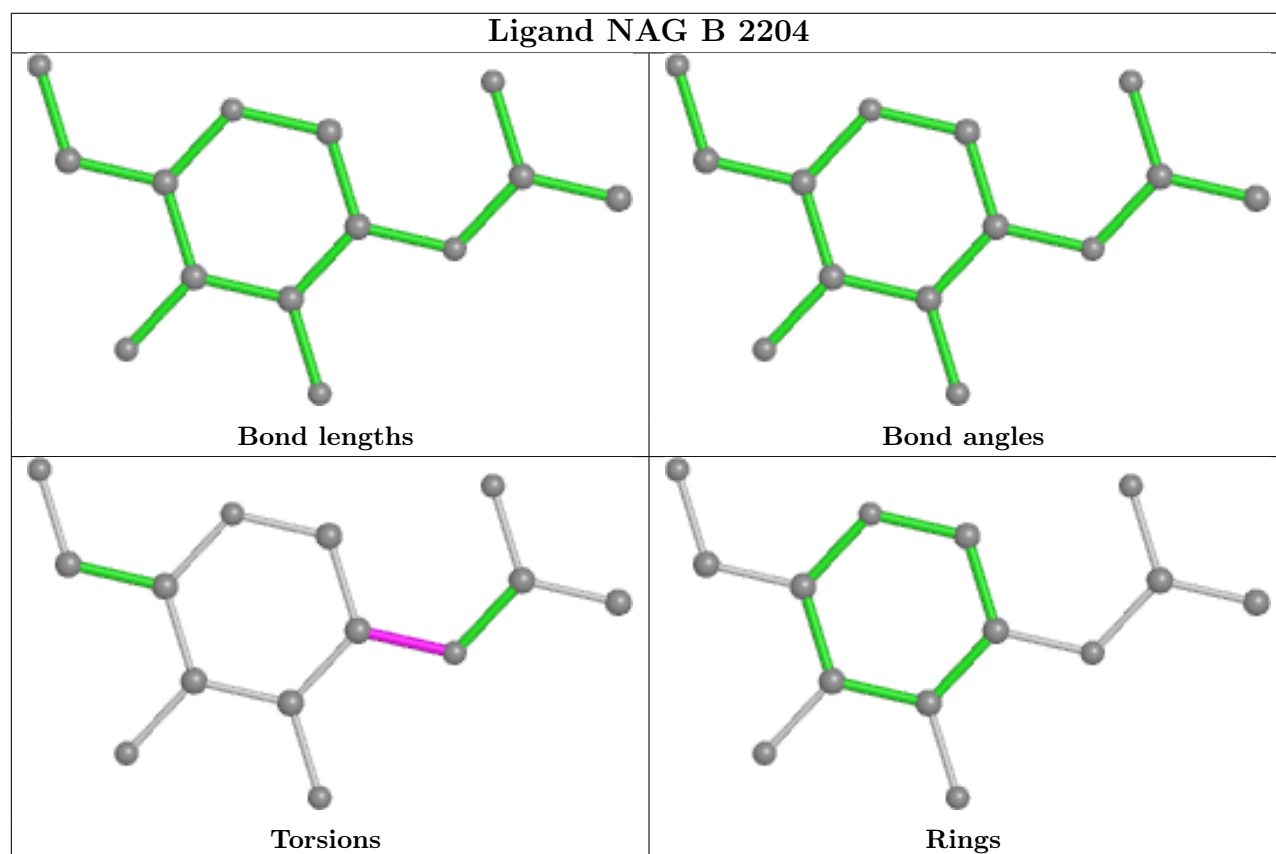
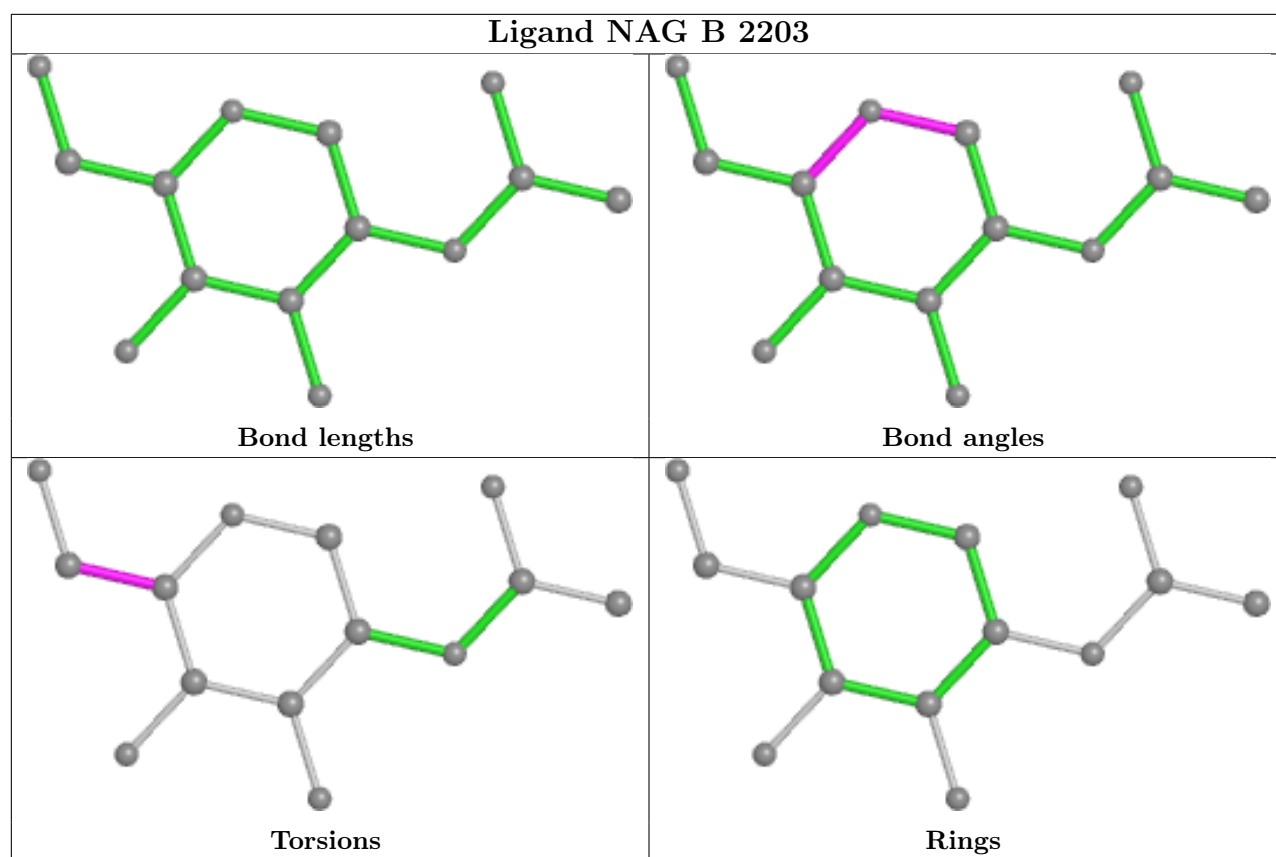






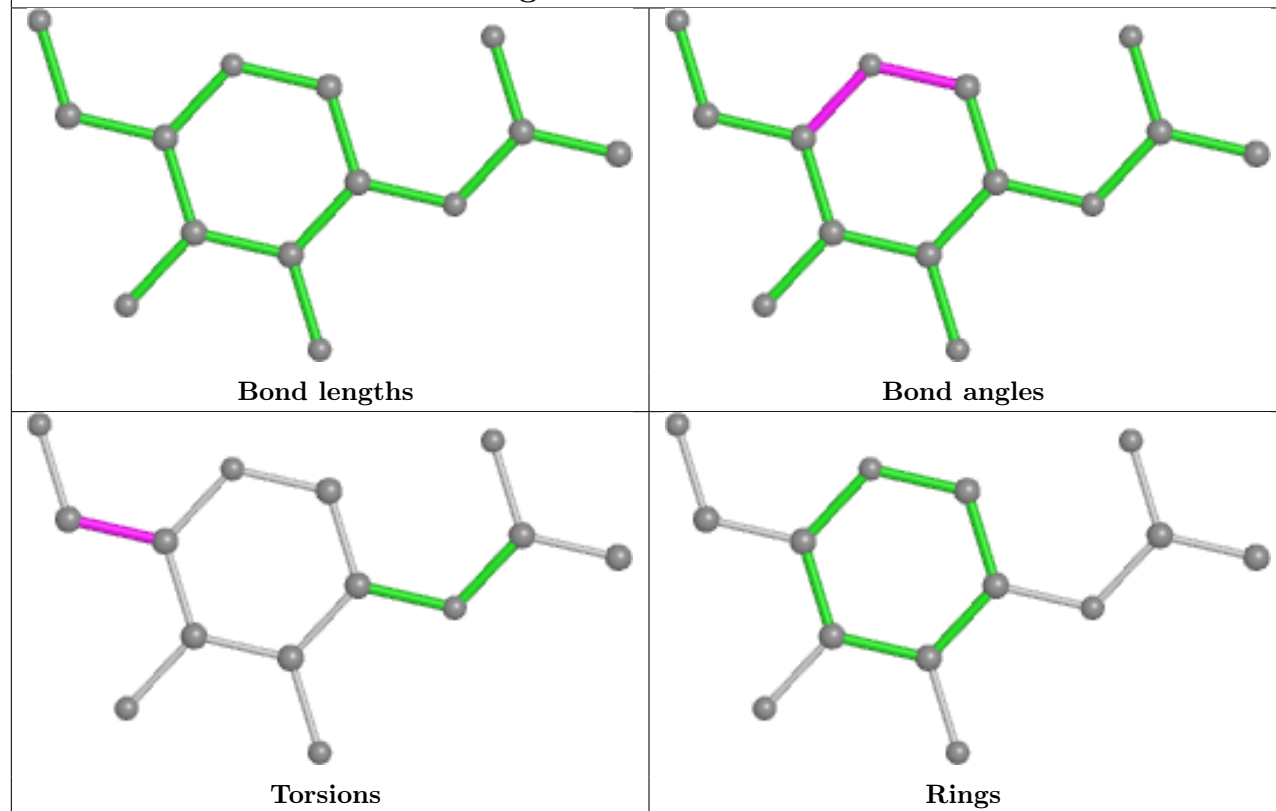




