



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2026 – 08:49 AM EDT

PDB ID : 9NFT / pdb_00009nft
EMDB ID : EMD-49372
Title : PRO-37587 bound to SARS-CoV-2 Spike protein
Authors : Zimmerman, M.I.; Jecrois, A.
Deposited on : 2025-02-21
Resolution : 3.00 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

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>.

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

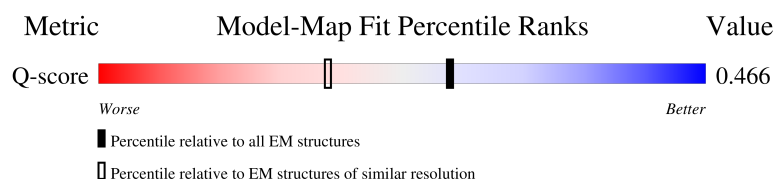
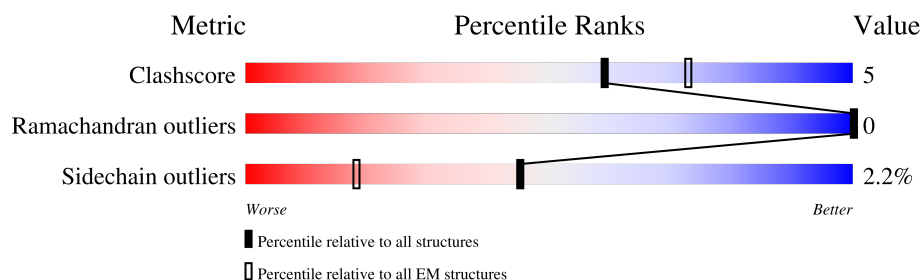
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.00 Å.

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



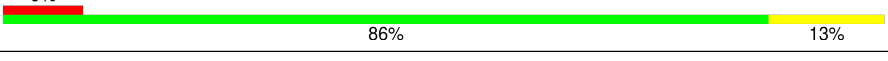
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 ≥ 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1141	
1	B	1141	
1	C	1141	
2	D	216	

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Mol	Chain	Length	Quality of chain
2	F	216	
2	H	216	
3	E	221	
3	G	221	
3	I	221	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34020 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 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1007	Total	C	N	O	S	0	0
			7887	5055	1310	1487	35		
1	B	1007	Total	C	N	O	S	0	0
			7887	5055	1310	1487	35		
1	C	1007	Total	C	N	O	S	0	0
			7887	5055	1310	1487	35		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	214B	GLU	-	insertion	UNP P0DTC2
A	214C	PRO	-	insertion	UNP P0DTC2
A	214D	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	214B	GLU	-	insertion	UNP P0DTC2
B	214C	PRO	-	insertion	UNP P0DTC2
B	214D	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	214B	GLU	-	insertion	UNP P0DTC2
C	214C	PRO	-	insertion	UNP P0DTC2
C	214D	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2

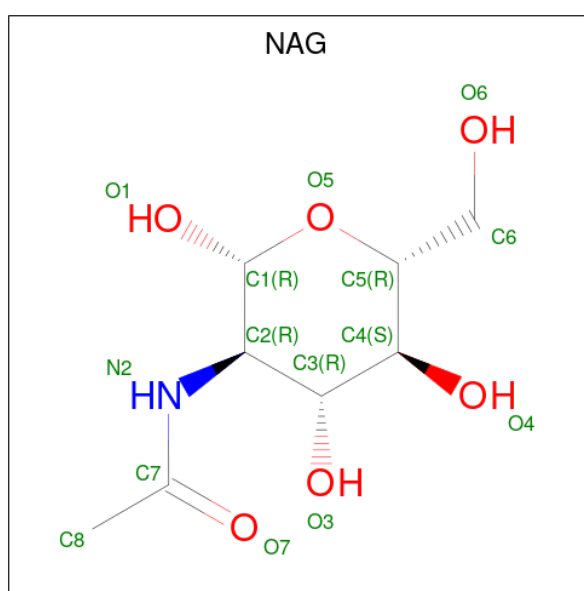
- Molecule 2 is a protein called PRO-37587 FAB light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	216	Total	C	N	O	S	0	0
			1609	1007	273	325	4		
2	F	216	Total	C	N	O	S	0	0
			1609	1007	273	325	4		
2	H	216	Total	C	N	O	S	0	0
			1609	1007	273	325	4		

- Molecule 3 is a protein called PRO-37587 FAB heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	221	Total	C	N	O	S	0	0
			1662	1049	275	332	6		
3	G	221	Total	C	N	O	S	0	0
			1662	1049	275	332	6		
3	I	221	Total	C	N	O	S	0	0
			1662	1049	275	332	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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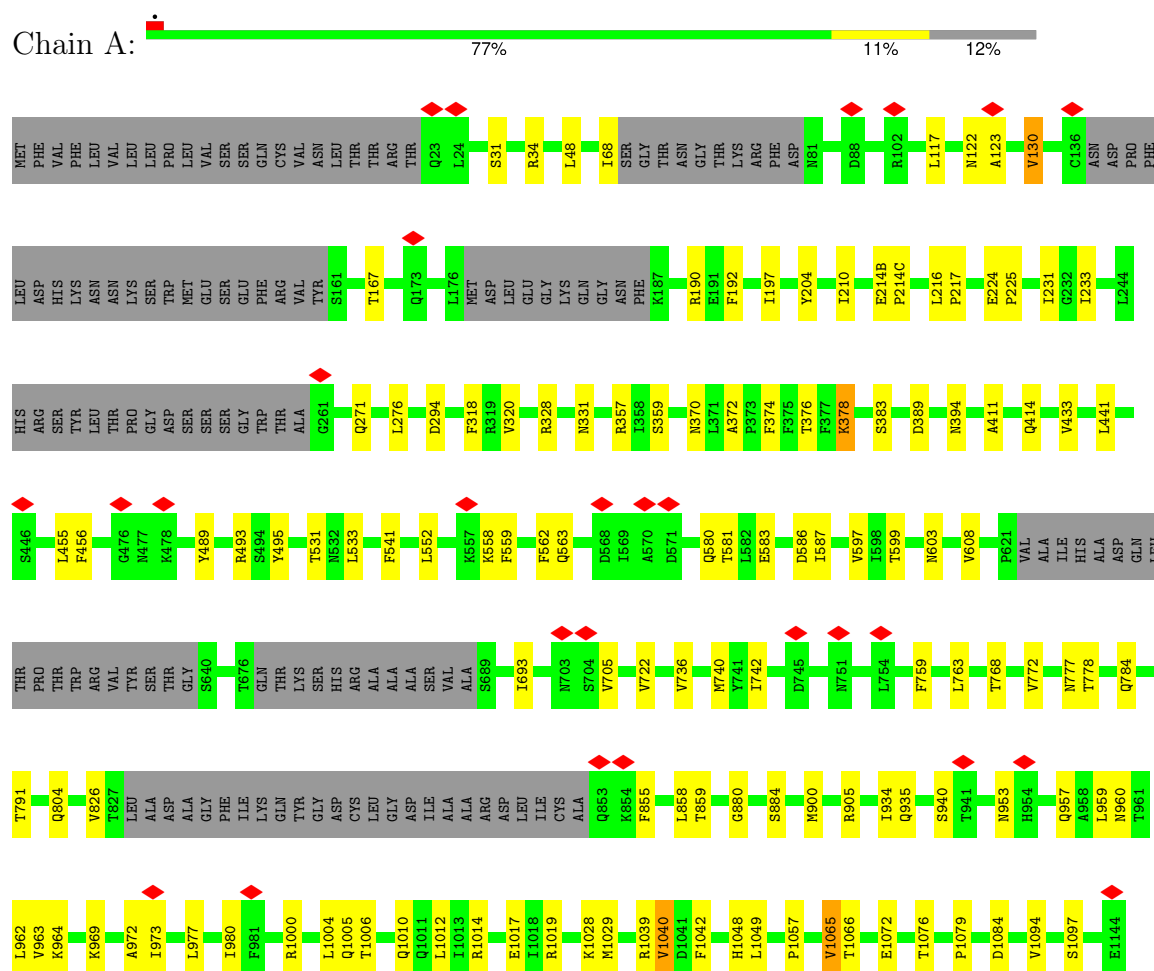
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

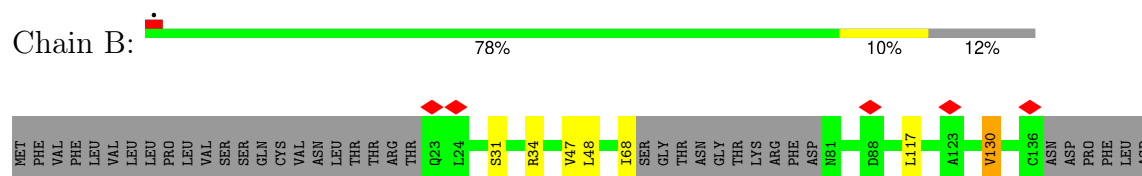
3 Residue-property plots

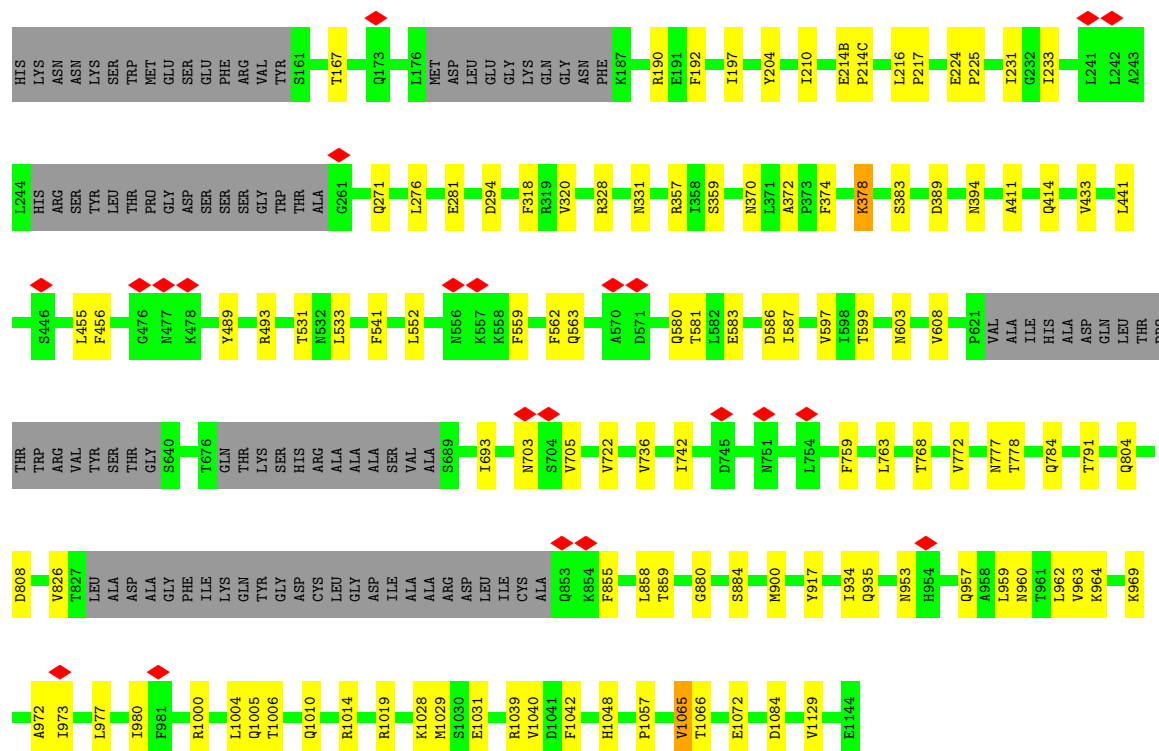
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 glycoprotein



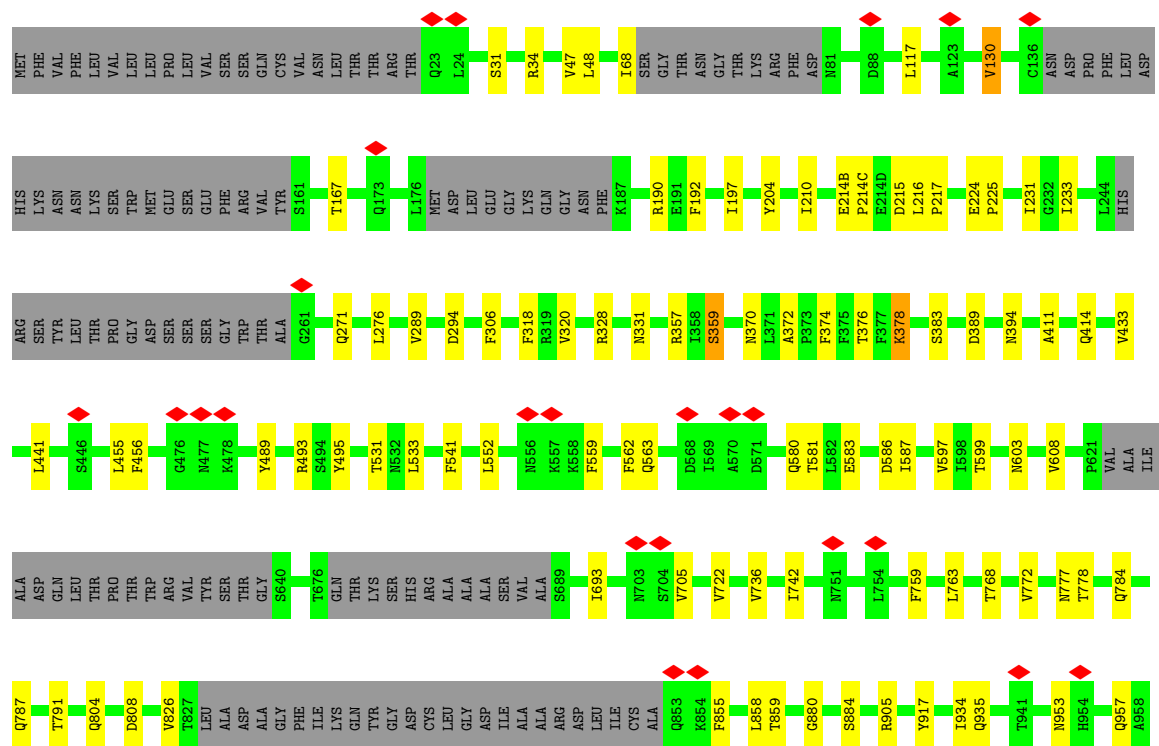
• Molecule 1: Spike glycoprotein

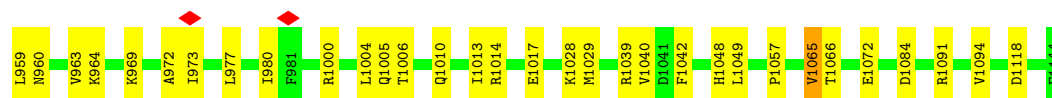




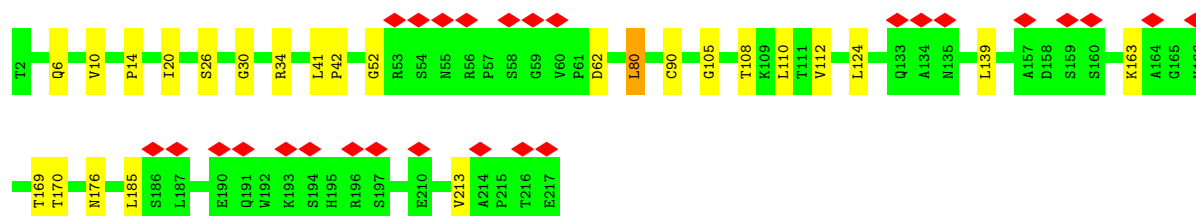
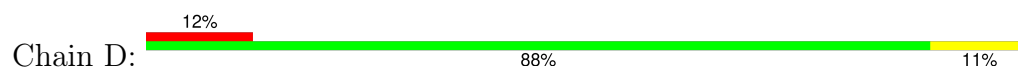
• Molecule 1: Spike glycoprotein

Chain C: 77% 11% 12%

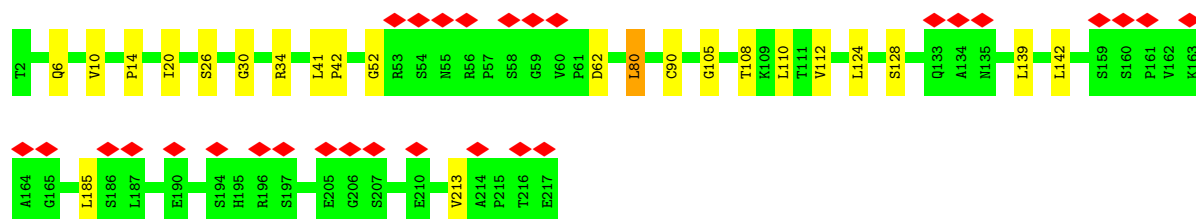
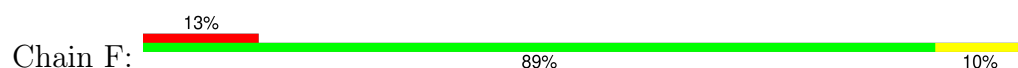




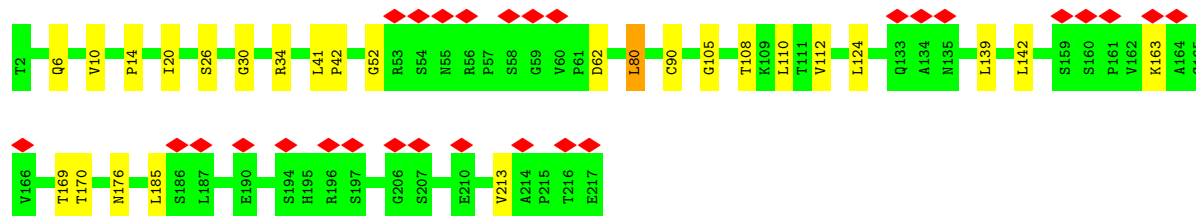
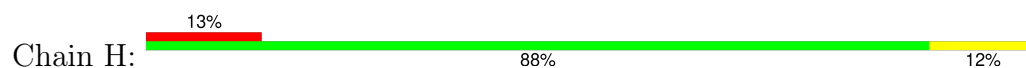
• Molecule 2: PRO-37587 FAB light chain



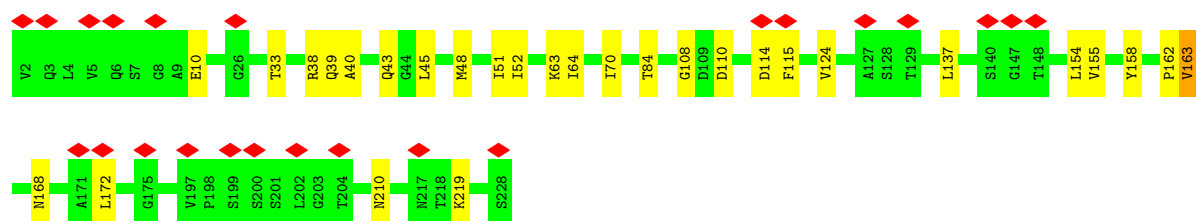
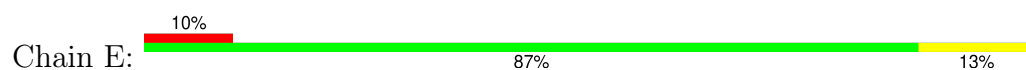
• Molecule 2: PRO-37587 FAB light chain



• Molecule 2: PRO-37587 FAB light chain

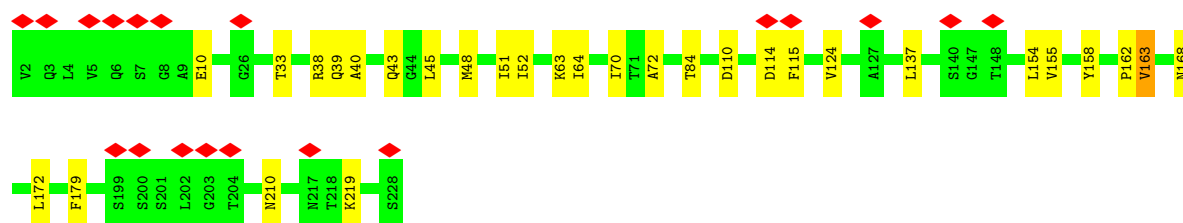


• Molecule 3: PRO-37587 FAB heavy chain



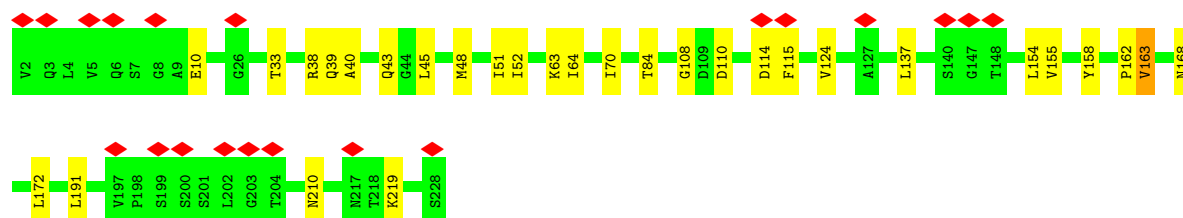
• Molecule 3: PRO-37587 FAB heavy chain

Chain G: 



• Molecule 3: PRO-37587 FAB heavy chain

Chain I: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	112195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.454	Depositor
Minimum map value	-2.819	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7151021, 0.7151021, 0.7151021	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	0.11	0/8073	0.29	0/10985
1	B	0.11	0/8073	0.29	0/10985
1	C	0.11	0/8073	0.29	0/10985
2	D	0.09	0/1651	0.25	0/2255
2	F	0.09	0/1651	0.25	0/2255
2	H	0.09	0/1651	0.25	0/2255
3	E	0.10	0/1702	0.27	0/2320
3	G	0.10	0/1702	0.27	0/2320
3	I	0.10	0/1702	0.27	0/2320
All	All	0.10	0/34278	0.28	0/46680

There are no bond length outliers.

There are no bond angle outliers.

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	7887	0	7737	74	0
1	B	7887	0	7737	69	0
1	C	7887	0	7737	71	0
2	D	1609	0	1557	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1609	0	1557	21	0
2	H	1609	0	1557	22	0
3	E	1662	0	1613	16	0
3	G	1662	0	1613	20	0
3	I	1662	0	1613	17	0
4	A	182	0	169	2	0
4	B	182	0	169	2	0
4	C	182	0	169	2	0
All	All	34020	0	33228	308	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 5.

The worst 5 of 308 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:C:759:PHE:HE1	1:C:1005:GLN:HE21	1.30	0.79
1:B:759:PHE:HE1	1:B:1005:GLN:HE21	1.30	0.79
2:F:34:ARG:NH2	3:G:110:ASP:O	2.17	0.78
1:A:759:PHE:HE1	1:A:1005:GLN:HE21	1.30	0.77
2:F:34:ARG:HG3	2:F:52:GLY:HA2	1.71	0.71

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	991/1141 (87%)	960 (97%)	31 (3%)	0	100	100
1	B	991/1141 (87%)	960 (97%)	31 (3%)	0	100	100
1	C	991/1141 (87%)	960 (97%)	31 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
2	F	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
2	H	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
3	E	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
3	G	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
3	I	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
All	All	4272/4734 (90%)	4146 (97%)	126 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	884/996 (89%)	862 (98%)	22 (2%)	42	72
1	B	884/996 (89%)	863 (98%)	21 (2%)	43	73
1	C	884/996 (89%)	861 (97%)	23 (3%)	40	72
2	D	179/179 (100%)	177 (99%)	2 (1%)	65	83
2	F	179/179 (100%)	177 (99%)	2 (1%)	65	83
2	H	179/179 (100%)	177 (99%)	2 (1%)	65	83
3	E	184/184 (100%)	180 (98%)	4 (2%)	45	74
3	G	184/184 (100%)	180 (98%)	4 (2%)	45	74
3	I	184/184 (100%)	180 (98%)	4 (2%)	45	74
All	All	3741/4077 (92%)	3657 (98%)	84 (2%)	45	74

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	599	THR
3	E	163	VAL

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Mol	Chain	Res	Type
1	C	705	VAL
1	C	1072	GLU
3	G	114	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	191	GLN
3	E	205	GLN
2	H	39	GLN
1	B	450	ASN
1	B	448	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

39 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	NAG	C	1210	1	14,14,15	0.72	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1210	1	14,14,15	0.72	0	17,19,21	0.80	0
4	NAG	B	1207	1	14,14,15	0.75	0	17,19,21	0.90	0
4	NAG	C	1201	1	14,14,15	0.72	0	17,19,21	2.34	3 (17%)
4	NAG	A	1210	1	14,14,15	0.72	0	17,19,21	0.79	0
4	NAG	B	1206	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	A	1202	1	14,14,15	0.71	0	17,19,21	0.78	0
4	NAG	A	1209	1	14,14,15	0.74	0	17,19,21	0.87	0
4	NAG	C	1211	1	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
4	NAG	B	1204	1	14,14,15	0.77	0	17,19,21	1.00	1 (5%)
4	NAG	B	1211	1	14,14,15	0.70	0	17,19,21	1.19	1 (5%)
4	NAG	C	1213	1	14,14,15	0.76	0	17,19,21	0.93	1 (5%)
4	NAG	A	1207	1	14,14,15	0.74	0	17,19,21	0.90	0
4	NAG	A	1212	1	14,14,15	0.72	0	17,19,21	0.82	0
4	NAG	A	1203	1	14,14,15	0.77	0	17,19,21	0.82	0
4	NAG	A	1206	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	A	1211	1	14,14,15	0.70	0	17,19,21	1.18	1 (5%)
4	NAG	A	1208	1	14,14,15	0.71	0	17,19,21	0.81	0
4	NAG	A	1201	1	14,14,15	0.72	0	17,19,21	2.34	3 (17%)
4	NAG	C	1207	1	14,14,15	0.72	0	17,19,21	0.90	0
4	NAG	C	1212	1	14,14,15	0.72	0	17,19,21	0.82	0
4	NAG	C	1202	1	14,14,15	0.72	0	17,19,21	0.78	0
4	NAG	C	1206	1	14,14,15	0.72	0	17,19,21	0.84	0
4	NAG	C	1209	1	14,14,15	0.73	0	17,19,21	0.87	0
4	NAG	B	1202	1	14,14,15	0.71	0	17,19,21	0.78	0
4	NAG	C	1205	1	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
4	NAG	B	1201	1	14,14,15	0.72	0	17,19,21	2.35	3 (17%)
4	NAG	B	1213	1	14,14,15	0.77	0	17,19,21	0.92	1 (5%)
4	NAG	B	1205	1	14,14,15	0.73	0	17,19,21	1.15	1 (5%)
4	NAG	B	1208	1	14,14,15	0.73	0	17,19,21	0.81	0
4	NAG	B	1209	1	14,14,15	0.74	0	17,19,21	0.87	0
4	NAG	C	1203	1	14,14,15	0.77	0	17,19,21	0.82	0
4	NAG	B	1212	1	14,14,15	0.72	0	17,19,21	0.82	0
4	NAG	C	1208	1	14,14,15	0.73	0	17,19,21	0.81	0
4	NAG	A	1205	1	14,14,15	0.72	0	17,19,21	1.15	1 (5%)
4	NAG	B	1203	1	14,14,15	0.77	0	17,19,21	0.82	0
4	NAG	C	1204	1	14,14,15	0.78	0	17,19,21	1.01	1 (5%)
4	NAG	A	1204	1	14,14,15	0.77	0	17,19,21	0.99	1 (5%)
4	NAG	A	1213	1	14,14,15	0.76	0	17,19,21	0.92	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
4	NAG	C	1210	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1210	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1210	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1209	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1211	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1211	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1213	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1212	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1211	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1208	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1212	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1202	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1213	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1209	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1203	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1212	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1203	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1213	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	NAG	C2-N2-C7	7.57	133.05	122.90
4	C	1201	NAG	C2-N2-C7	7.57	133.04	122.90
4	A	1201	NAG	C2-N2-C7	7.54	133.01	122.90
4	A	1201	NAG	C1-C2-N2	4.04	116.80	110.43
4	C	1201	NAG	C1-C2-N2	4.01	116.75	110.43

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1201	NAG	C1-C2-N2-C7
4	B	1201	NAG	C1-C2-N2-C7
4	C	1201	NAG	C1-C2-N2-C7
4	A	1203	NAG	C8-C7-N2-C2
4	A	1203	NAG	O7-C7-N2-C2

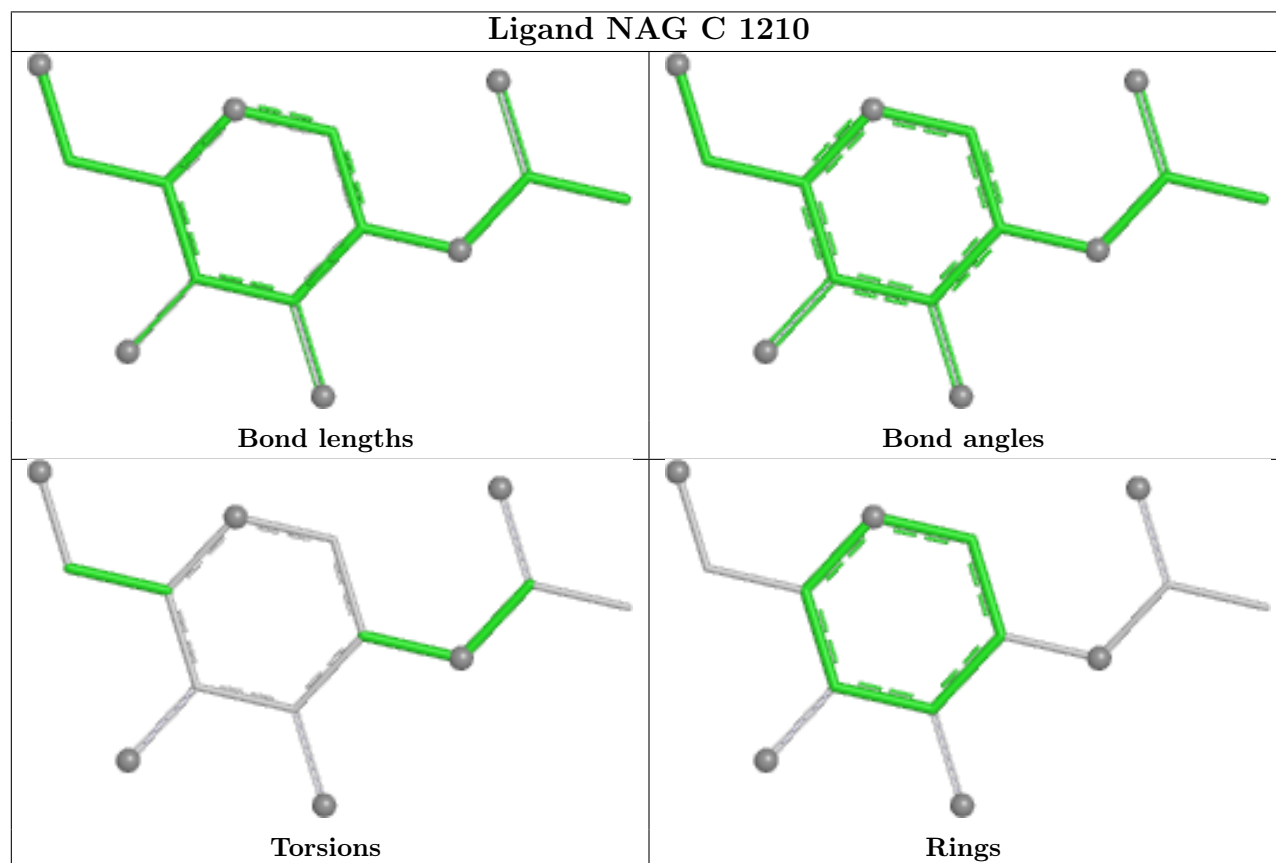
There are no ring outliers.

3 monomers are involved in 6 short contacts:

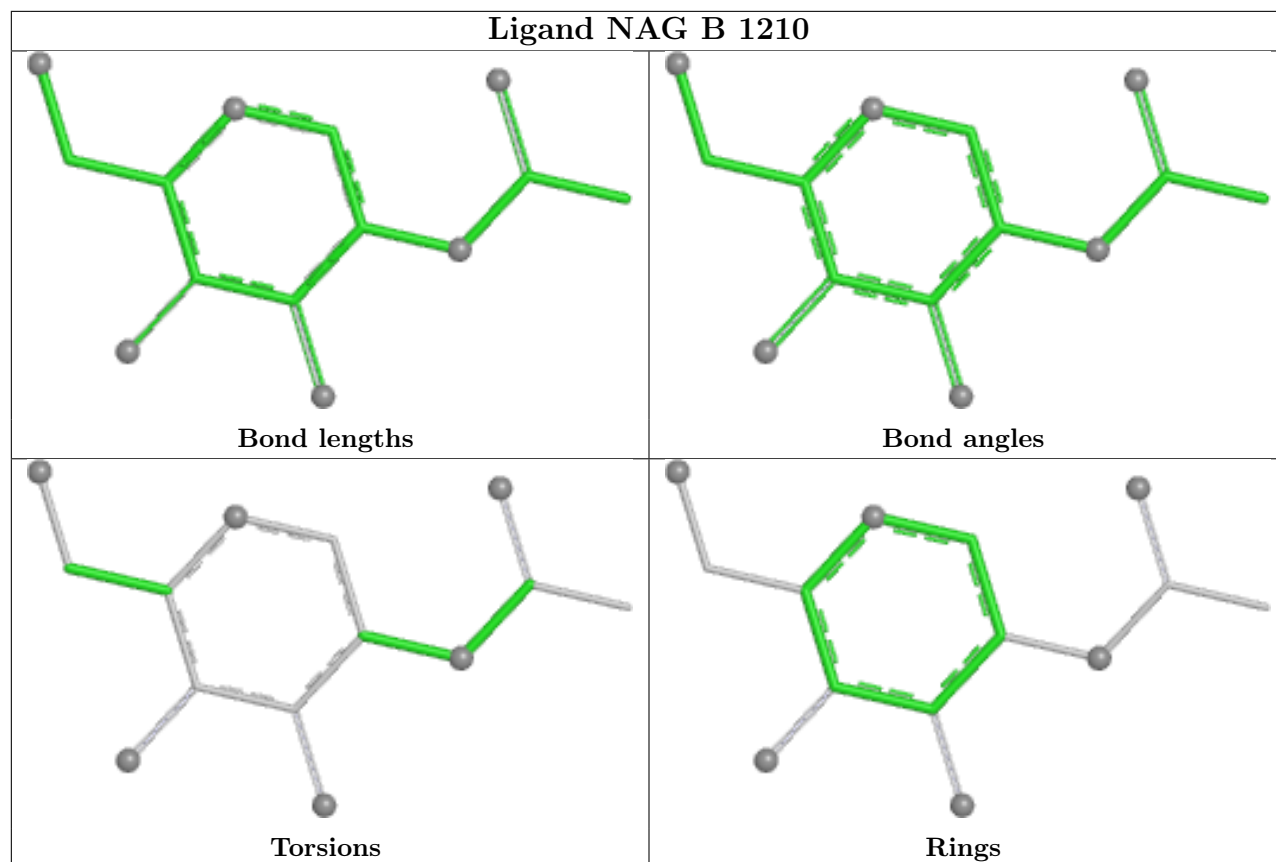
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1204	NAG	2	0
4	C	1204	NAG	2	0
4	A	1204	NAG	2	0

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

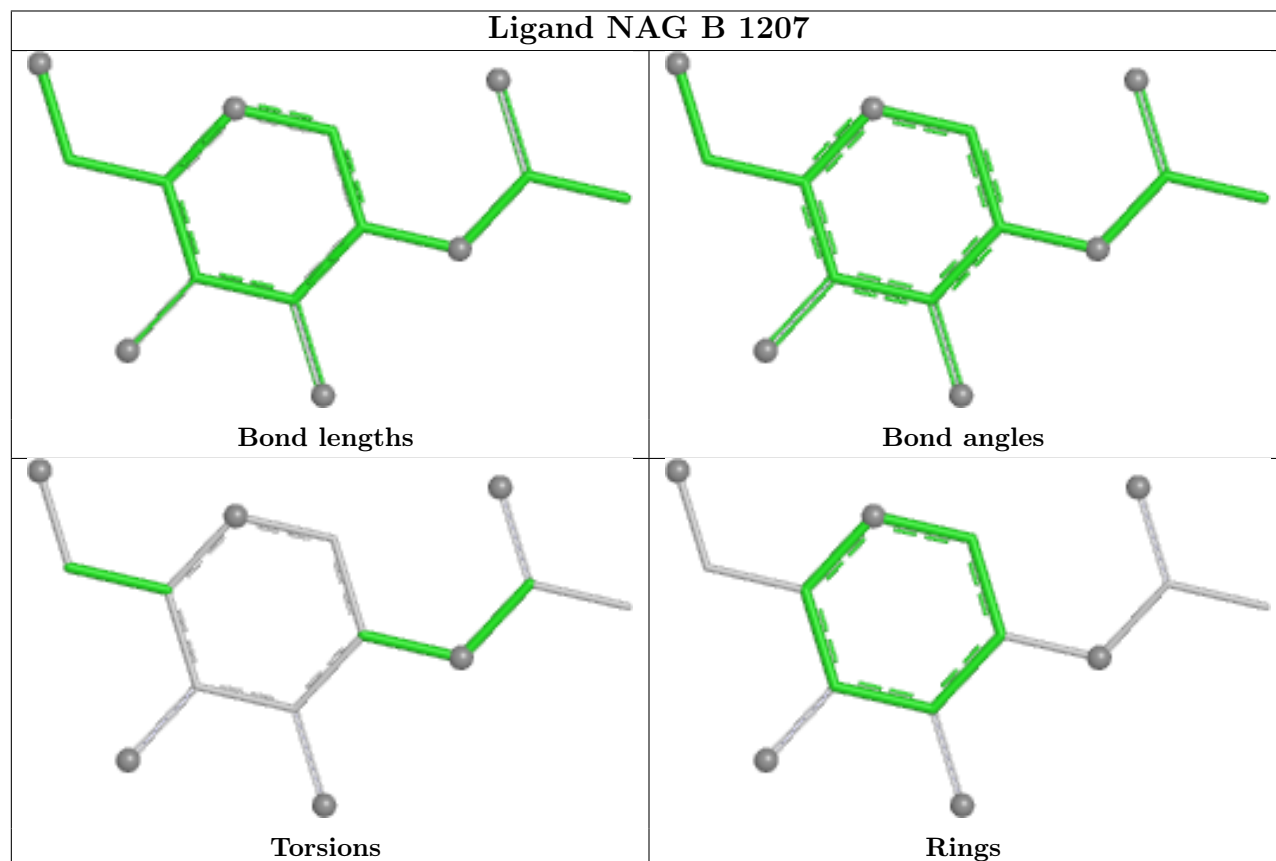
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