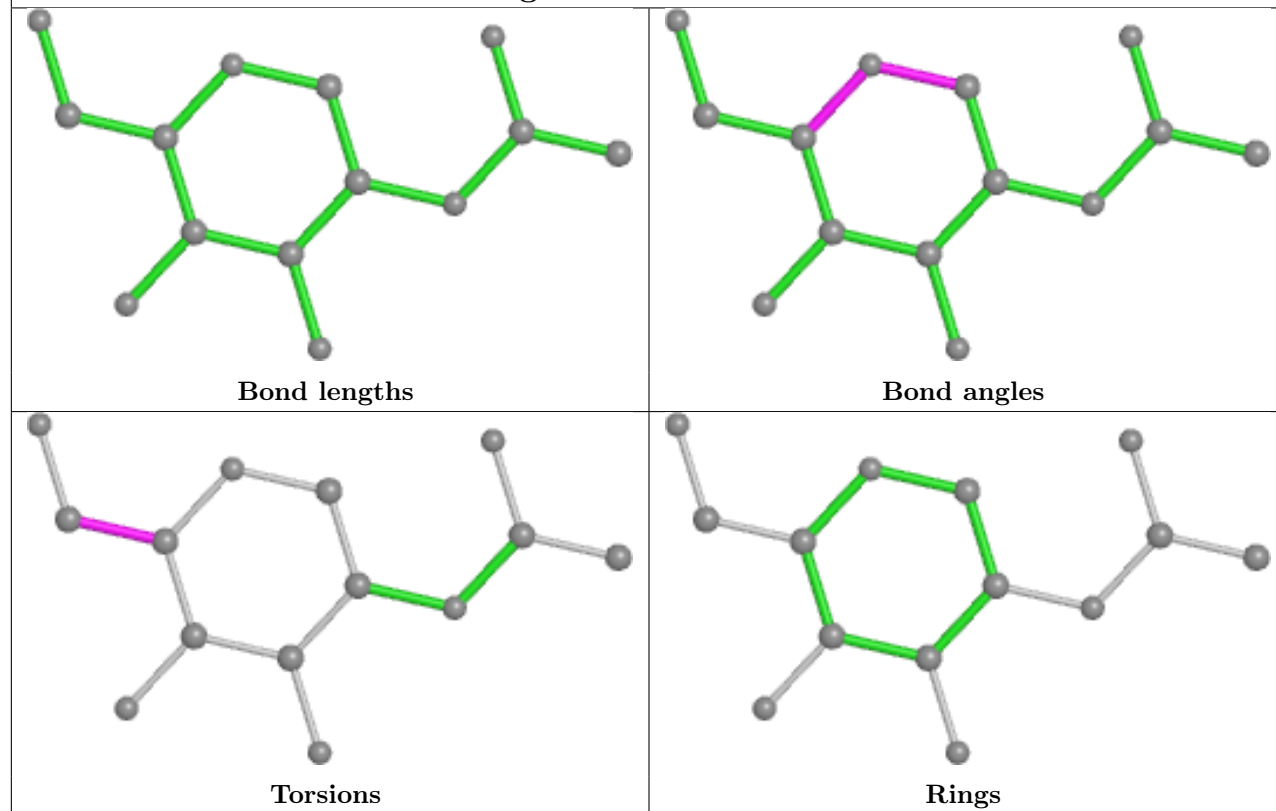


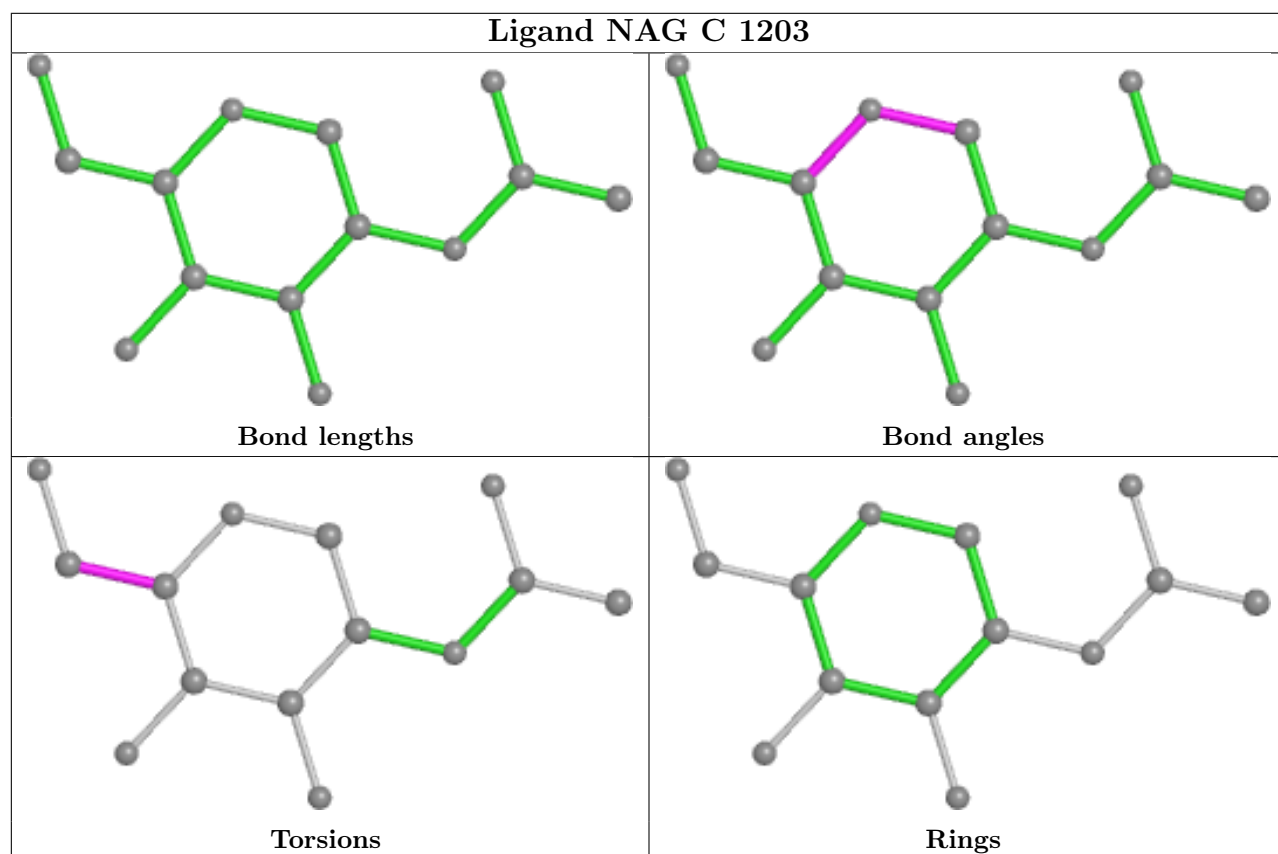
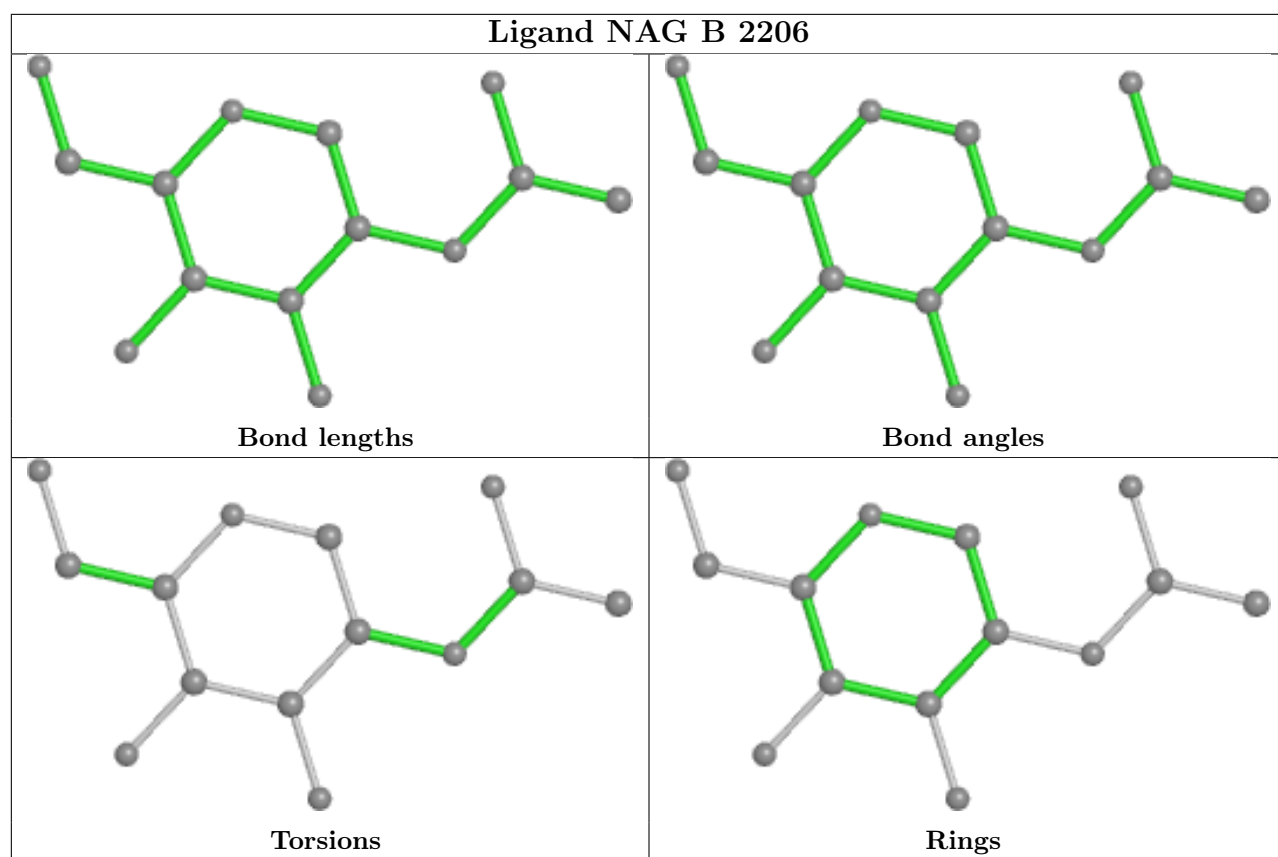