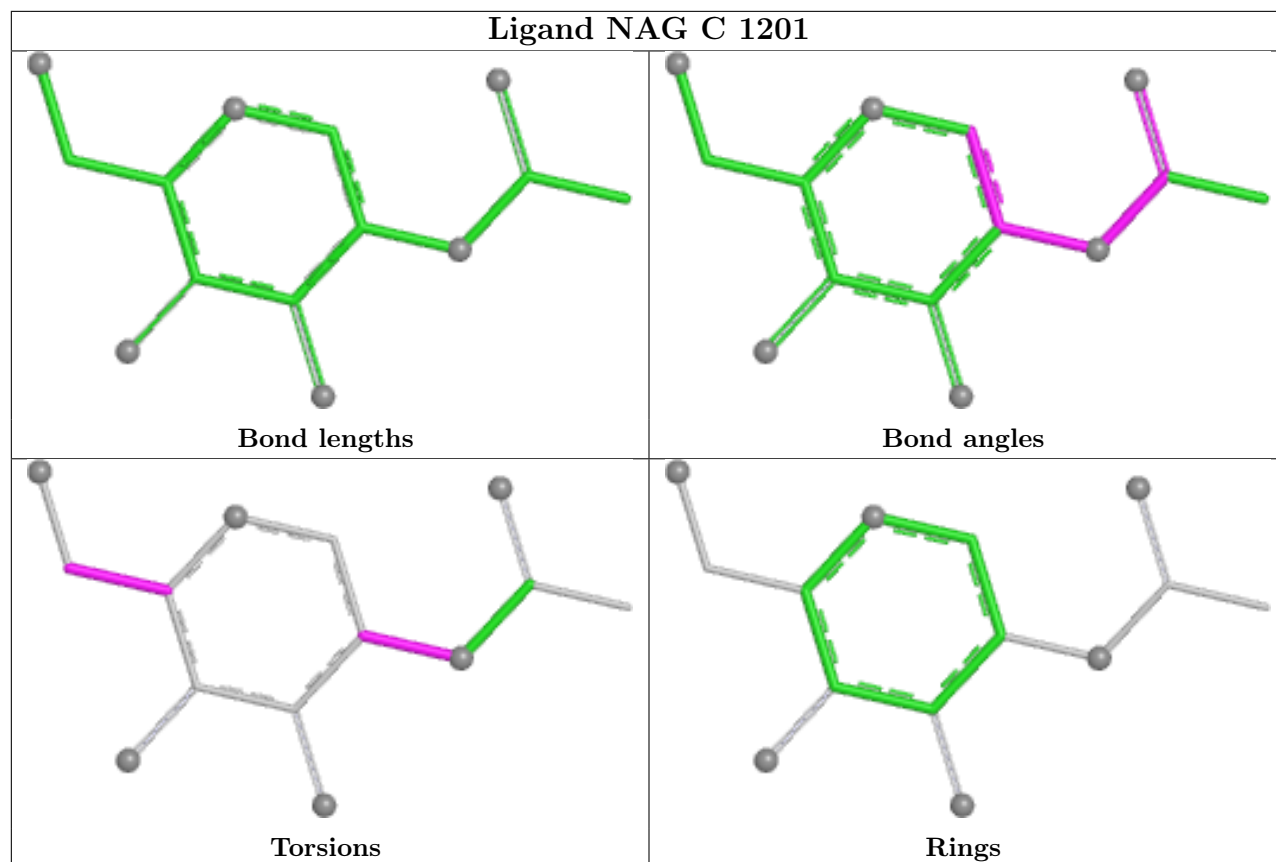
Ligand NAG B 1210



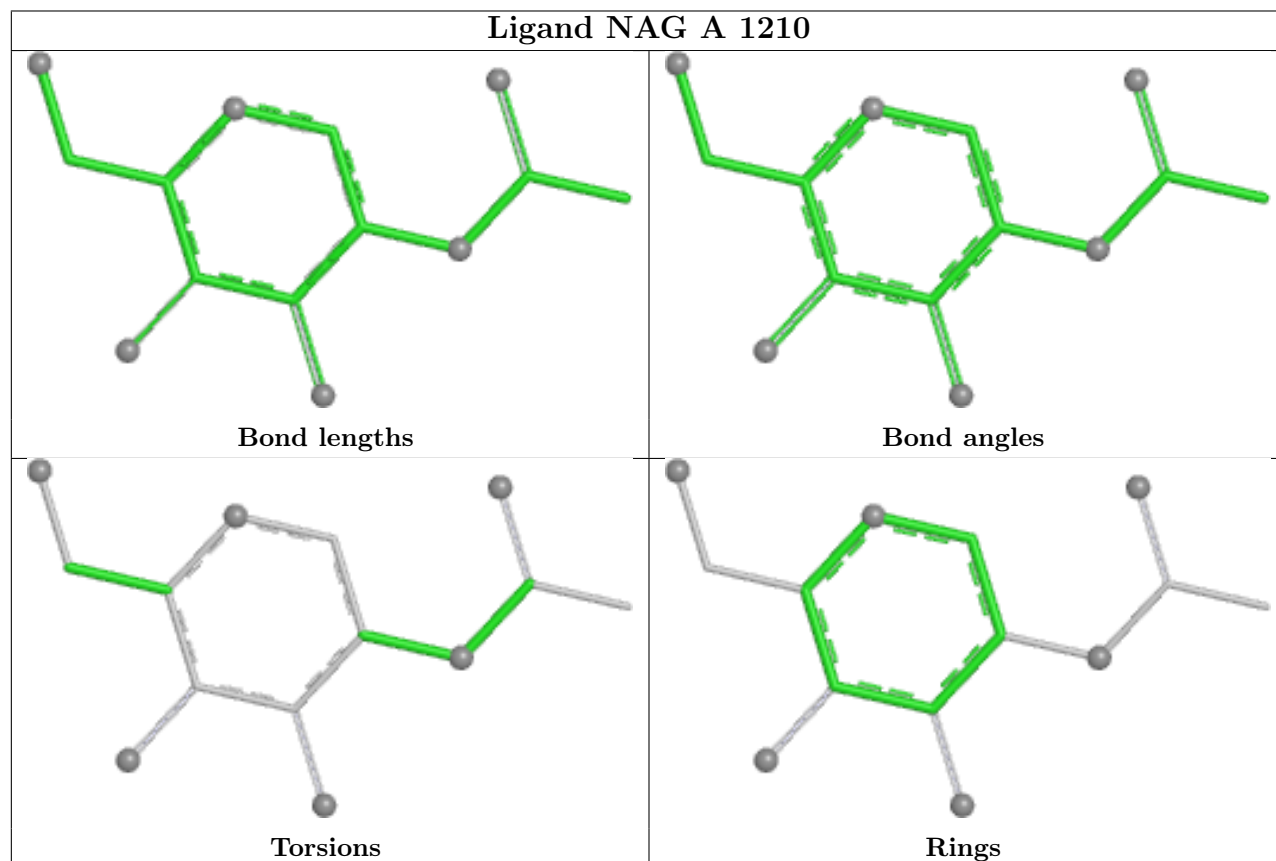
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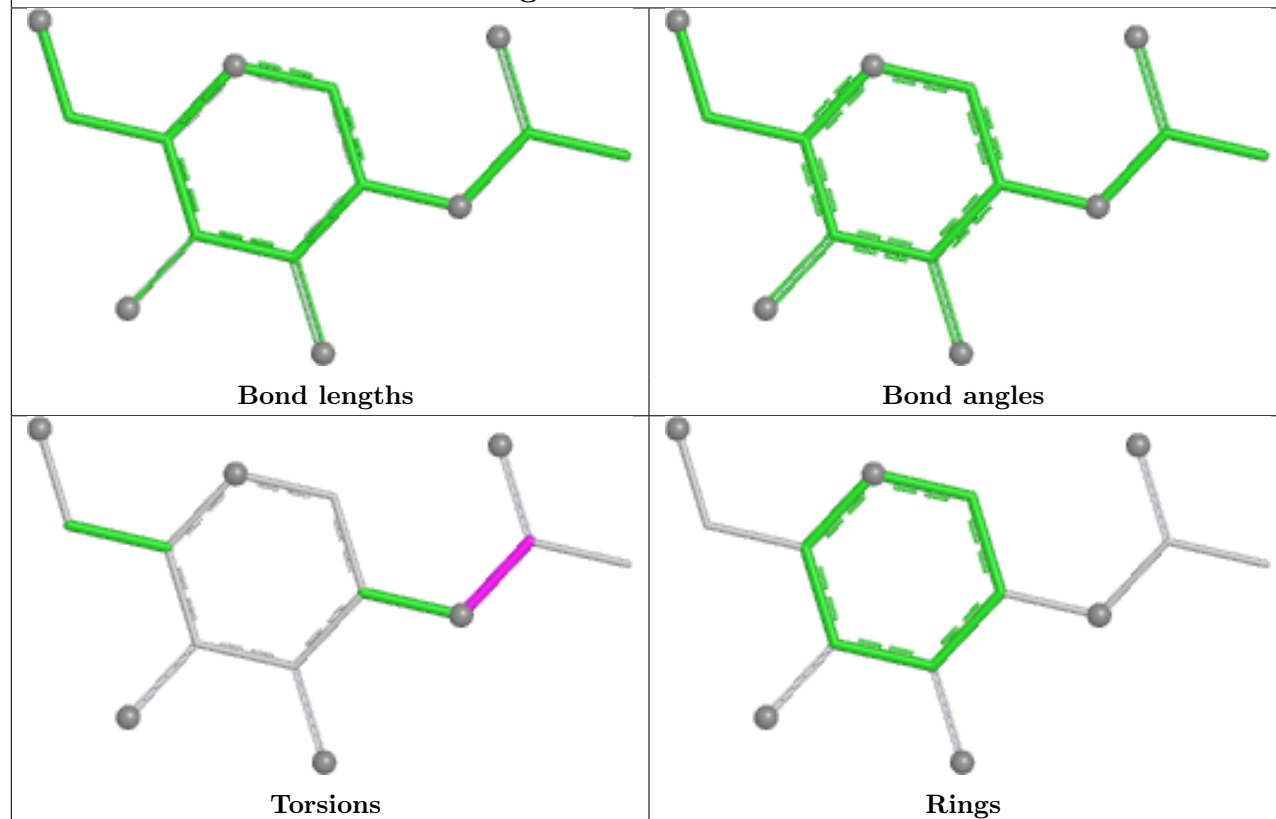
Ligand NAG C 1201