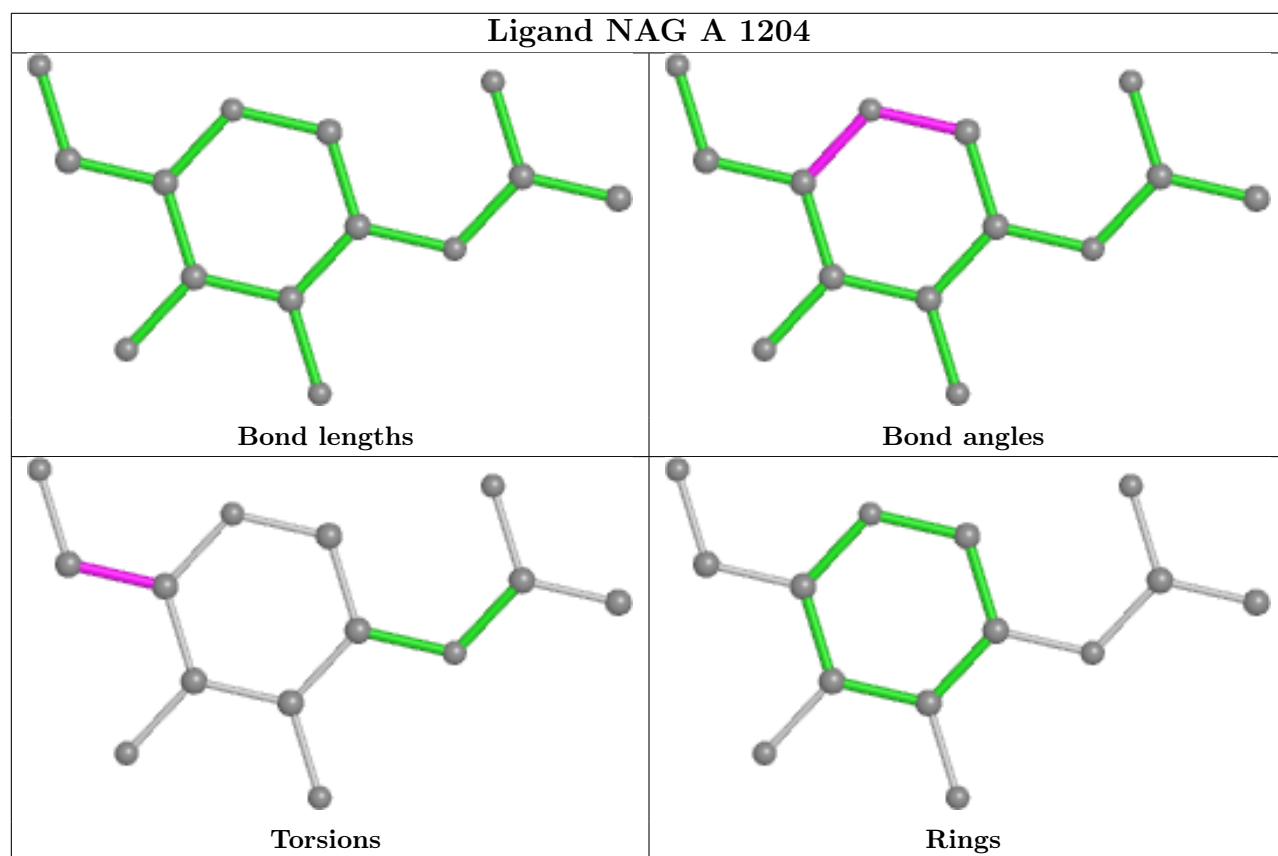
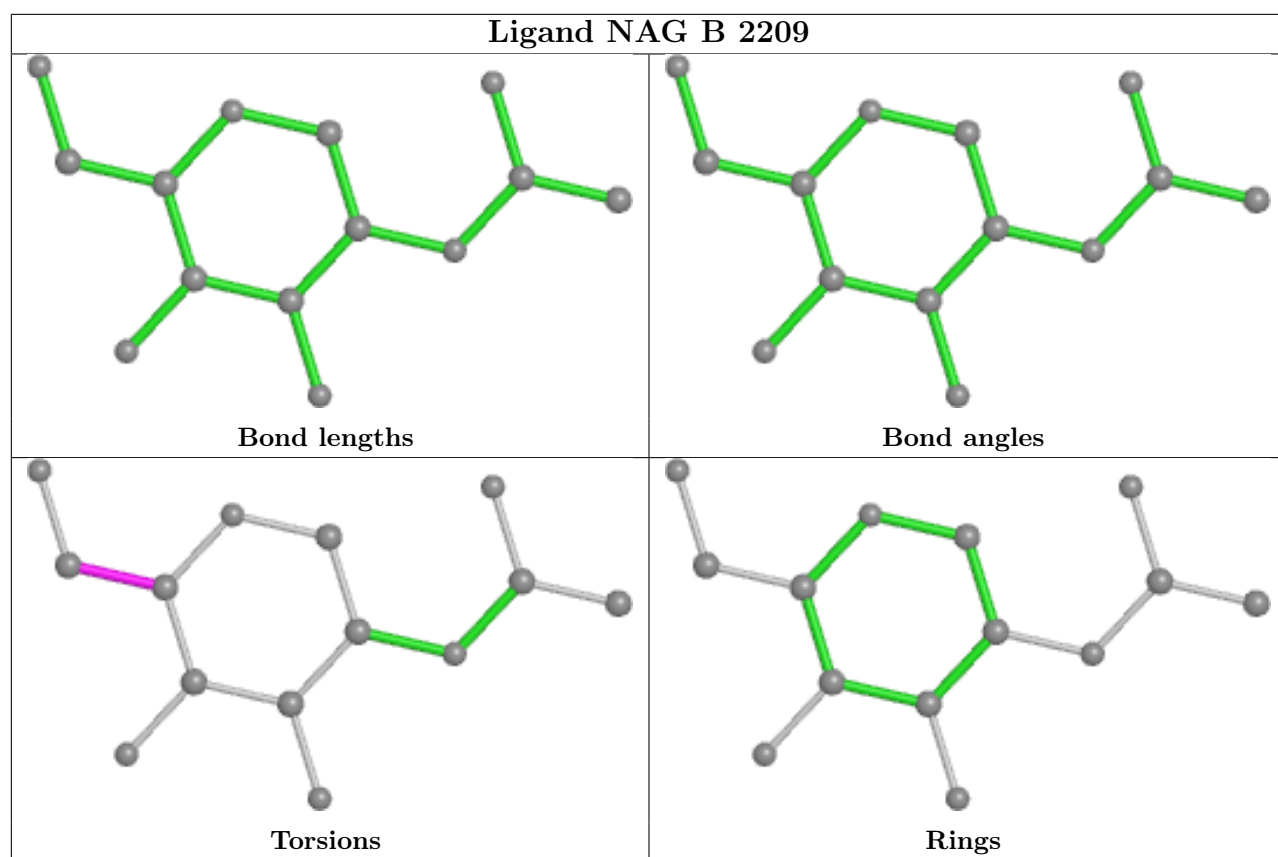
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