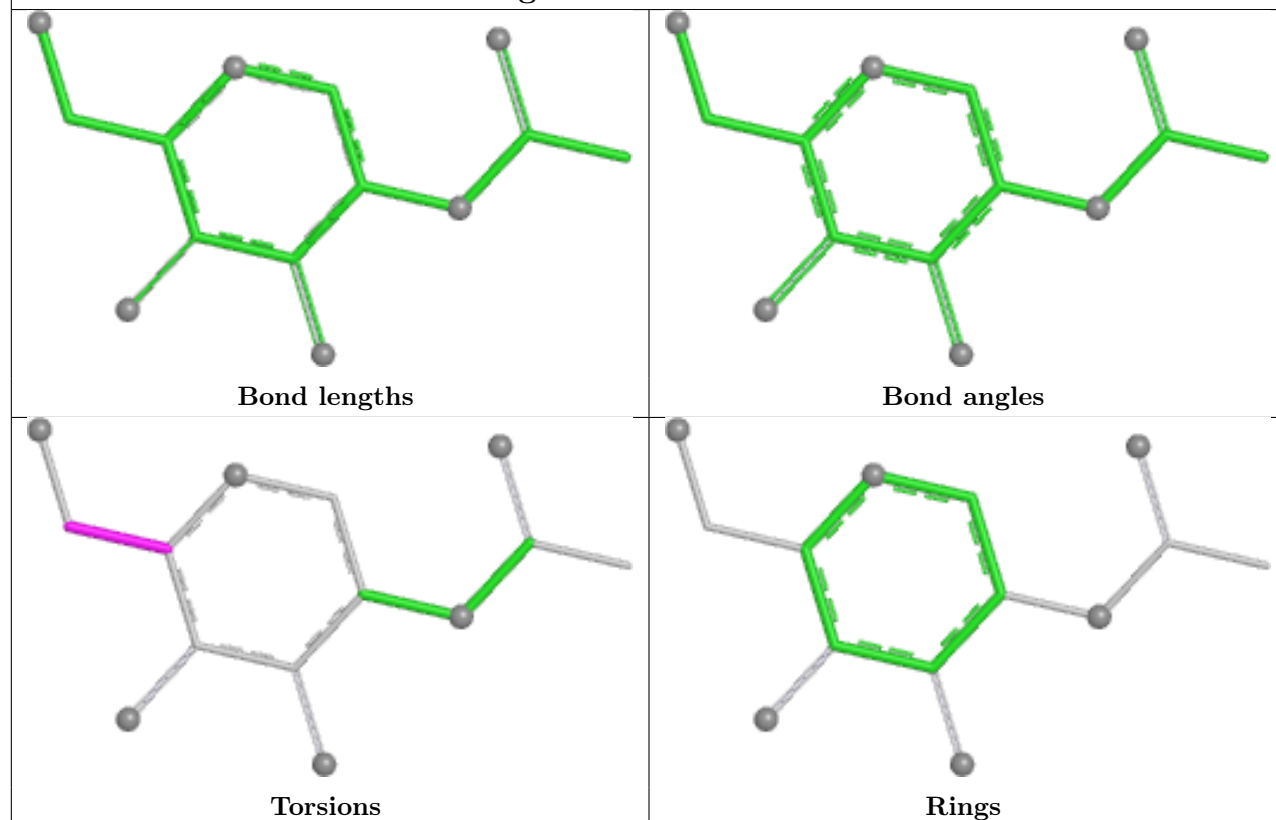
Ligand NAG A 1210



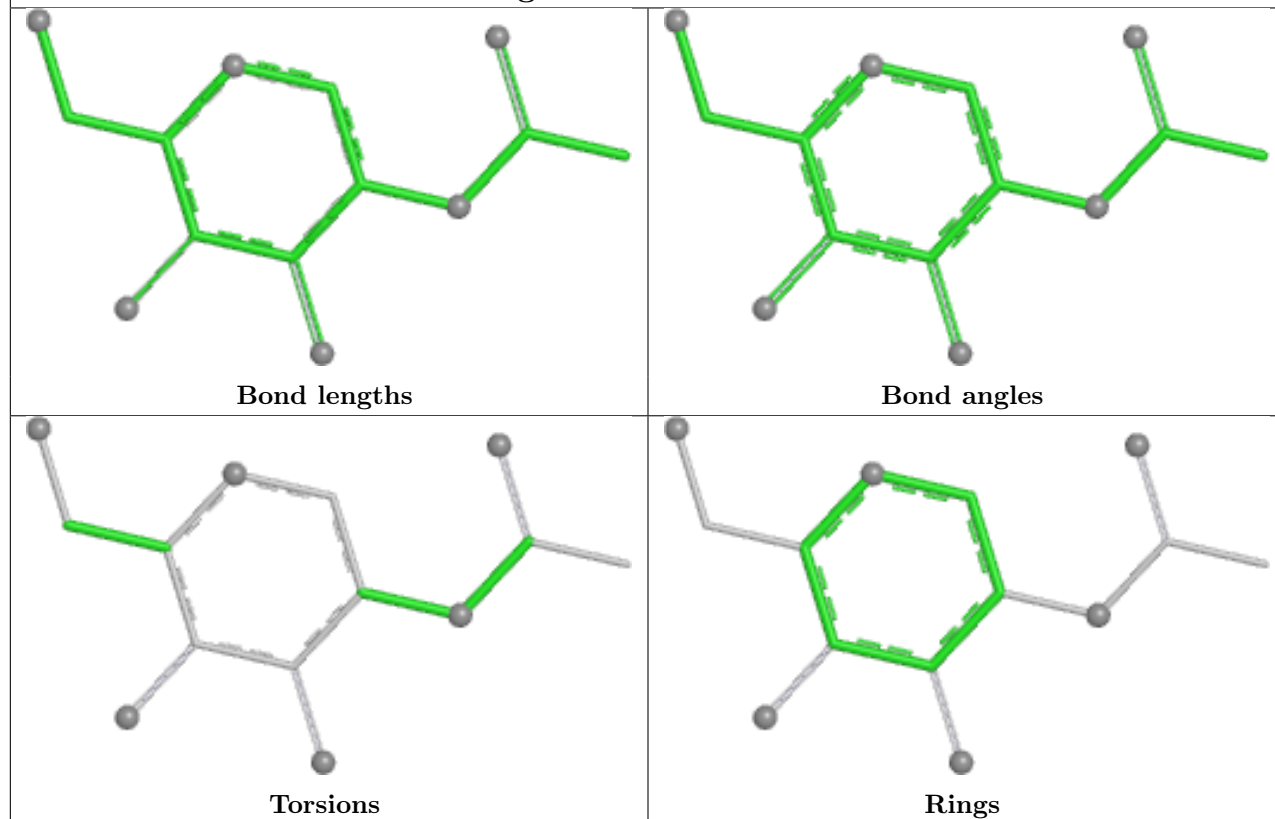
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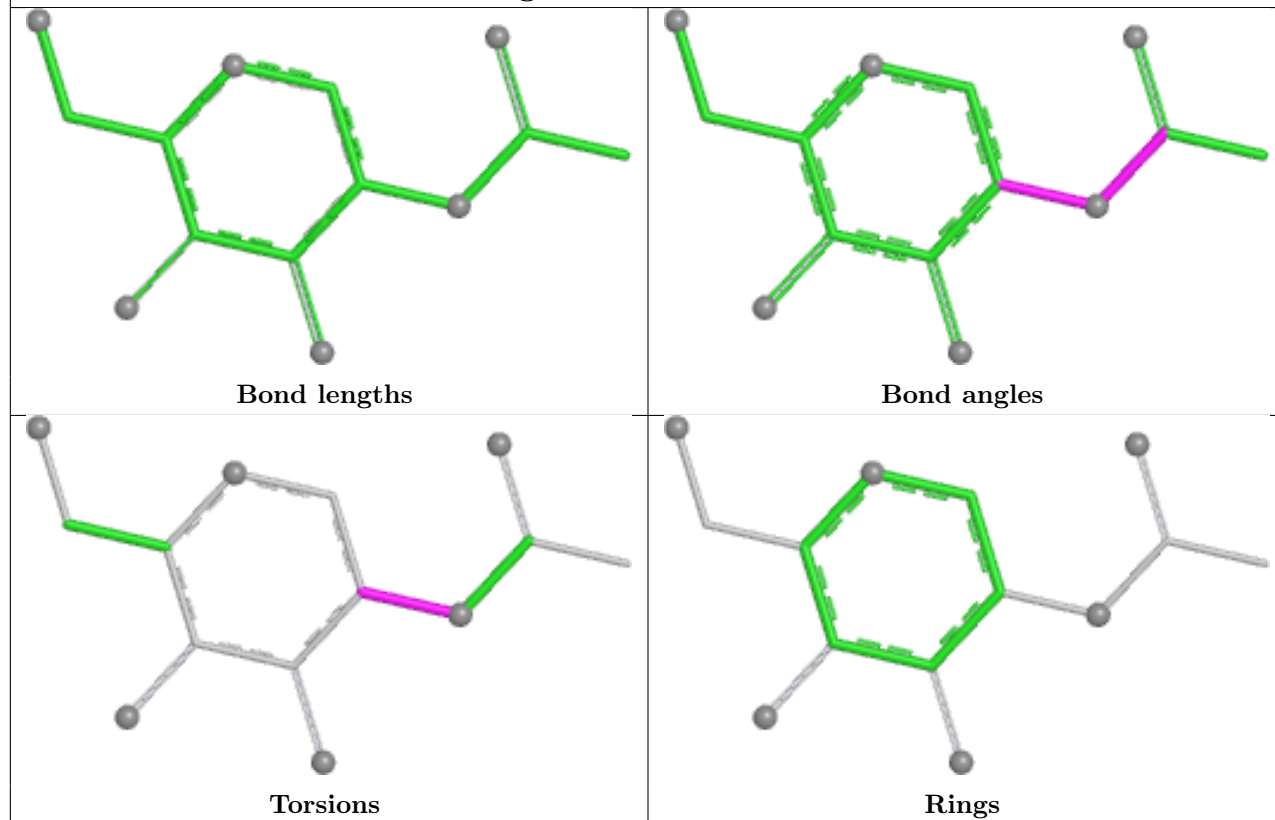
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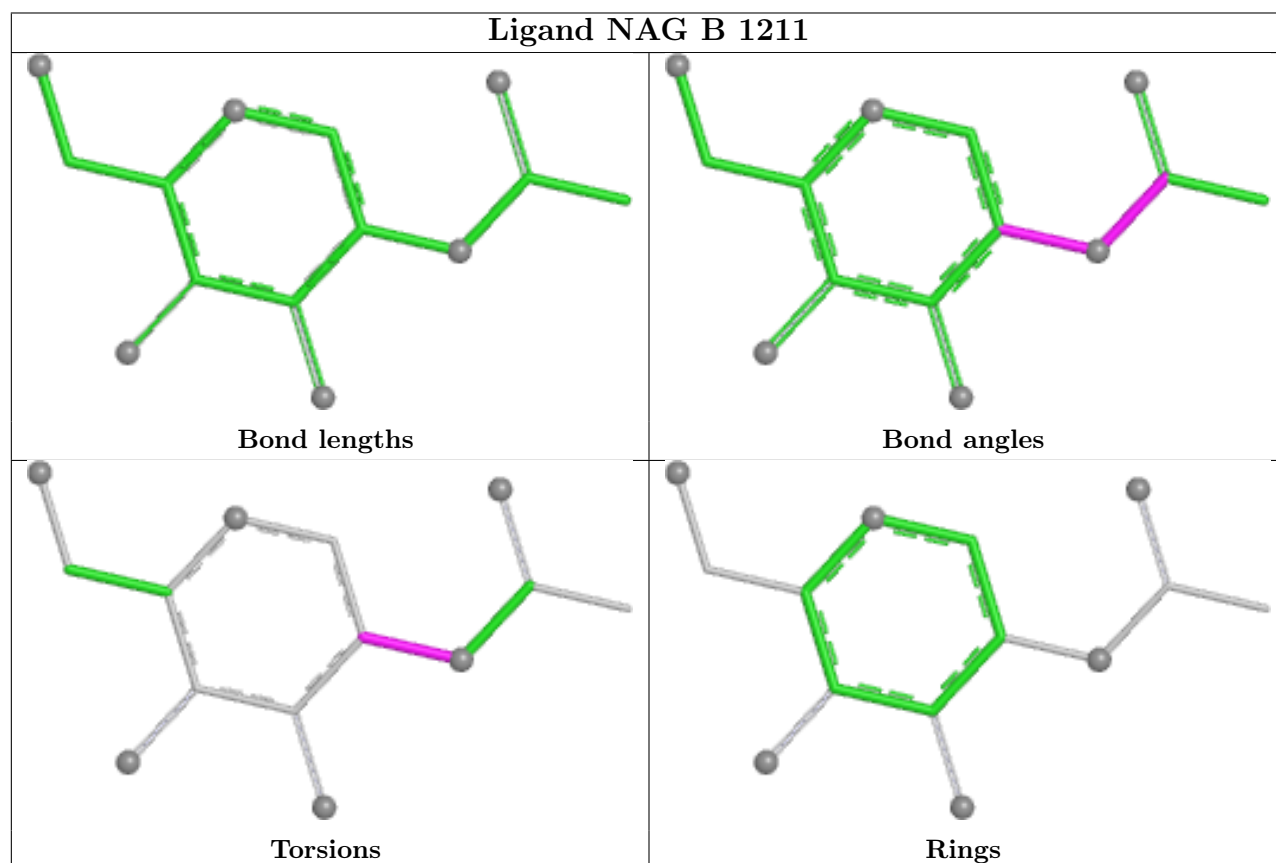
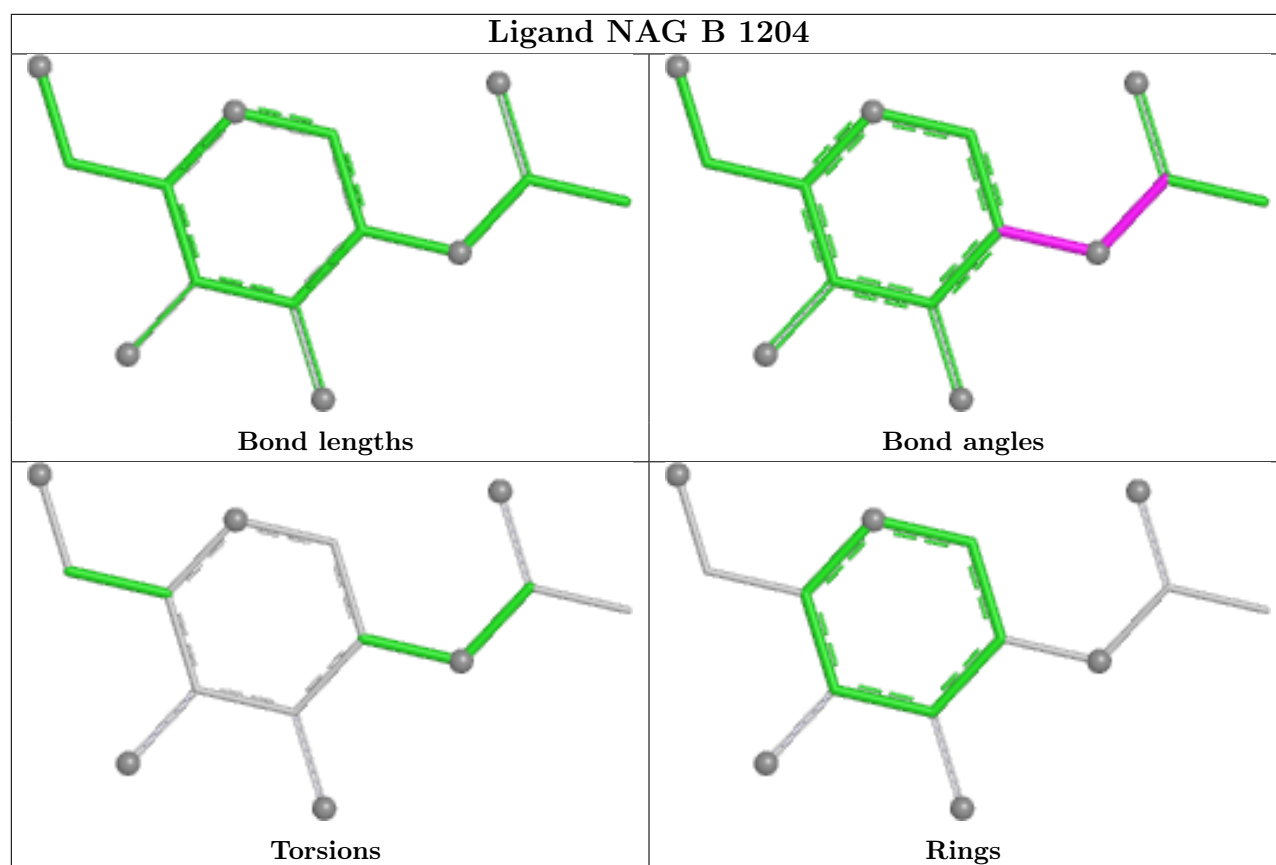


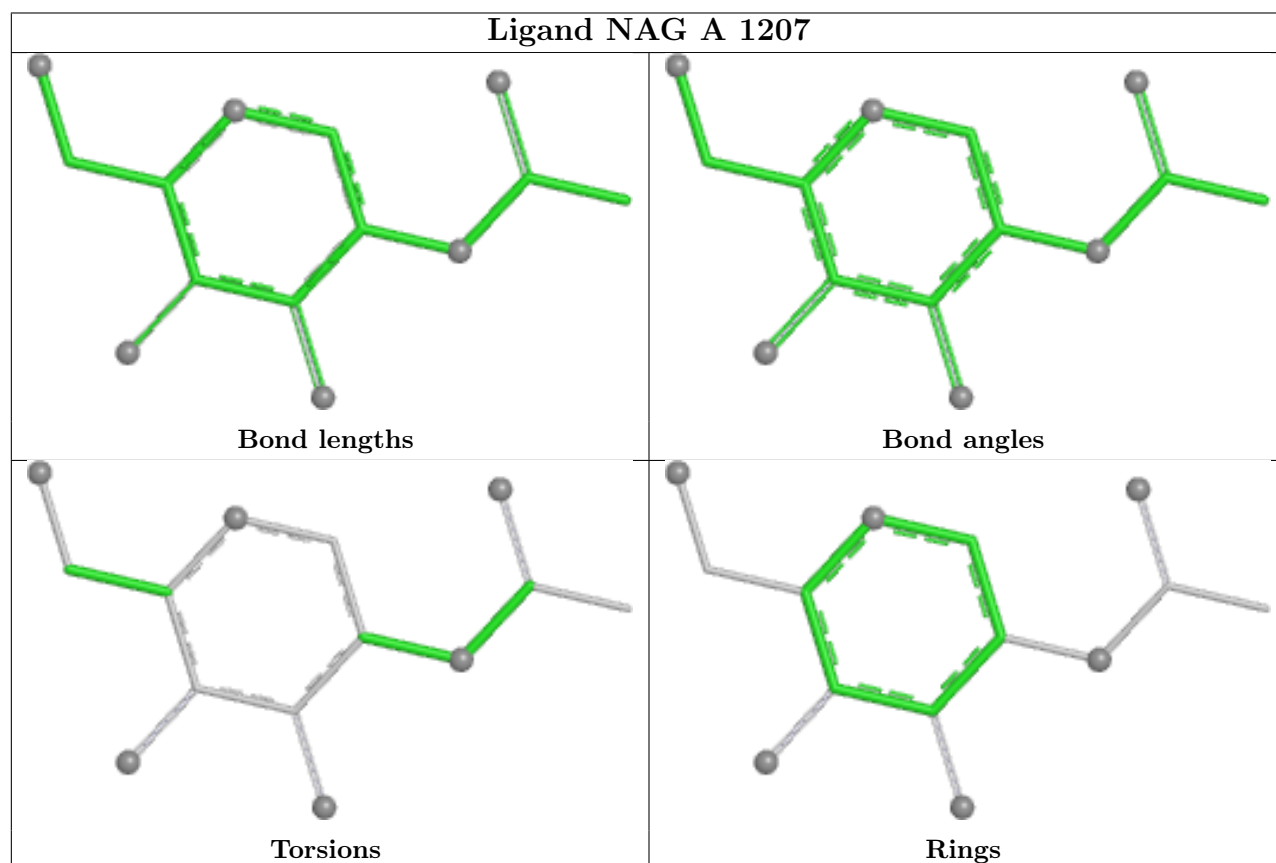
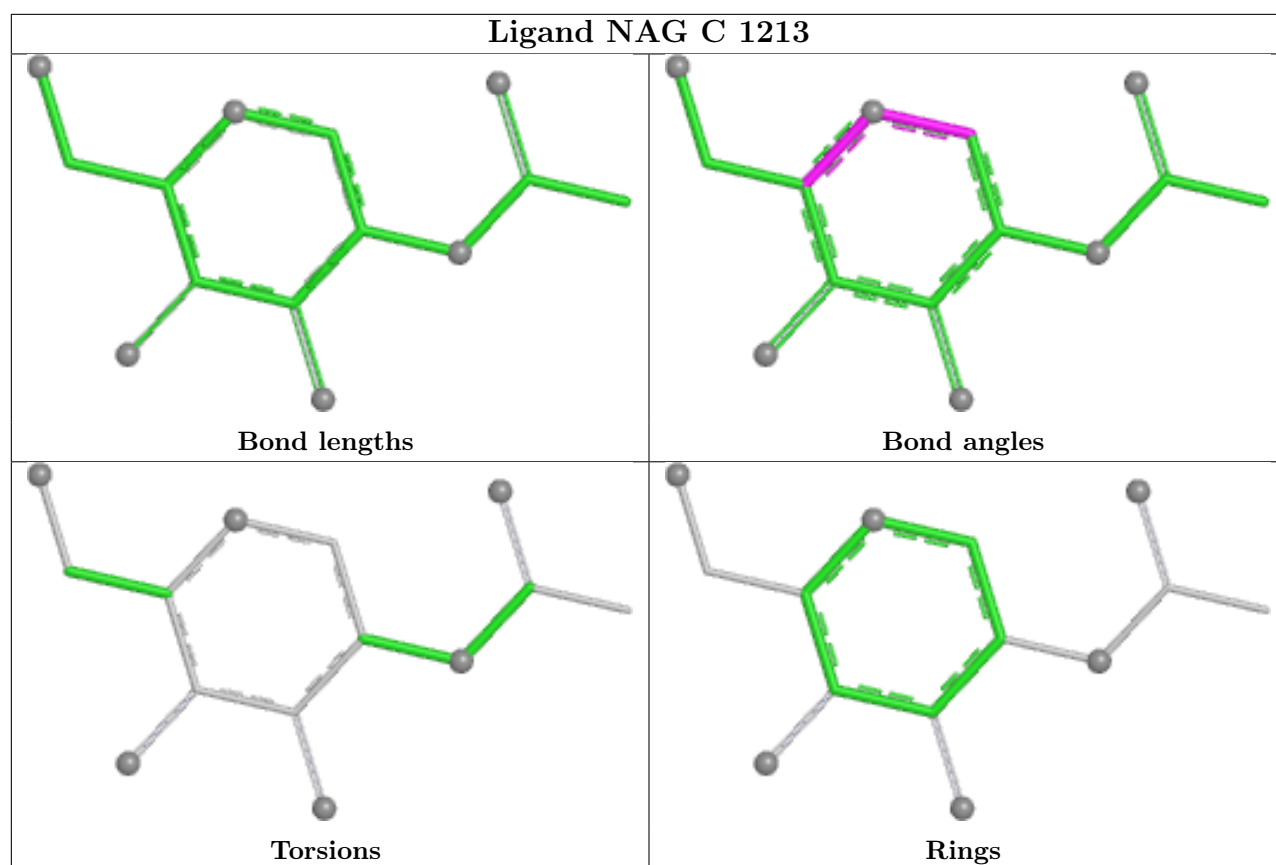
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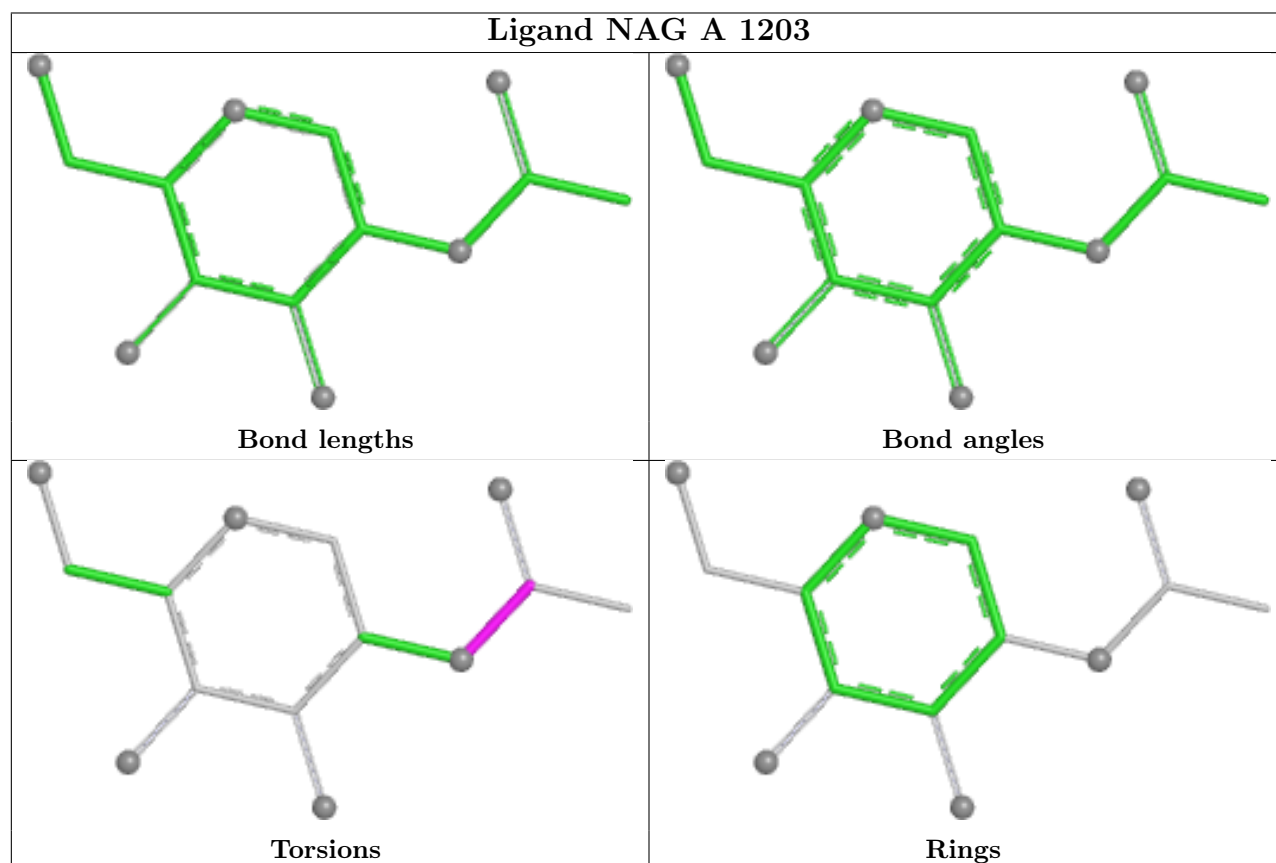
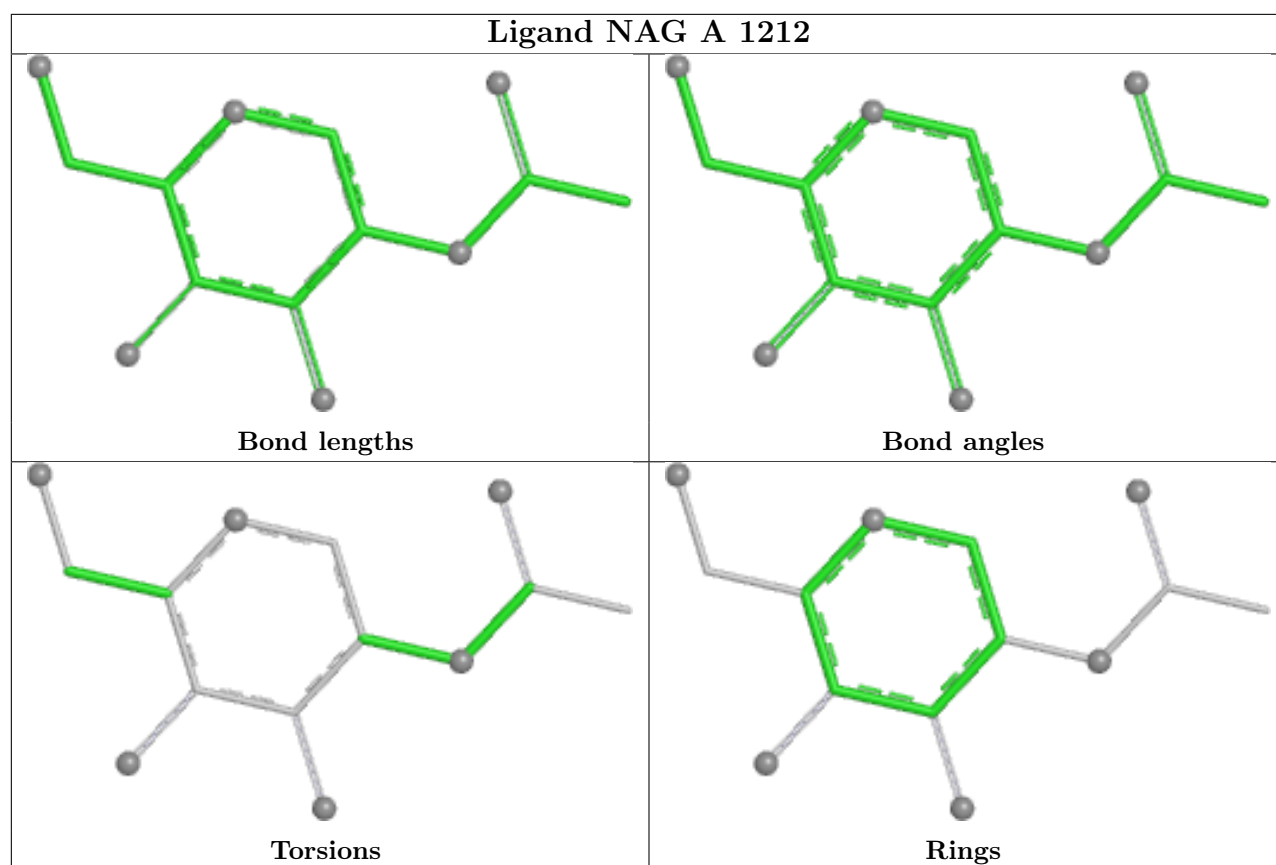