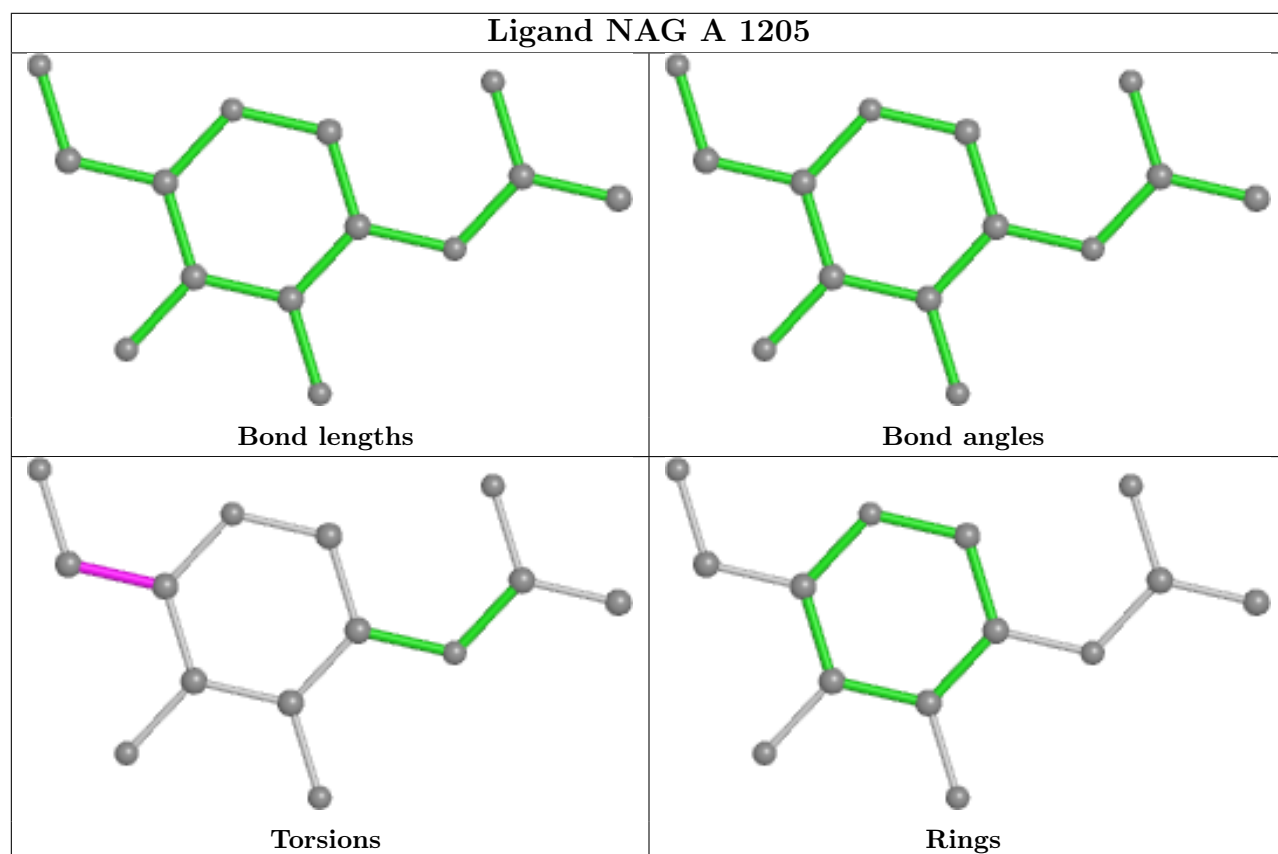
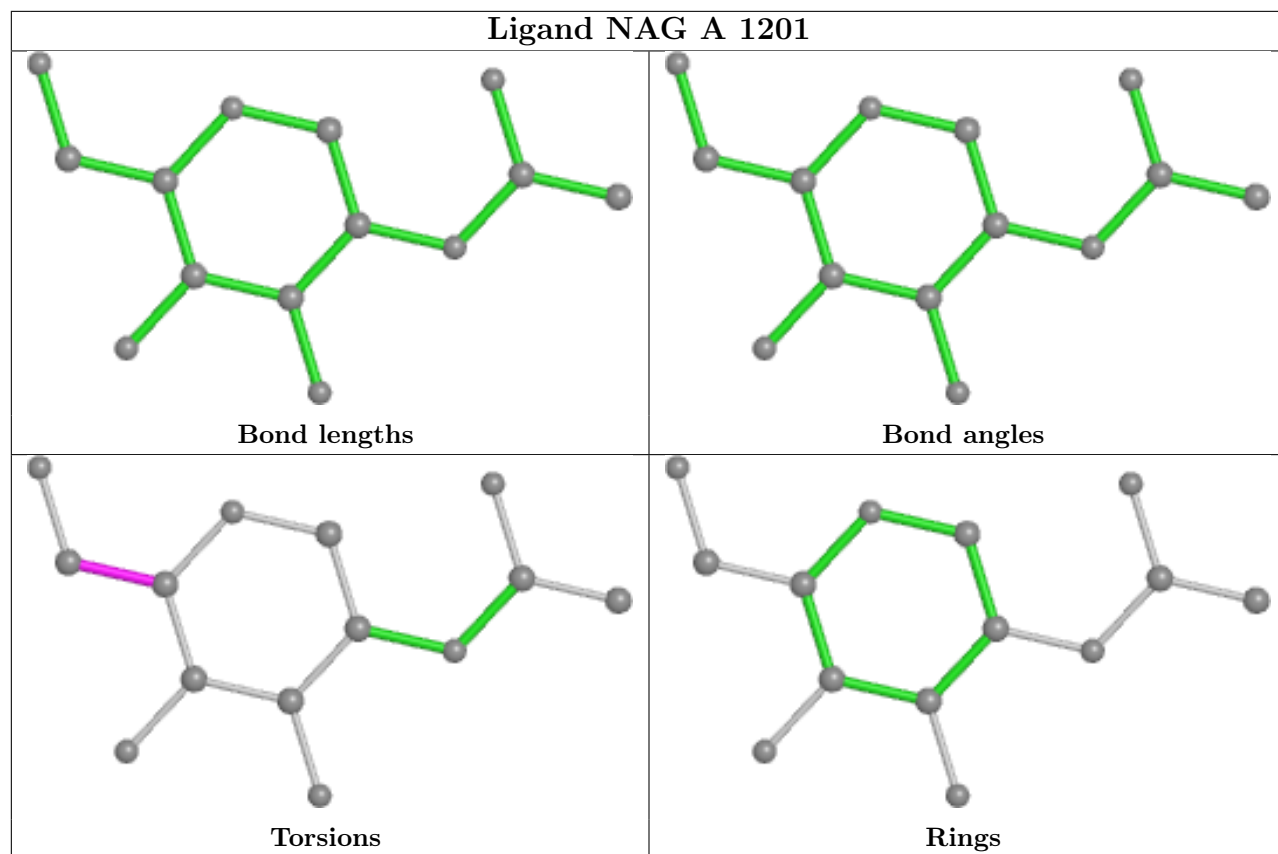


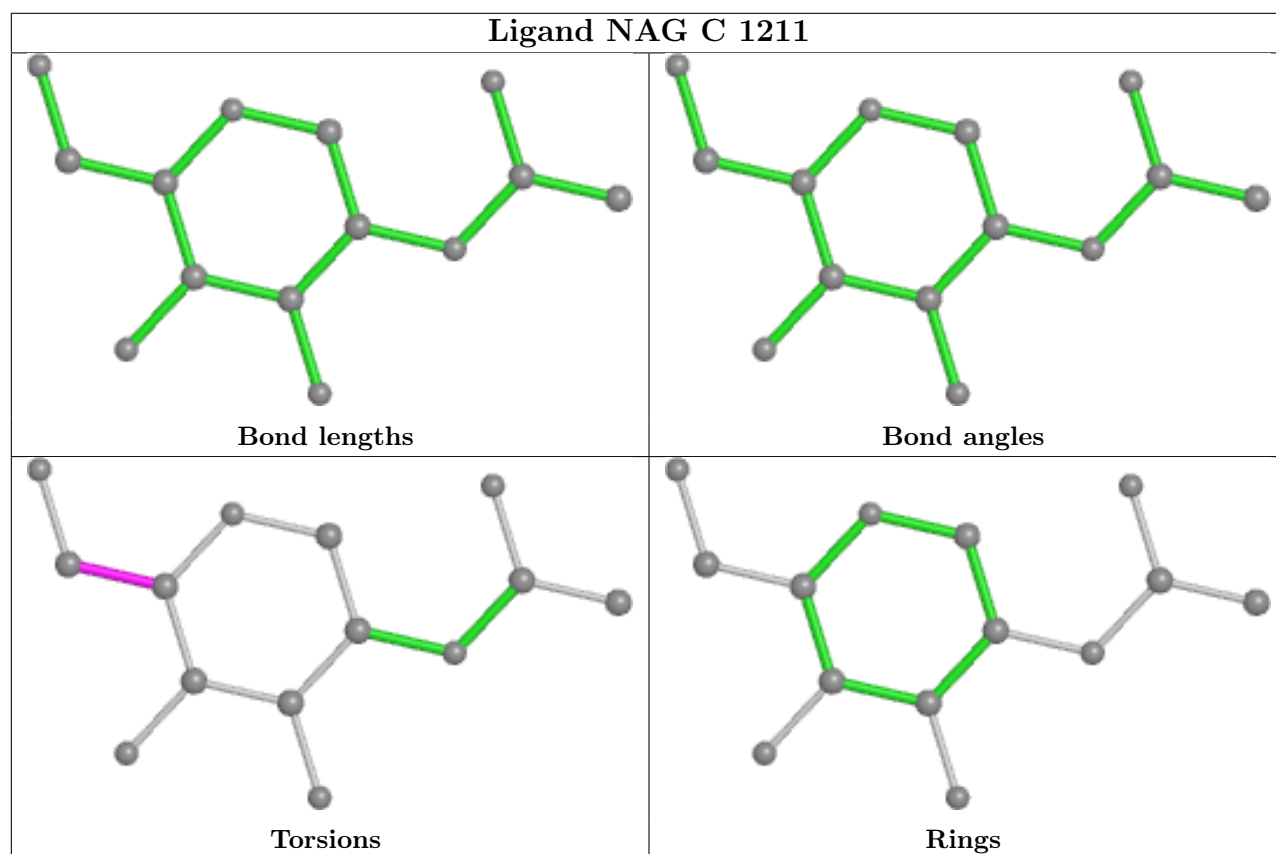