Ligand NAG C 1211

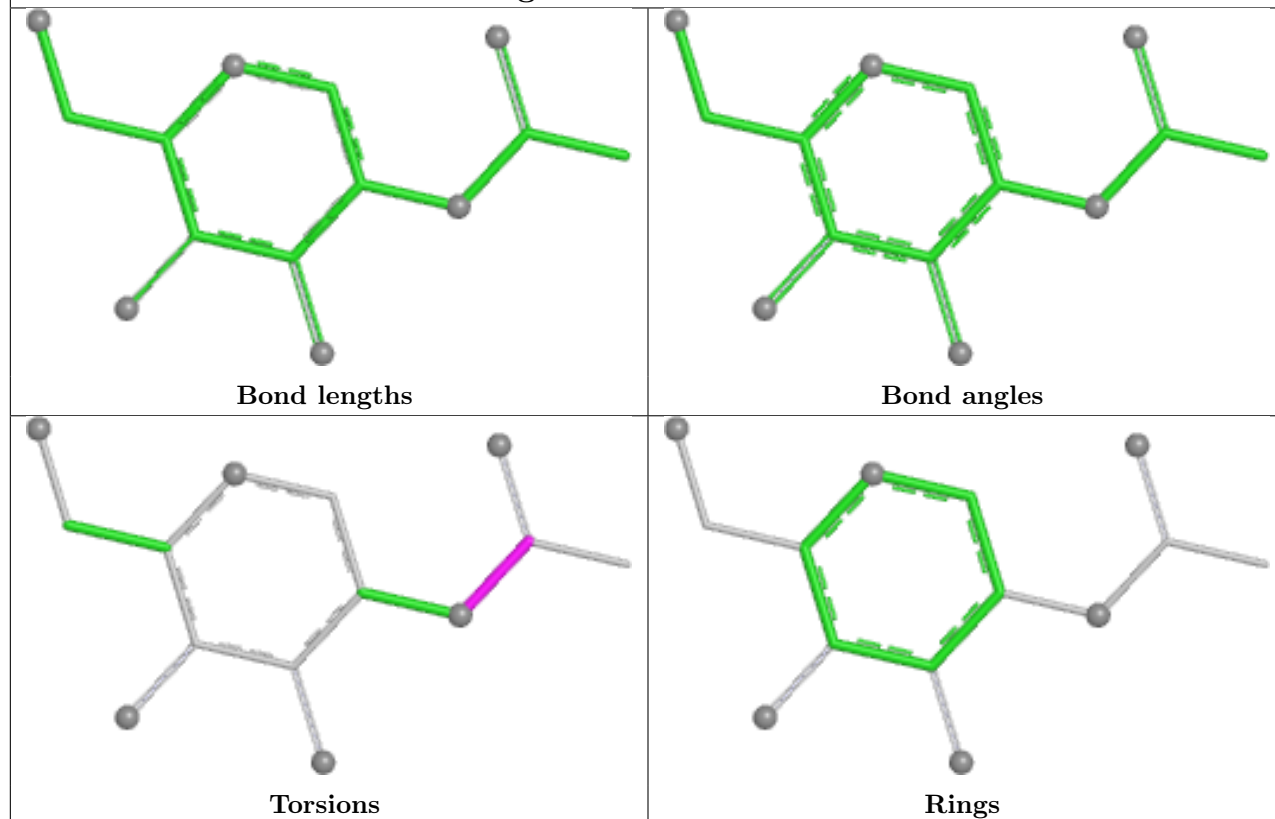




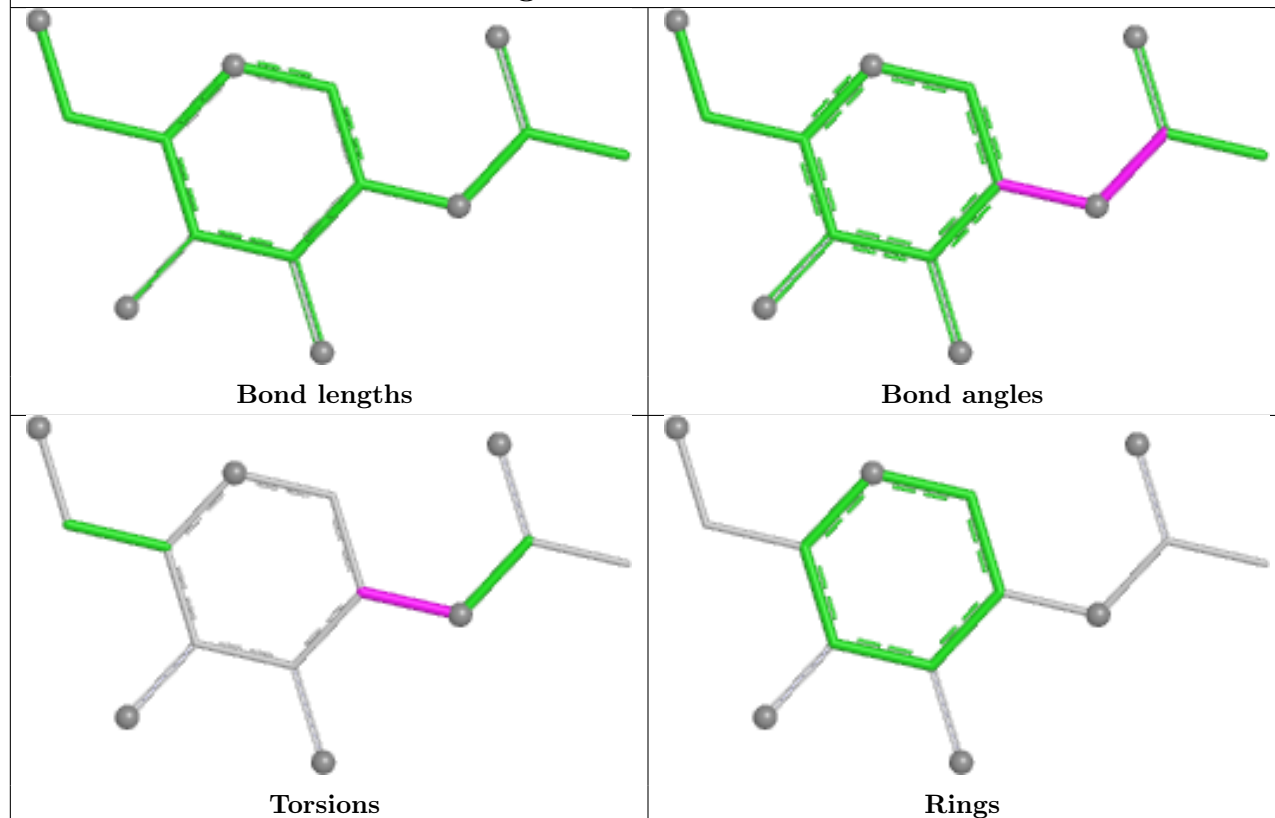


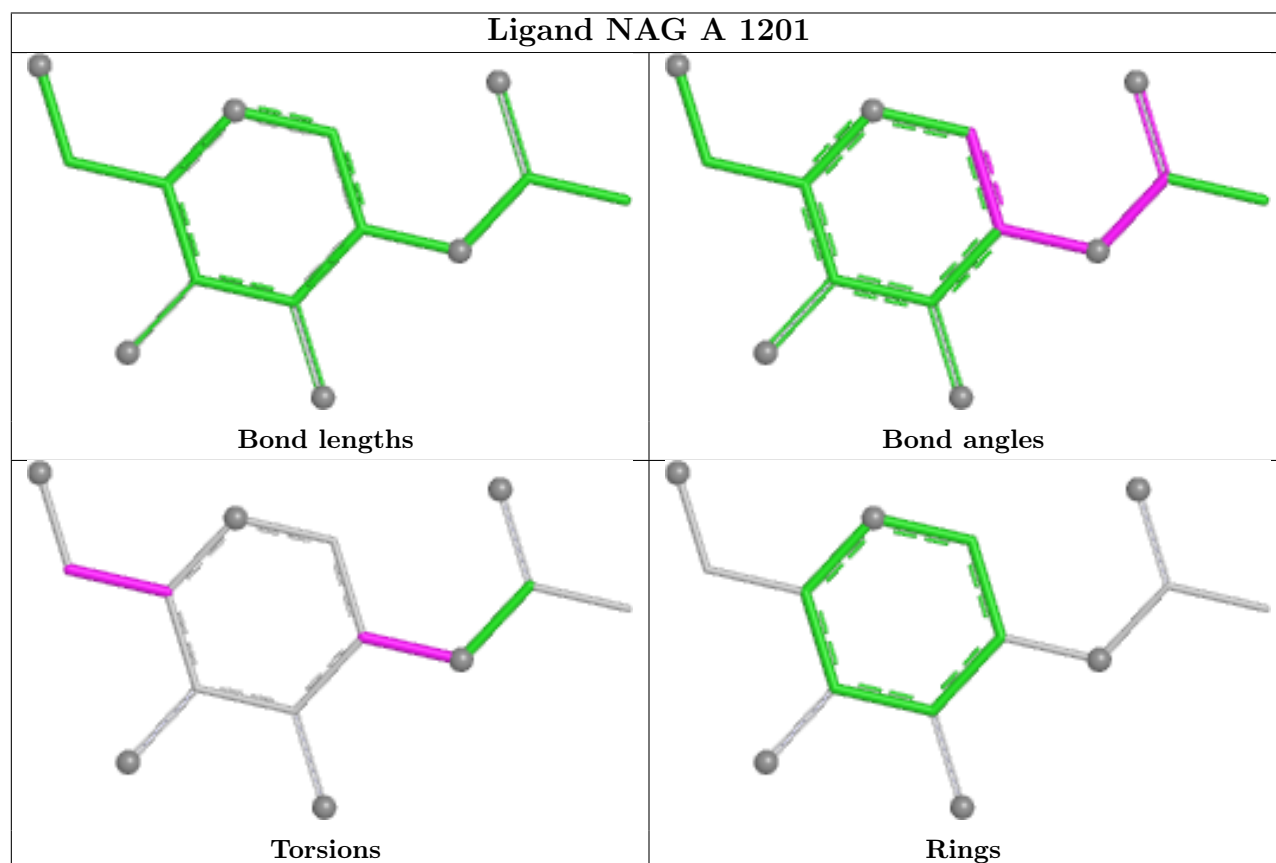
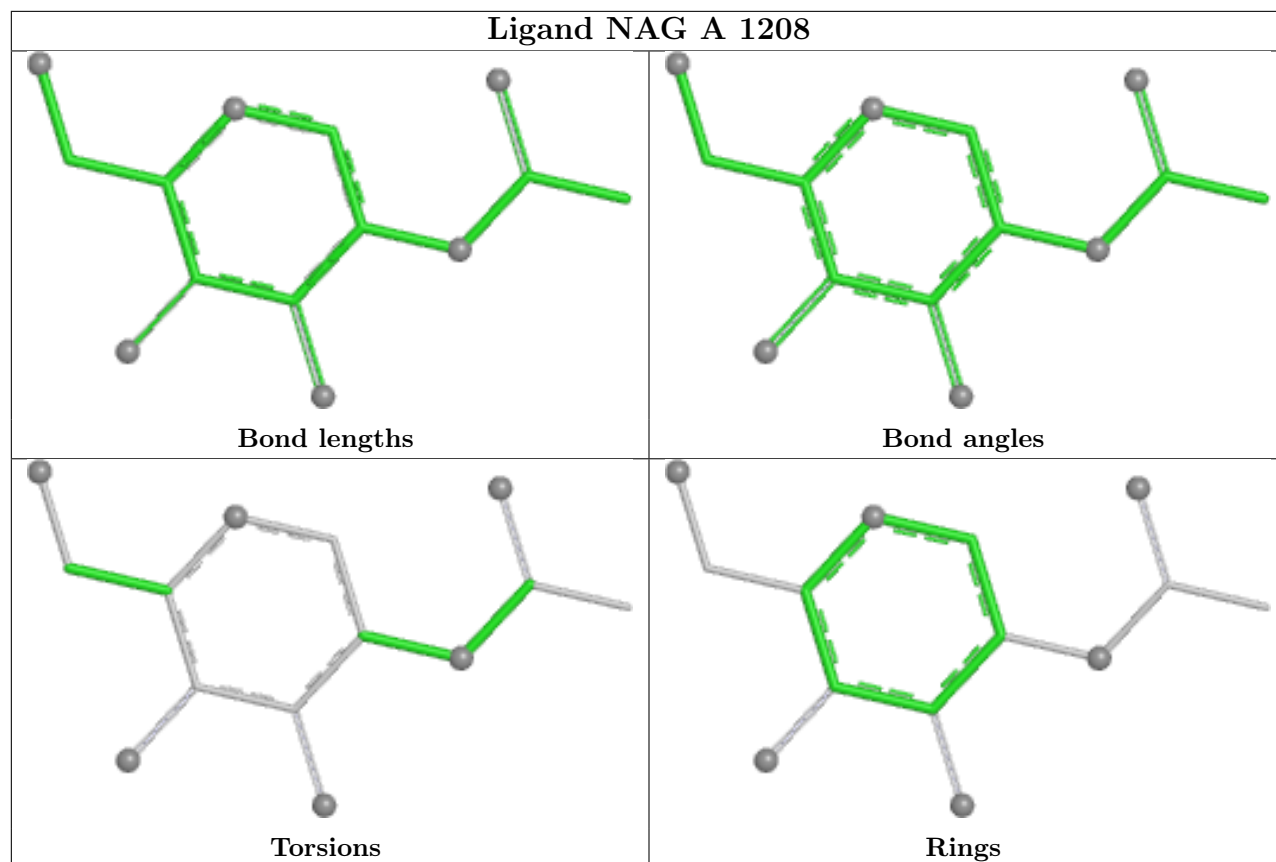


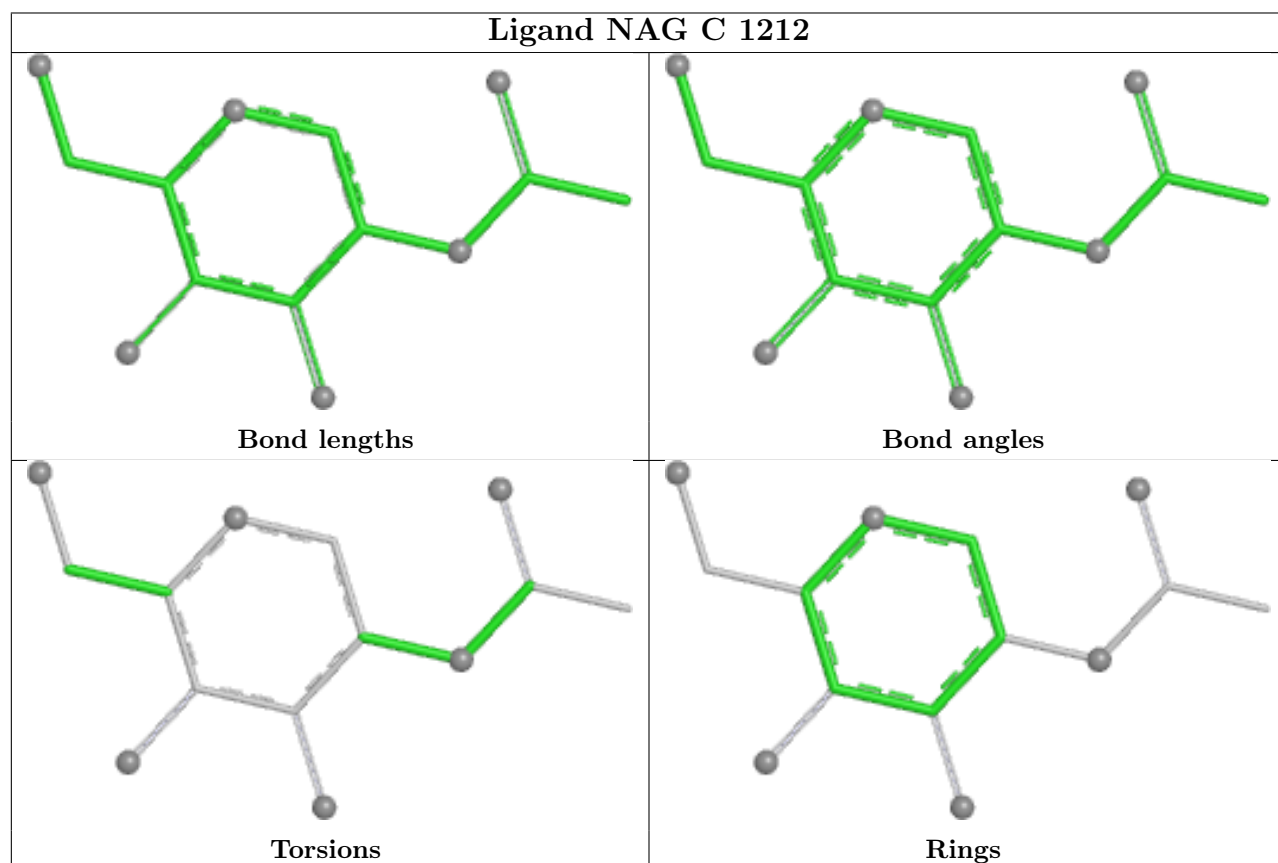
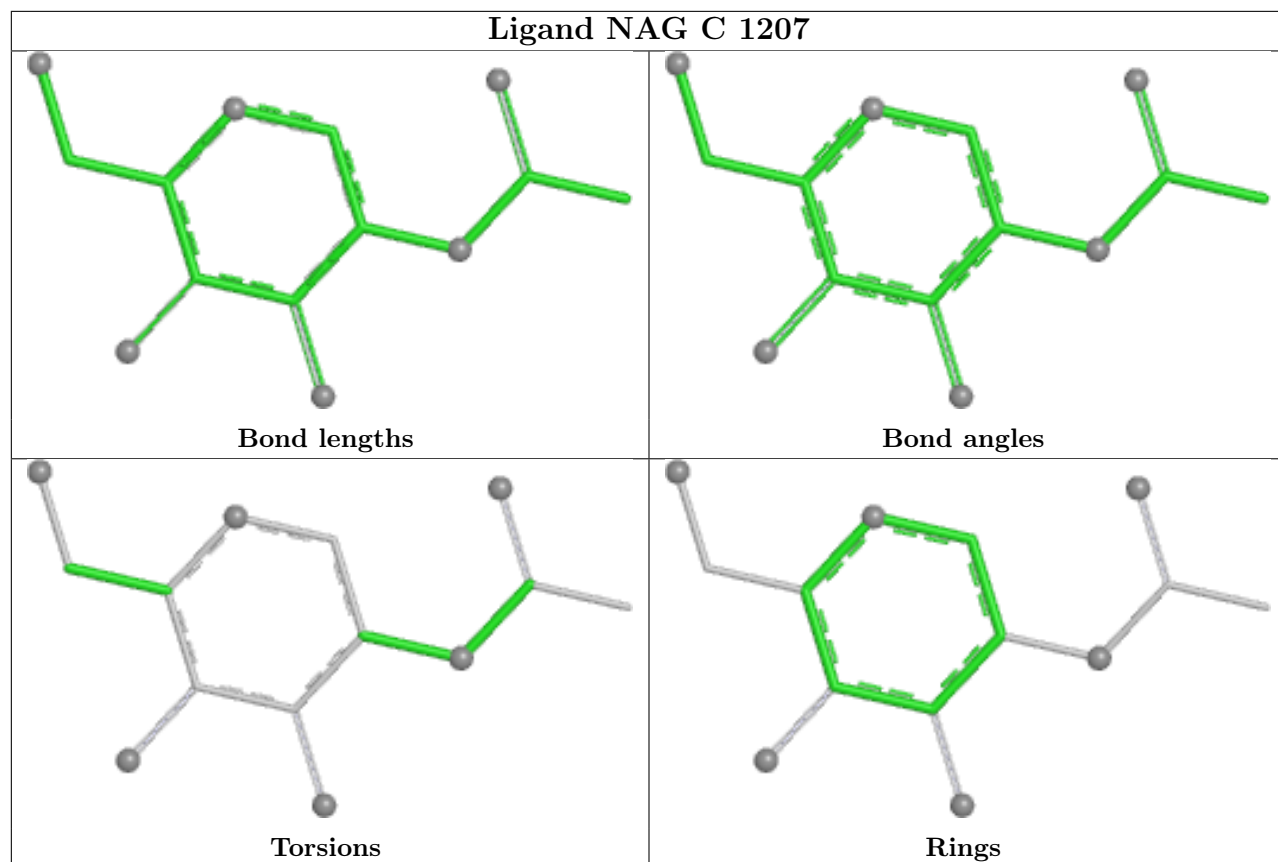
Ligand NAG A 1206

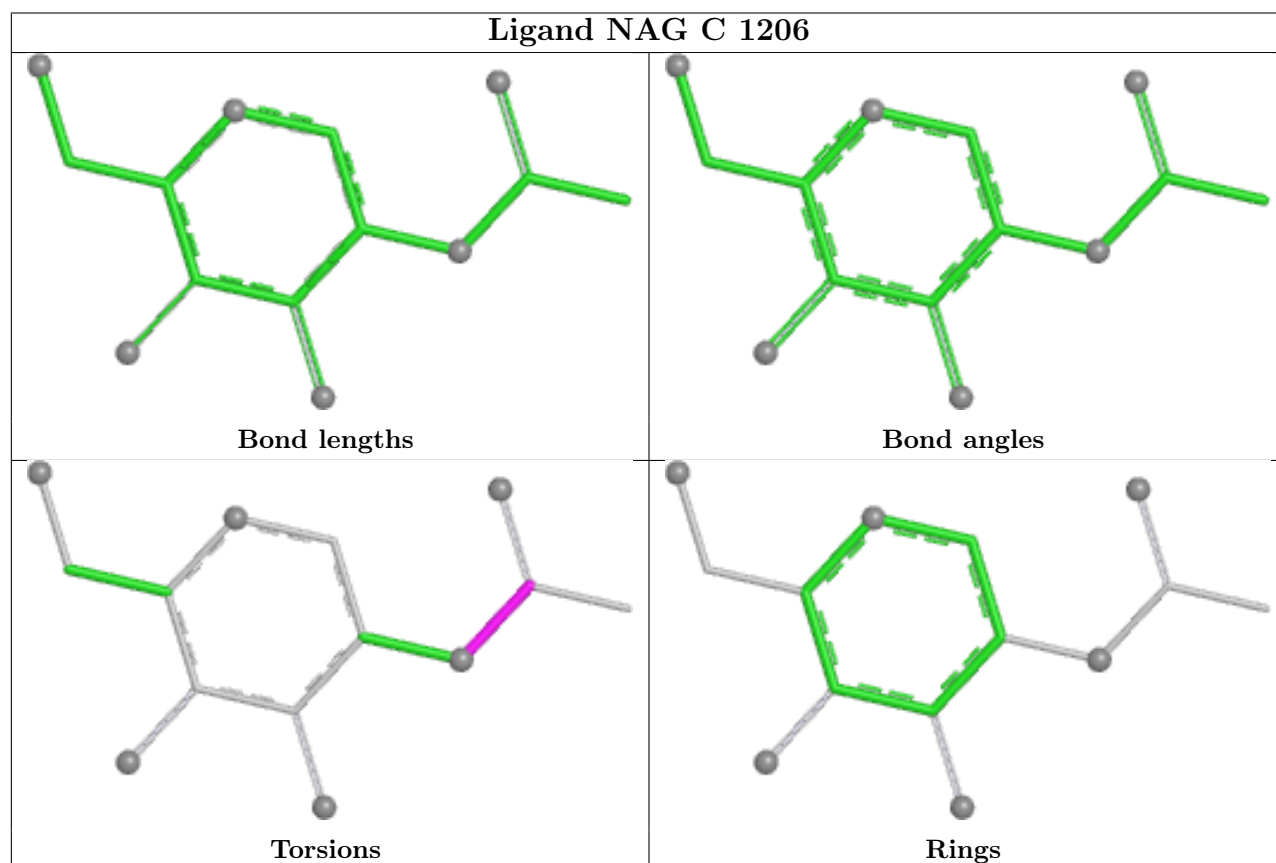
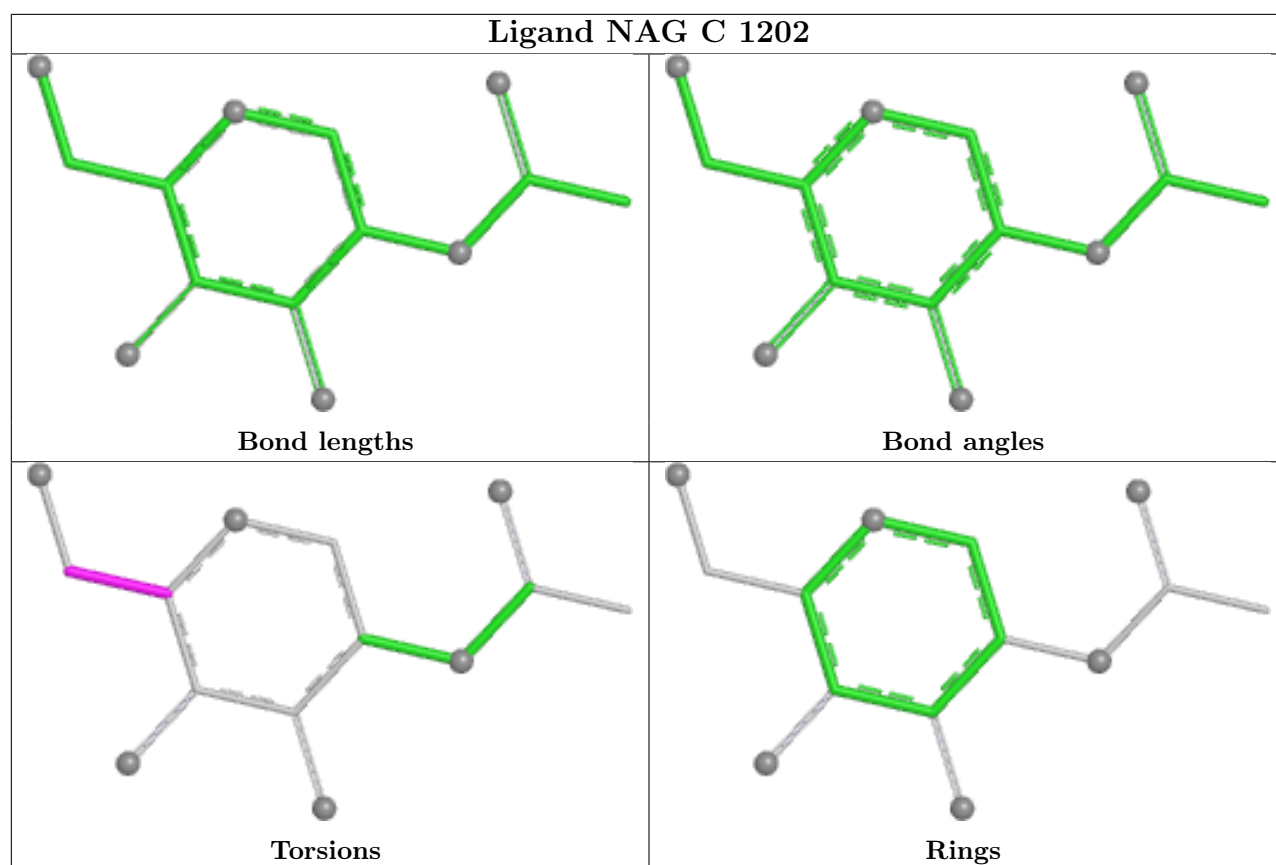


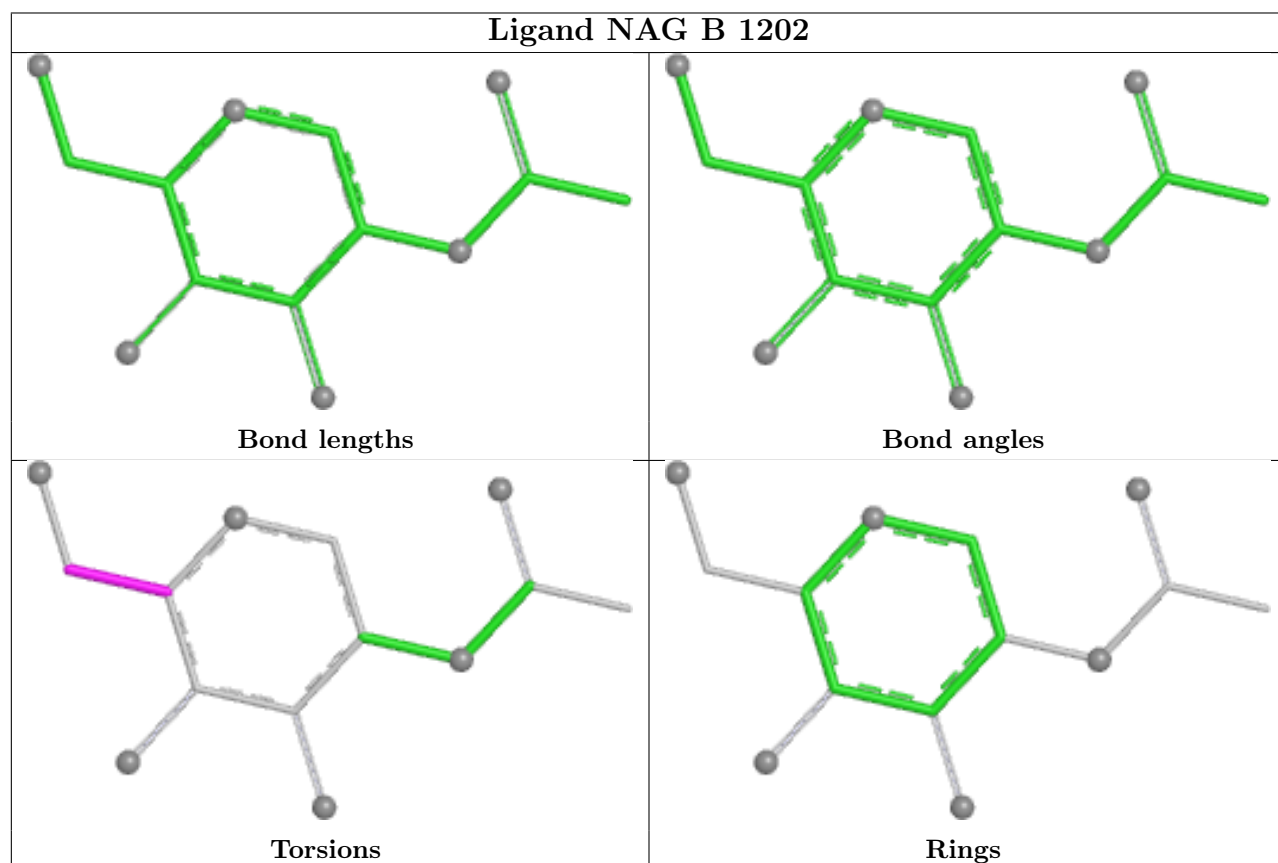
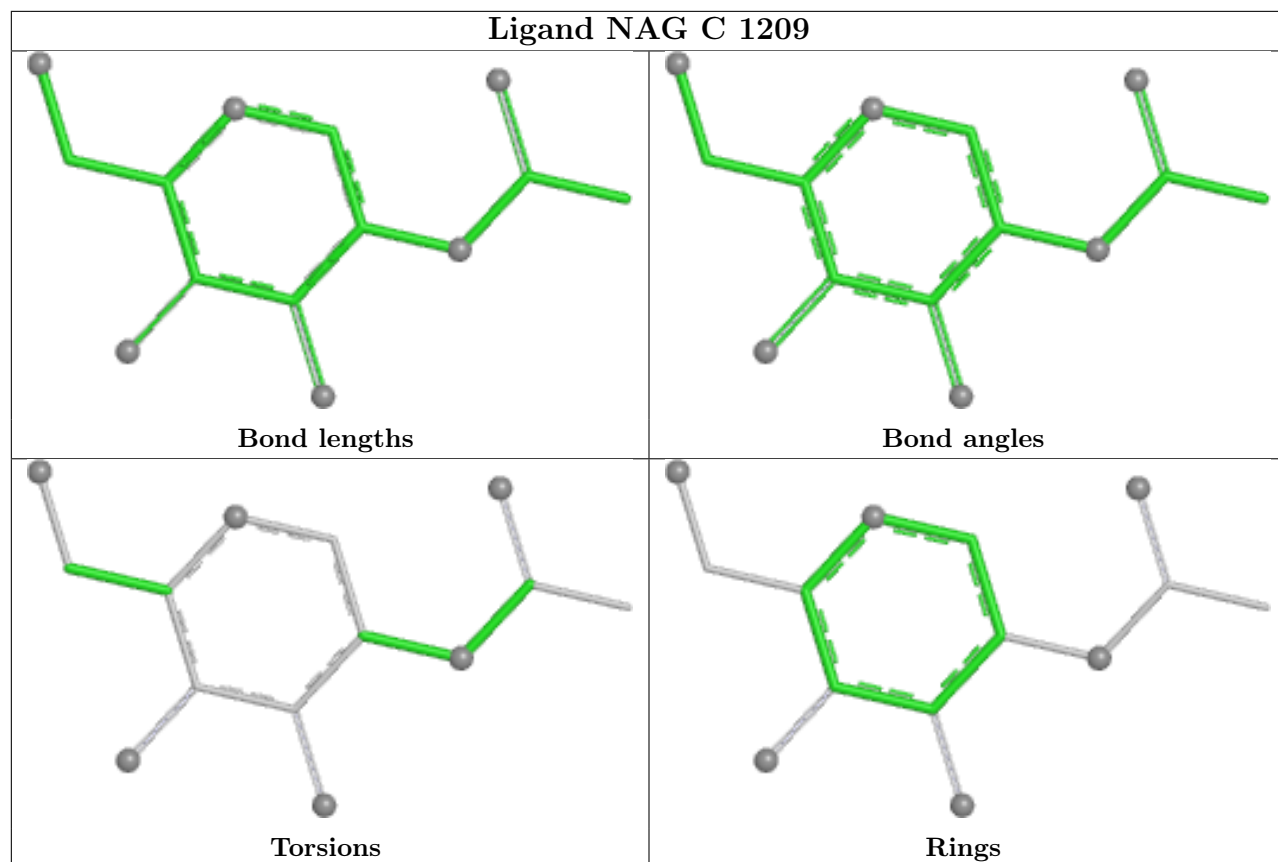
Ligand NAG A 1211