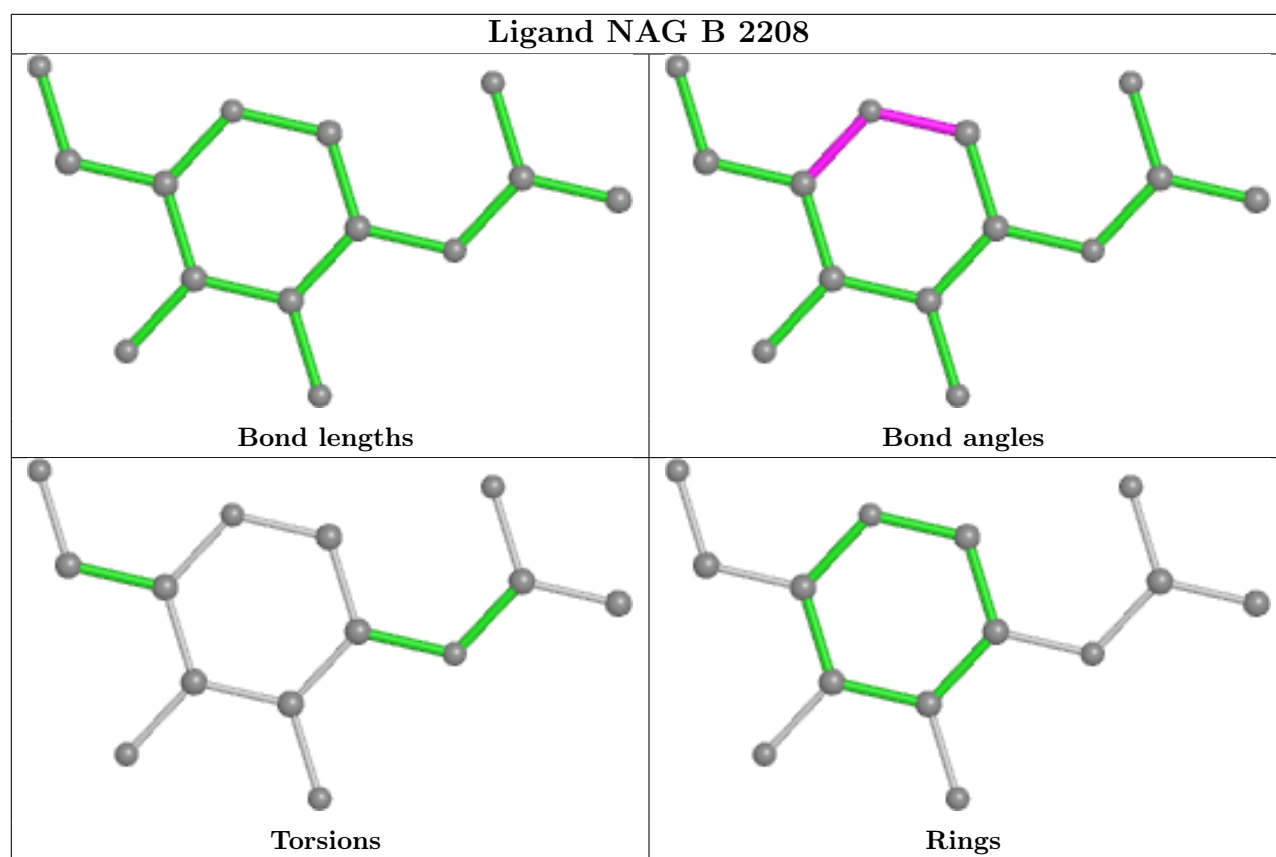
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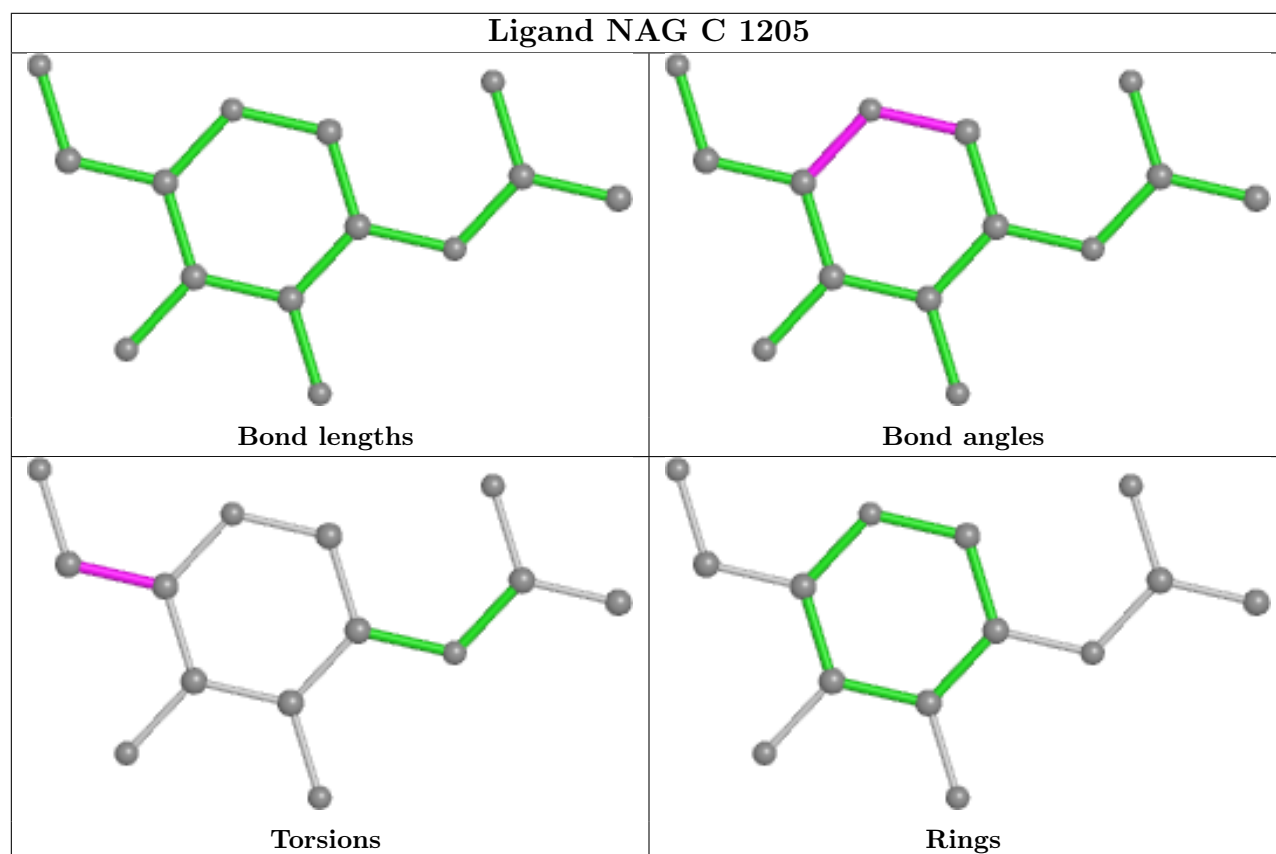