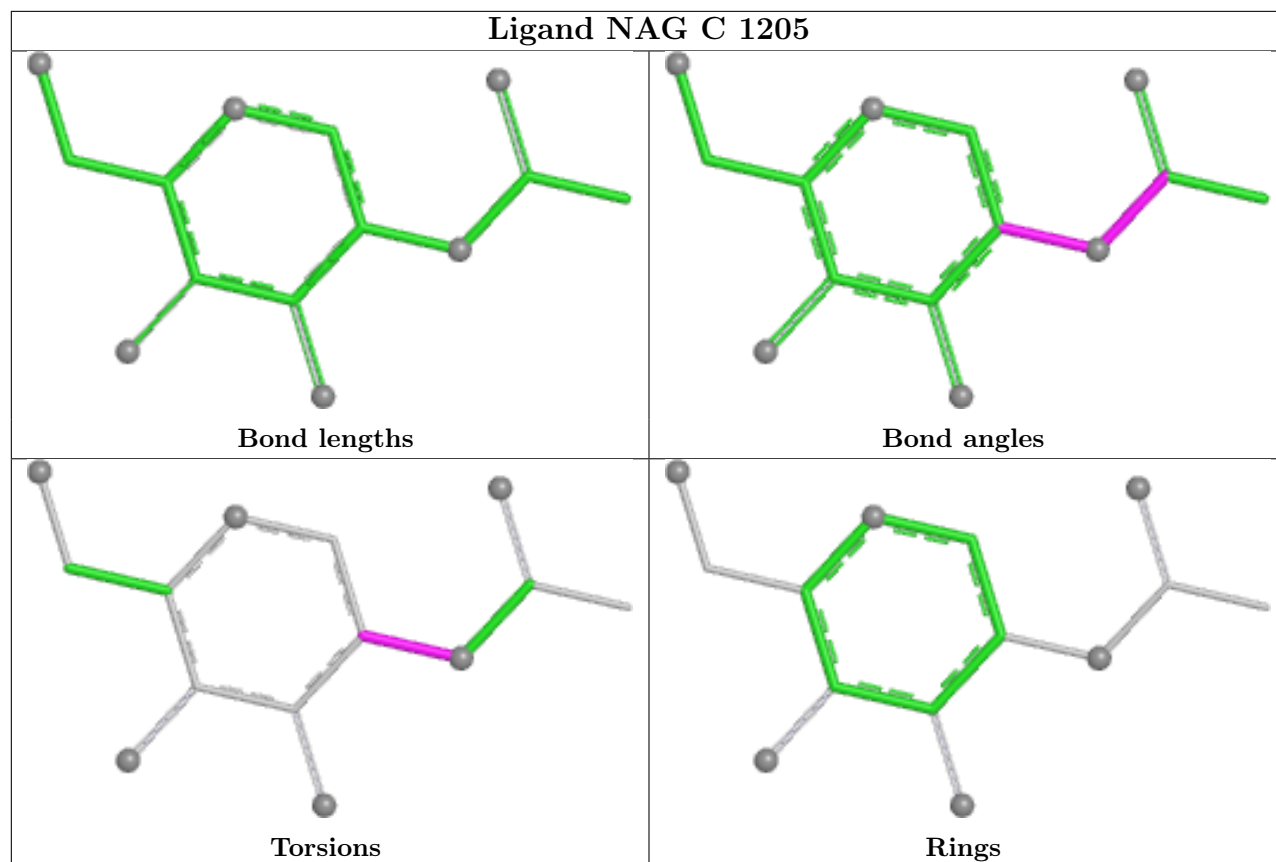




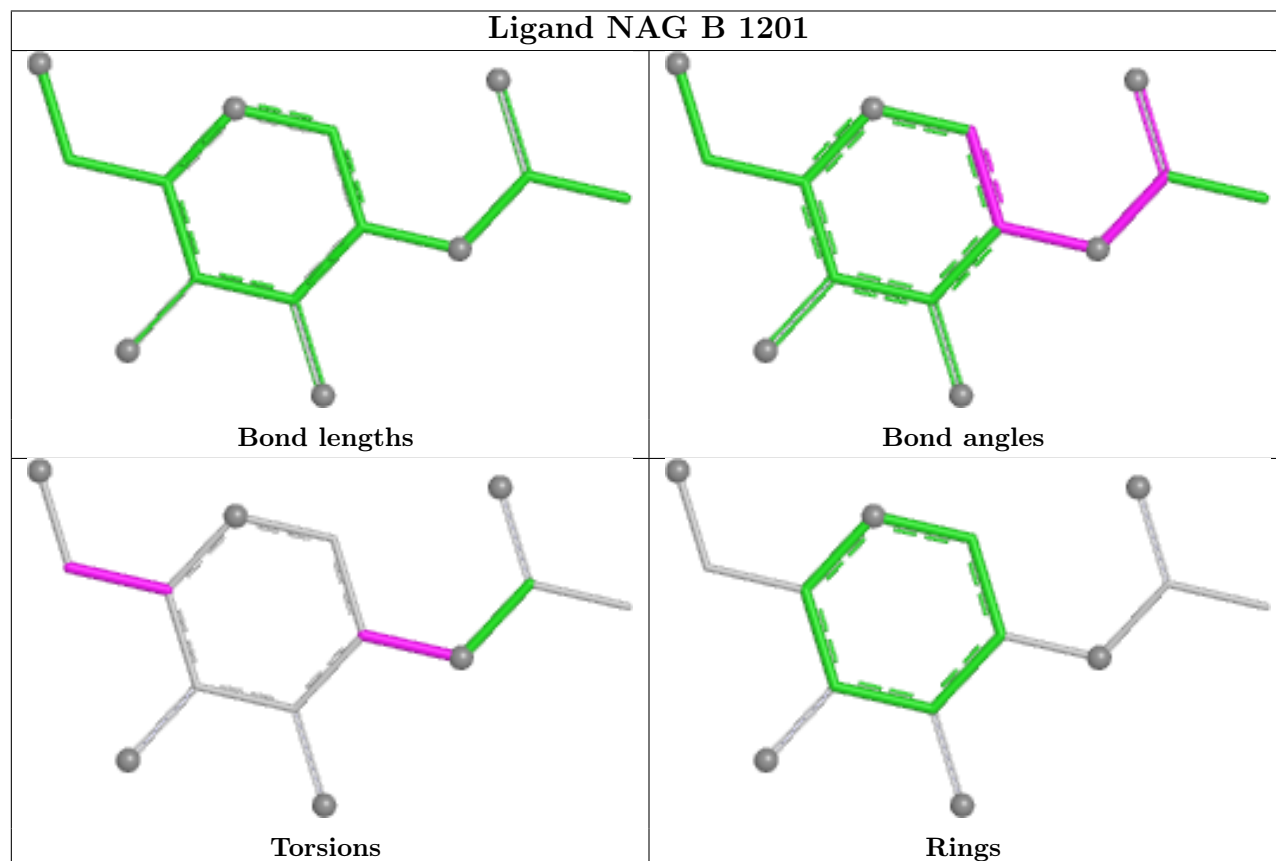


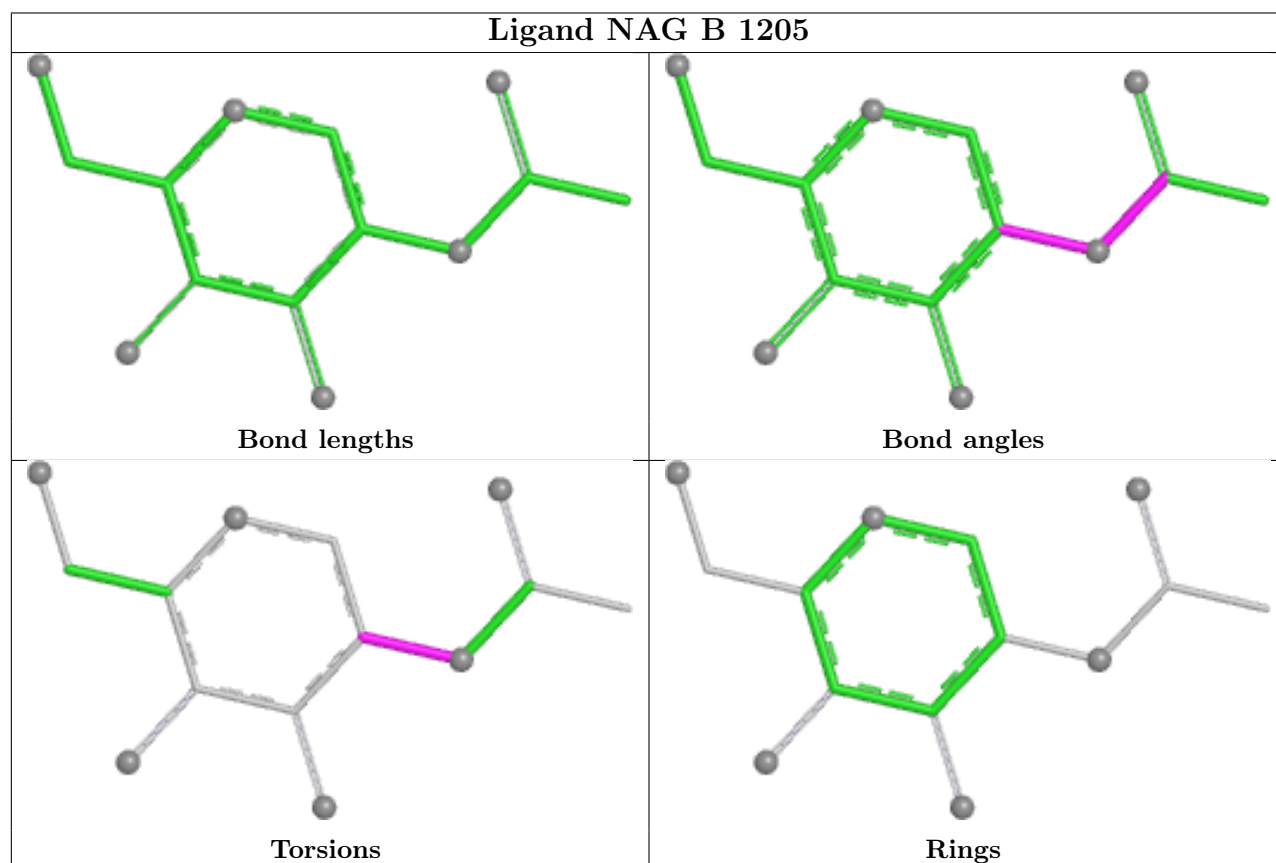
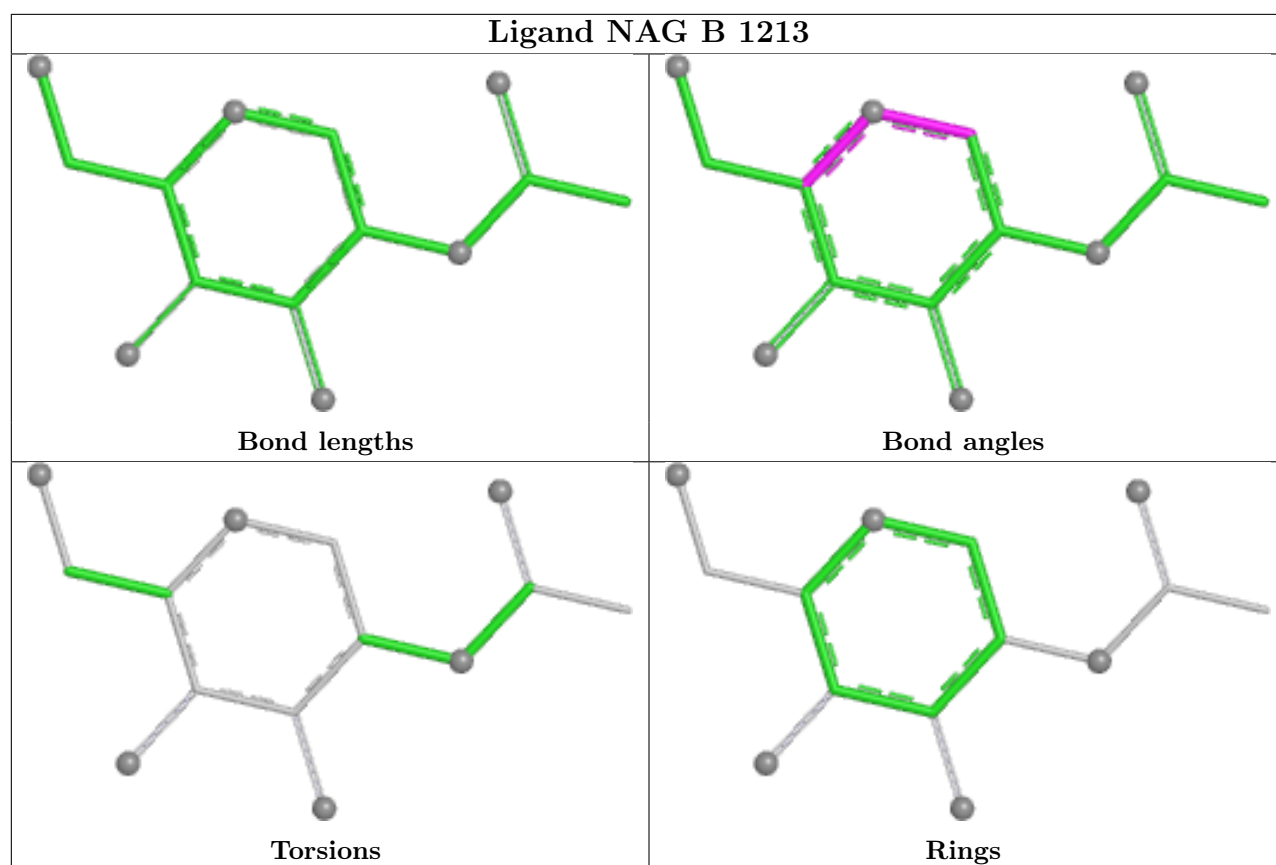


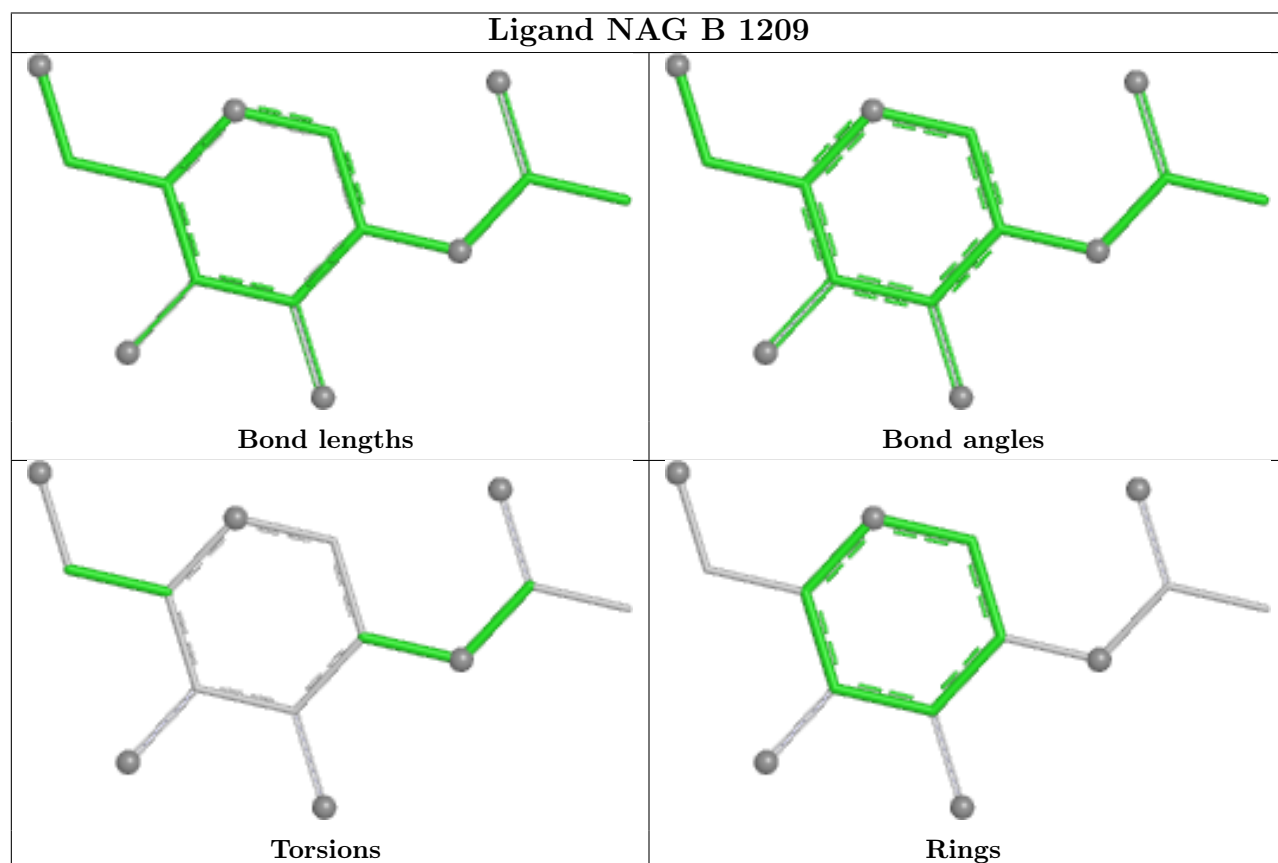
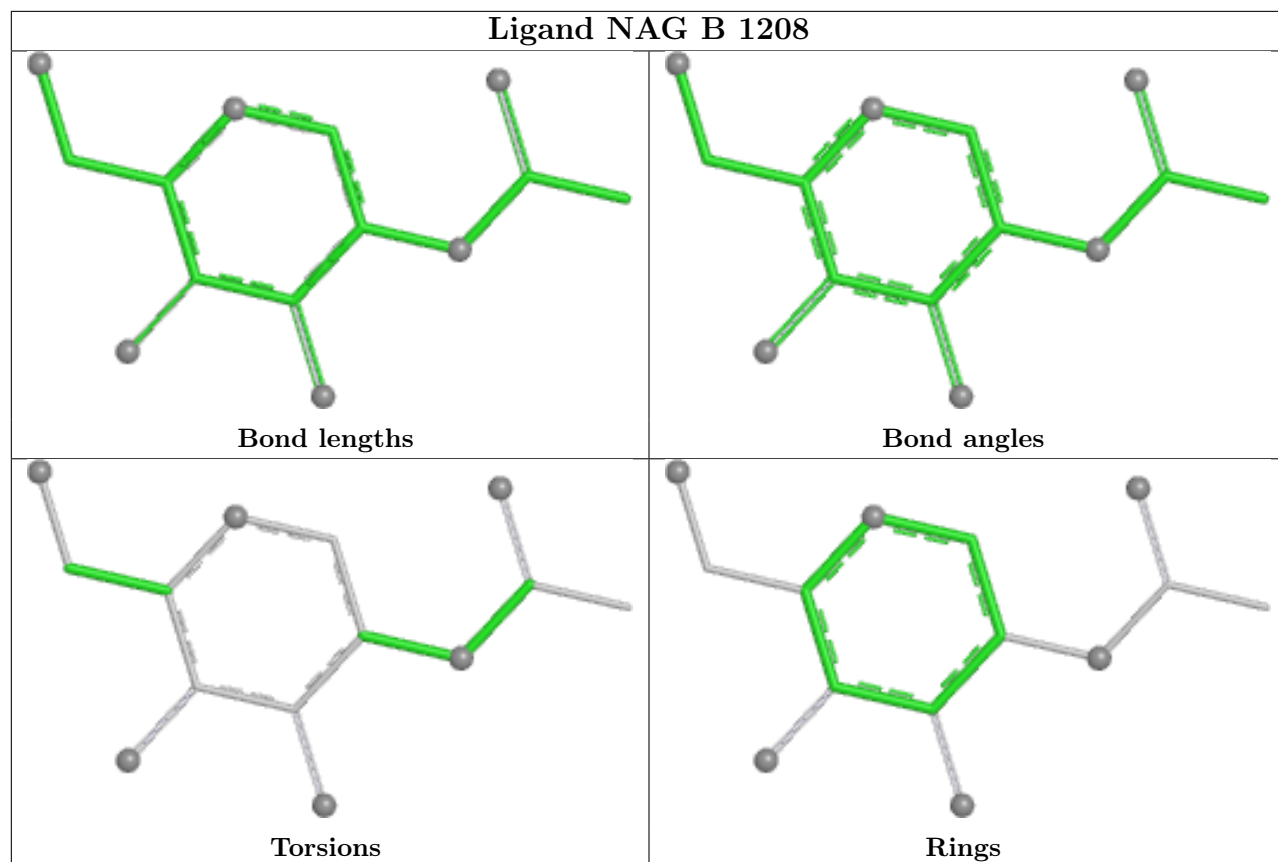
Ligand NAG C 1205