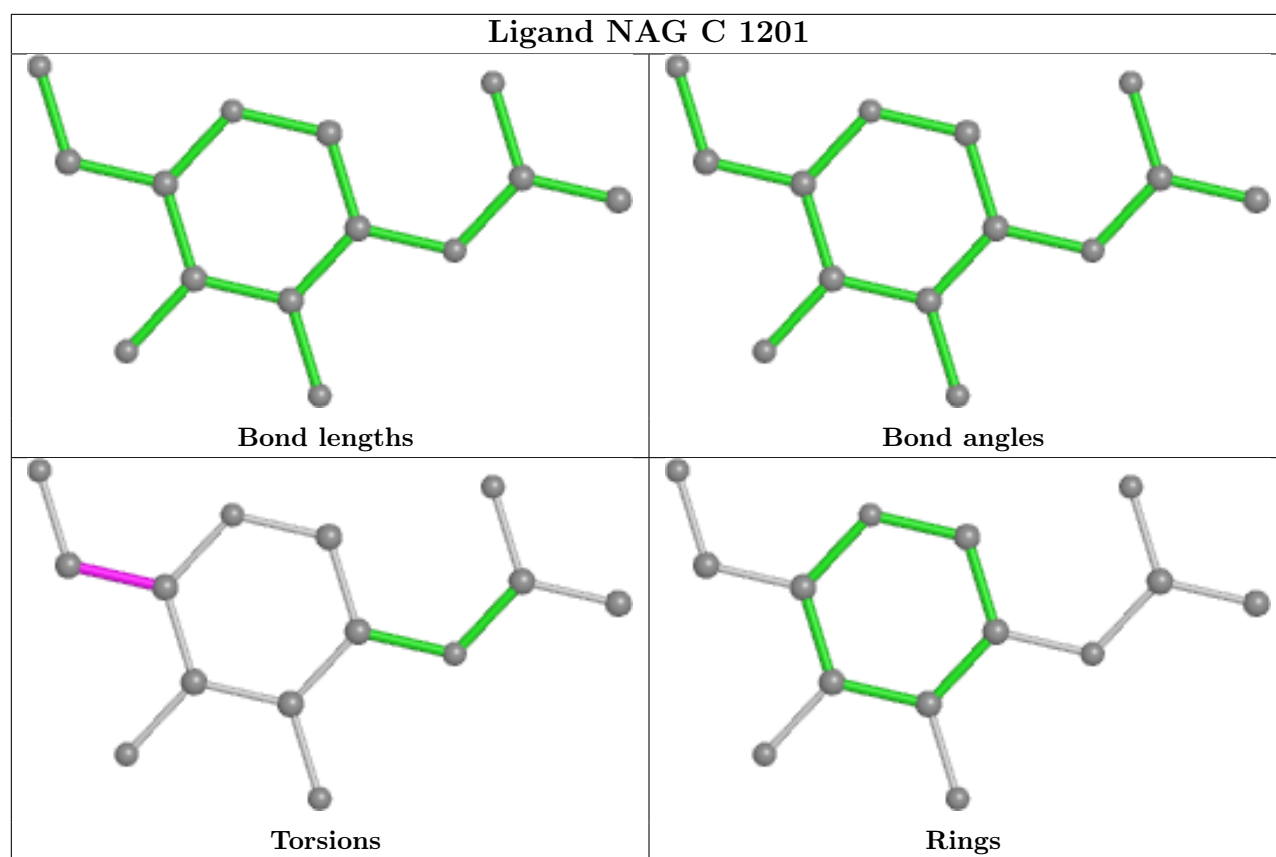


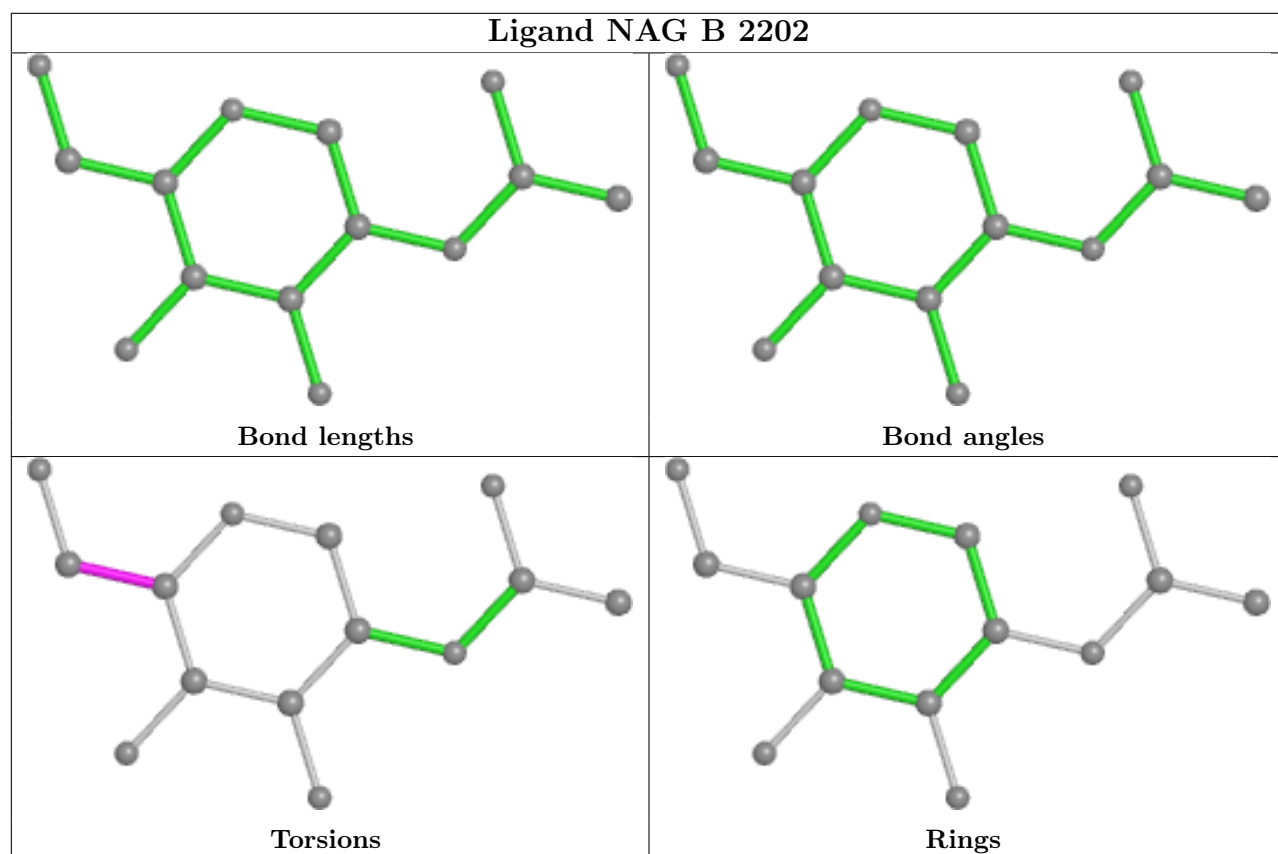
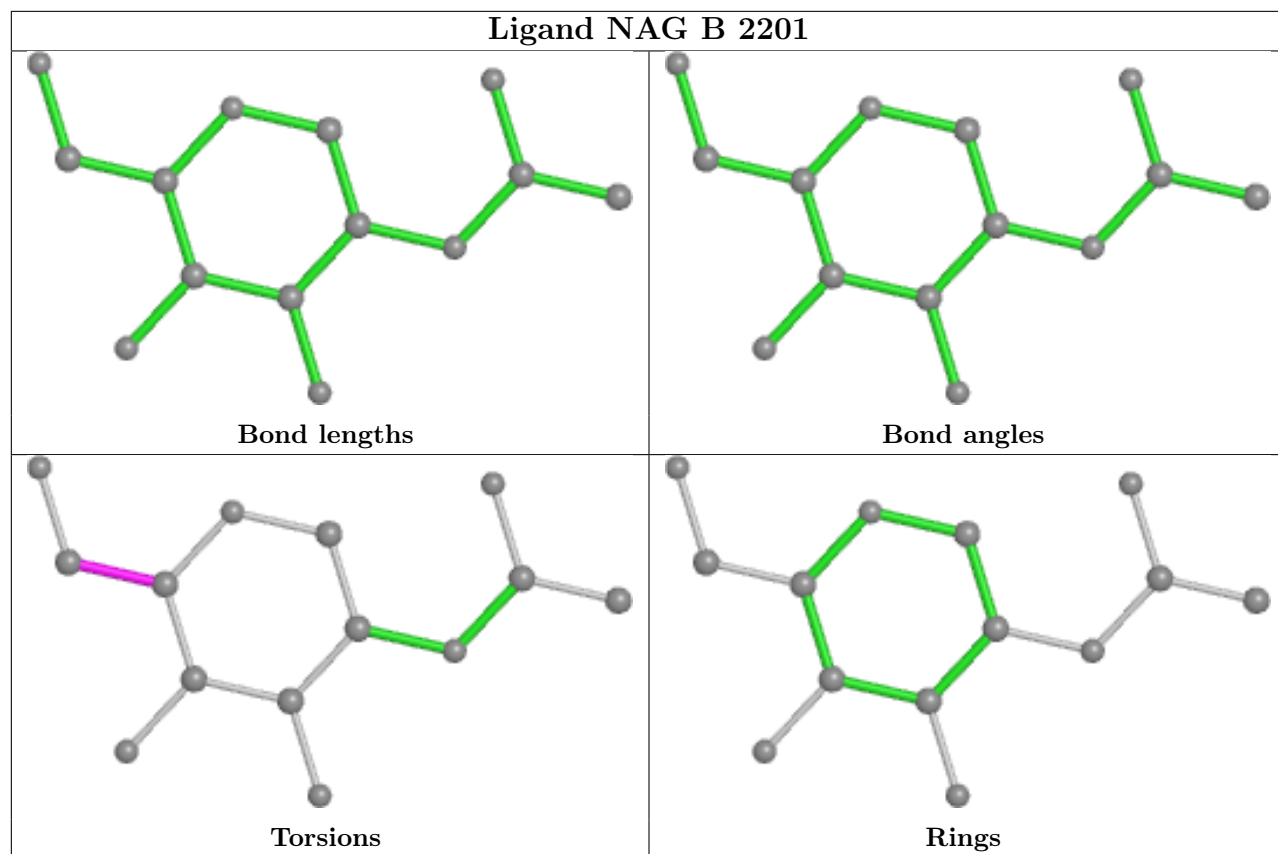


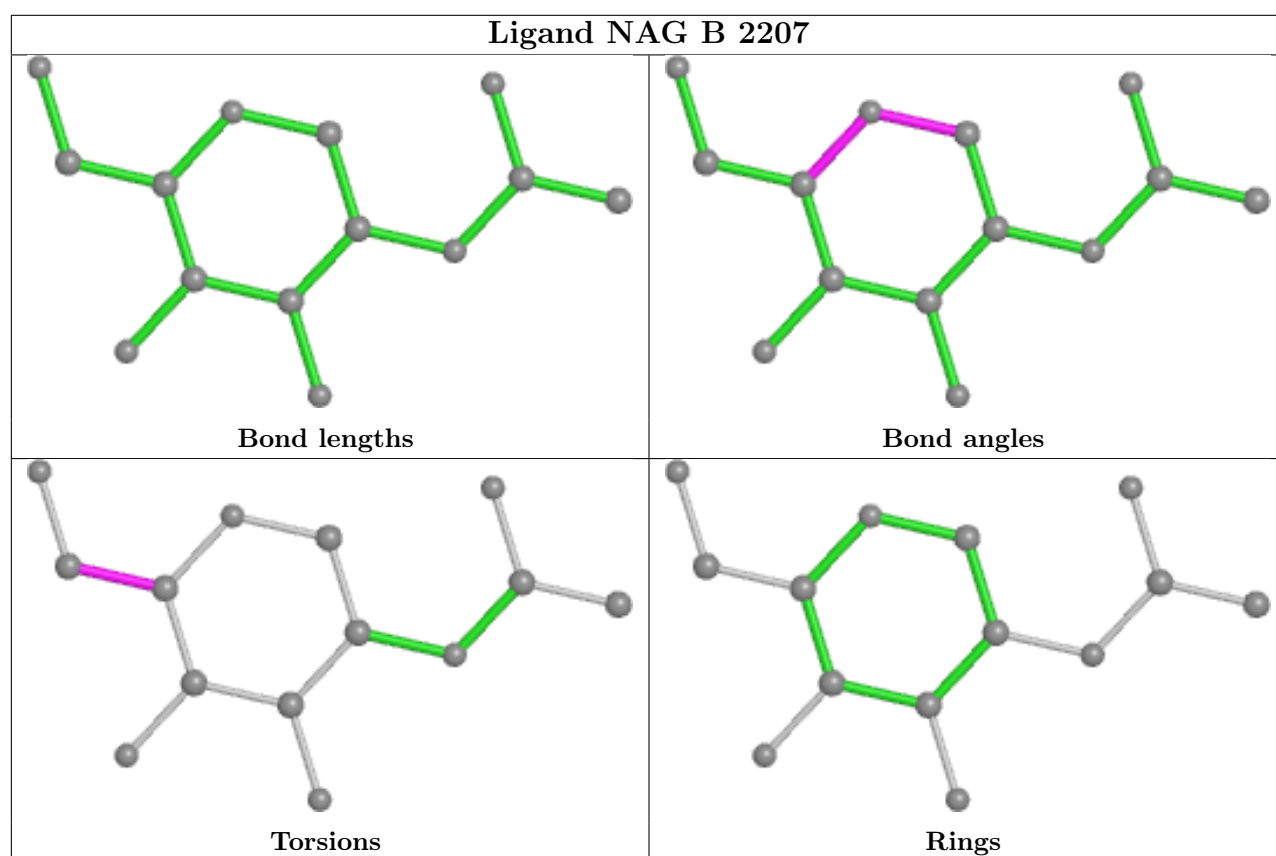
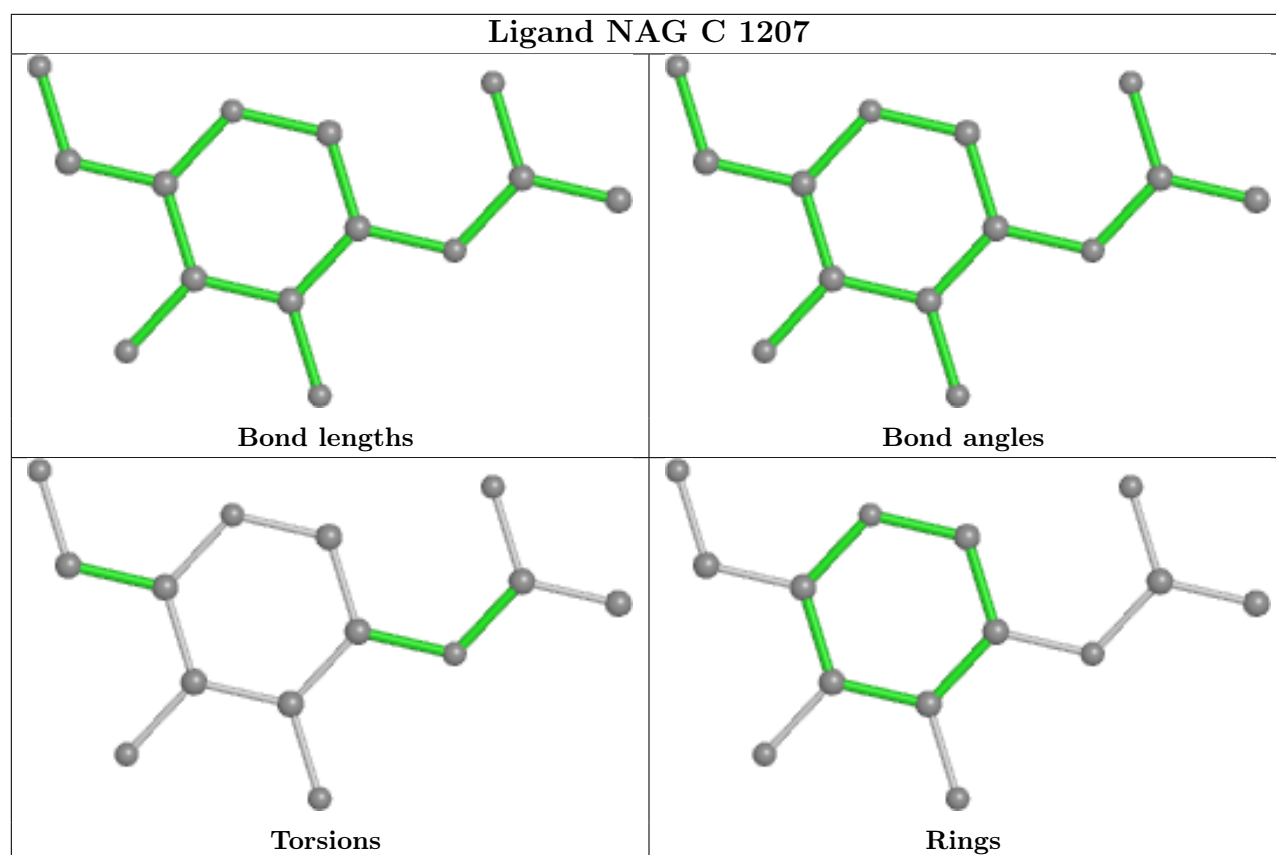




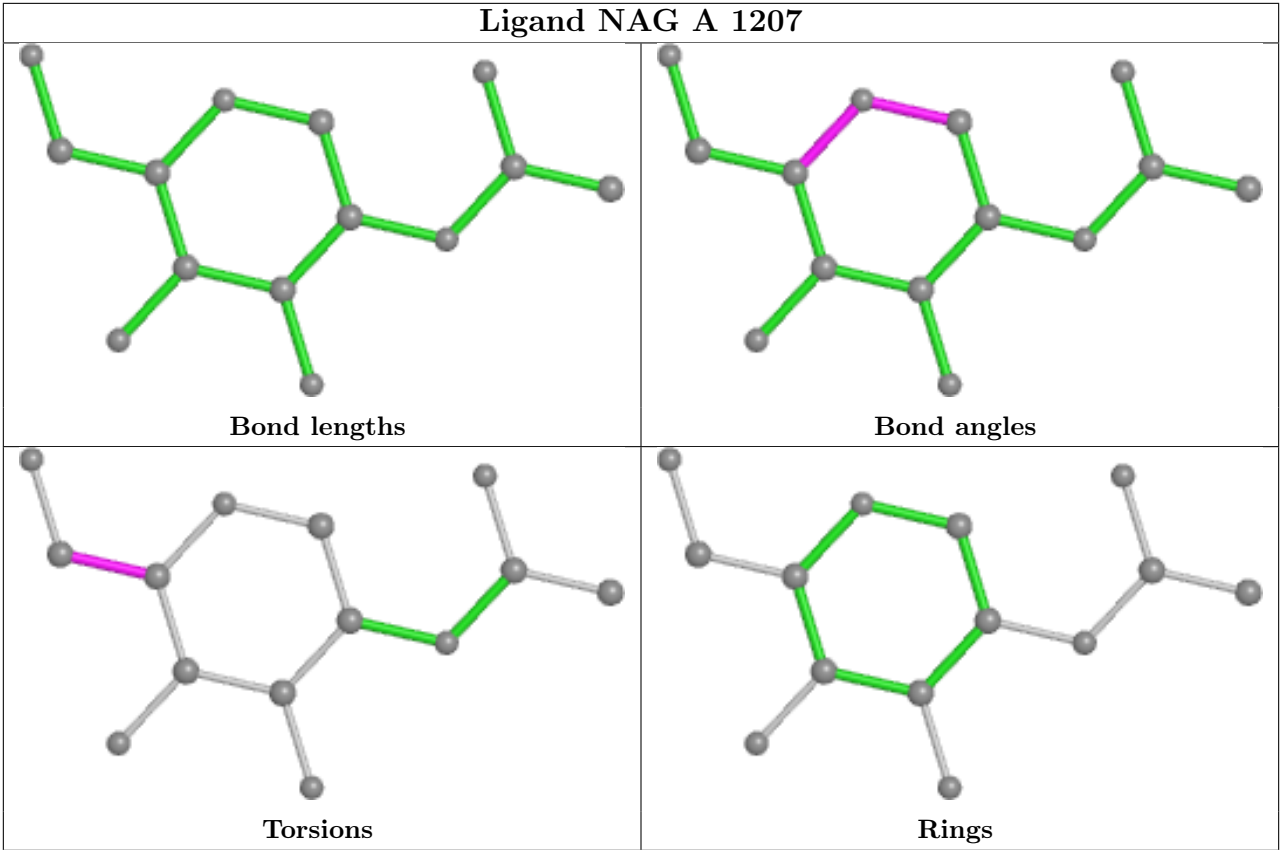












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	548:ASN	C	549:LEU	N	4.10
1	C	821:ILE	C	822:LEU	N	1.18