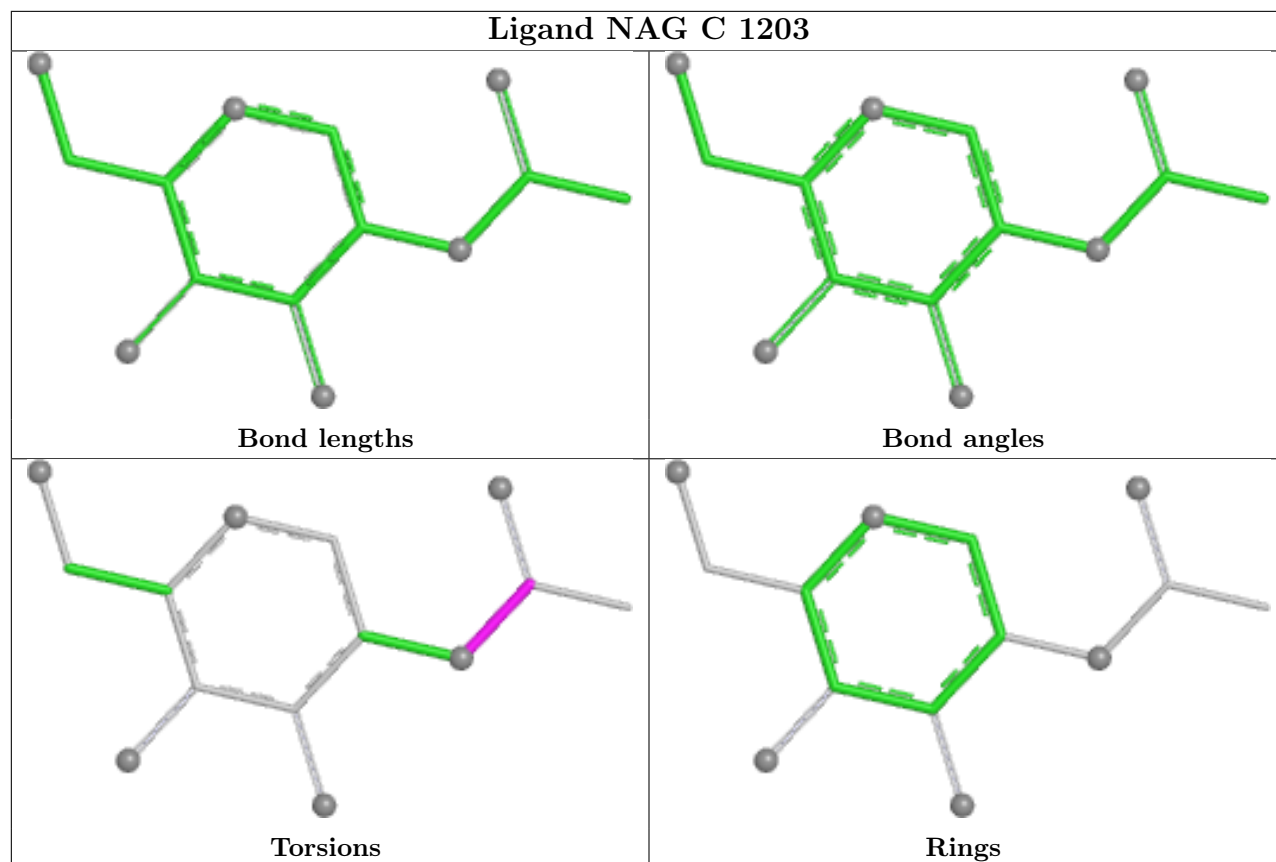
Ligand NAG B 1201



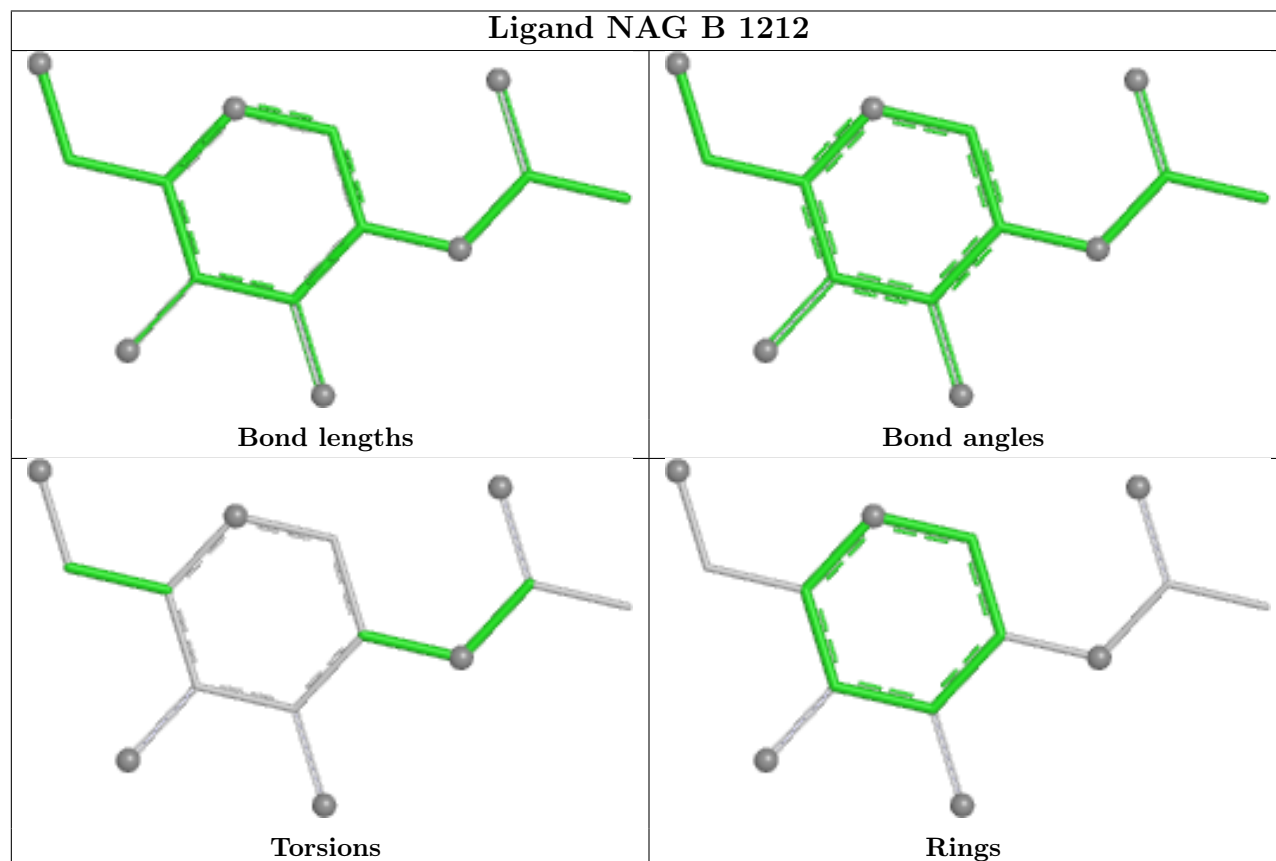


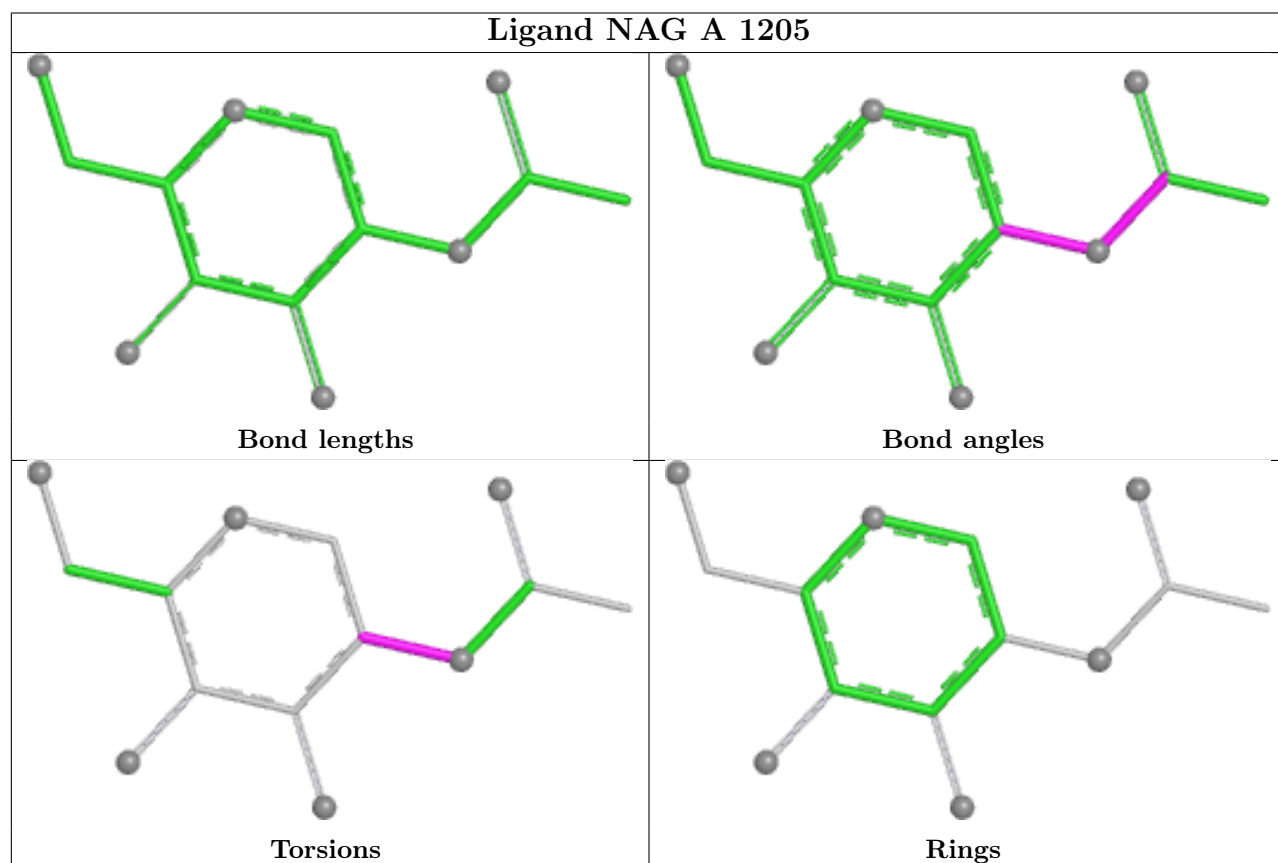
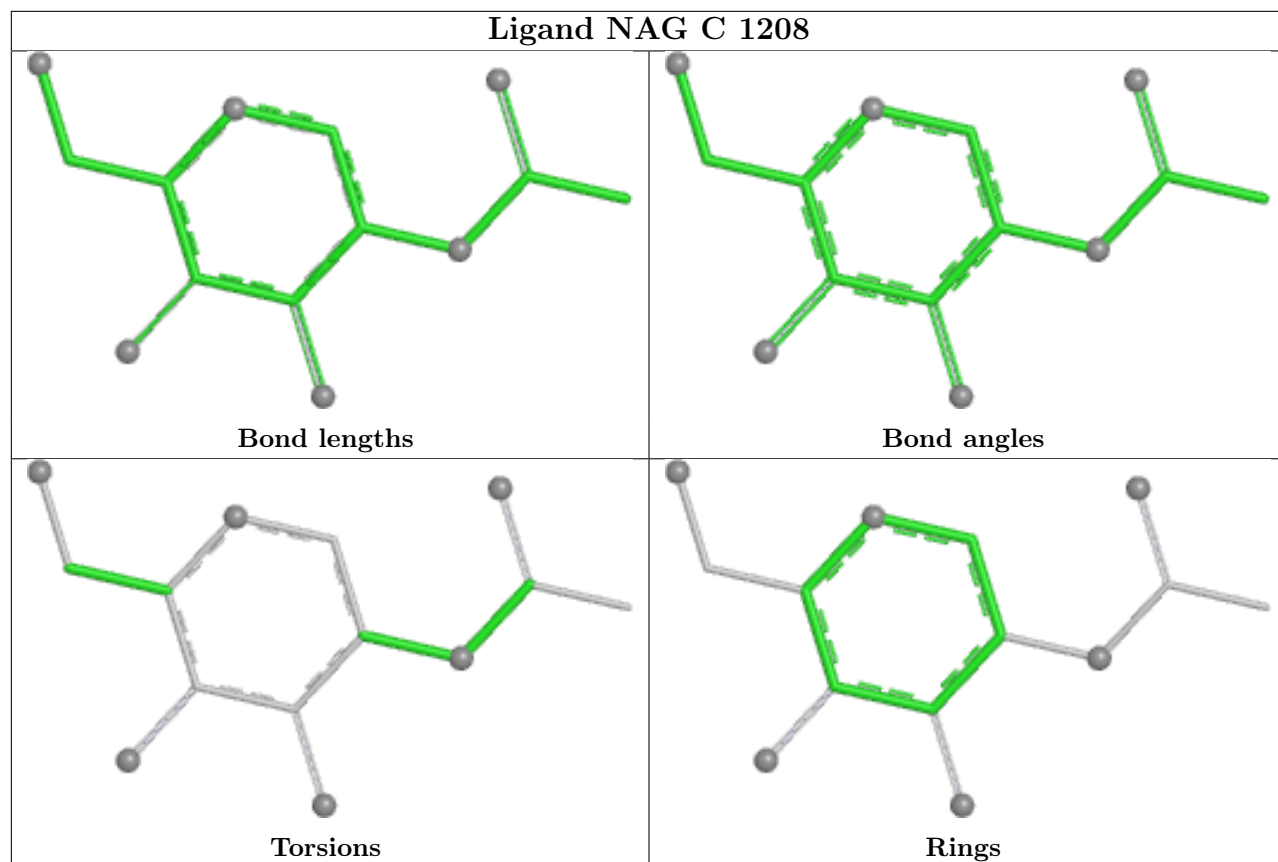


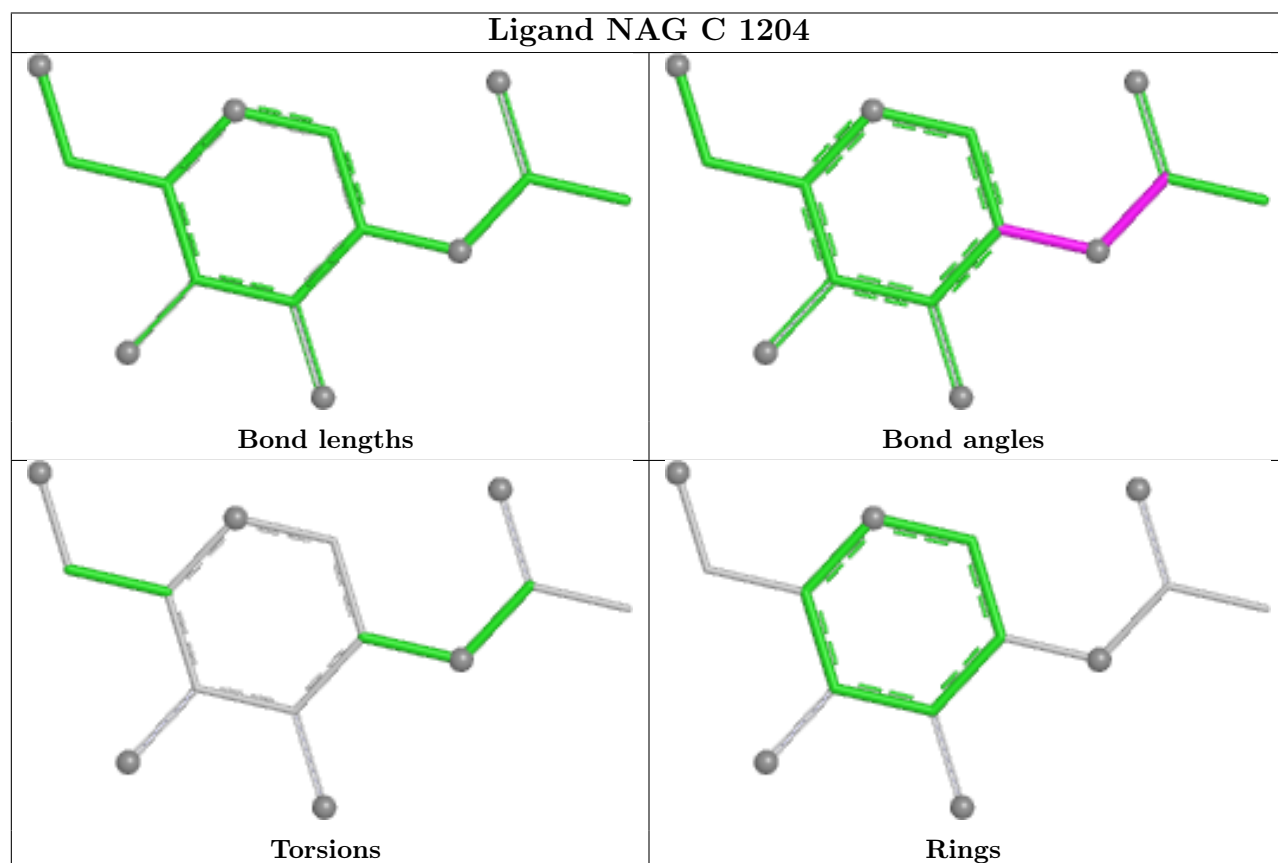
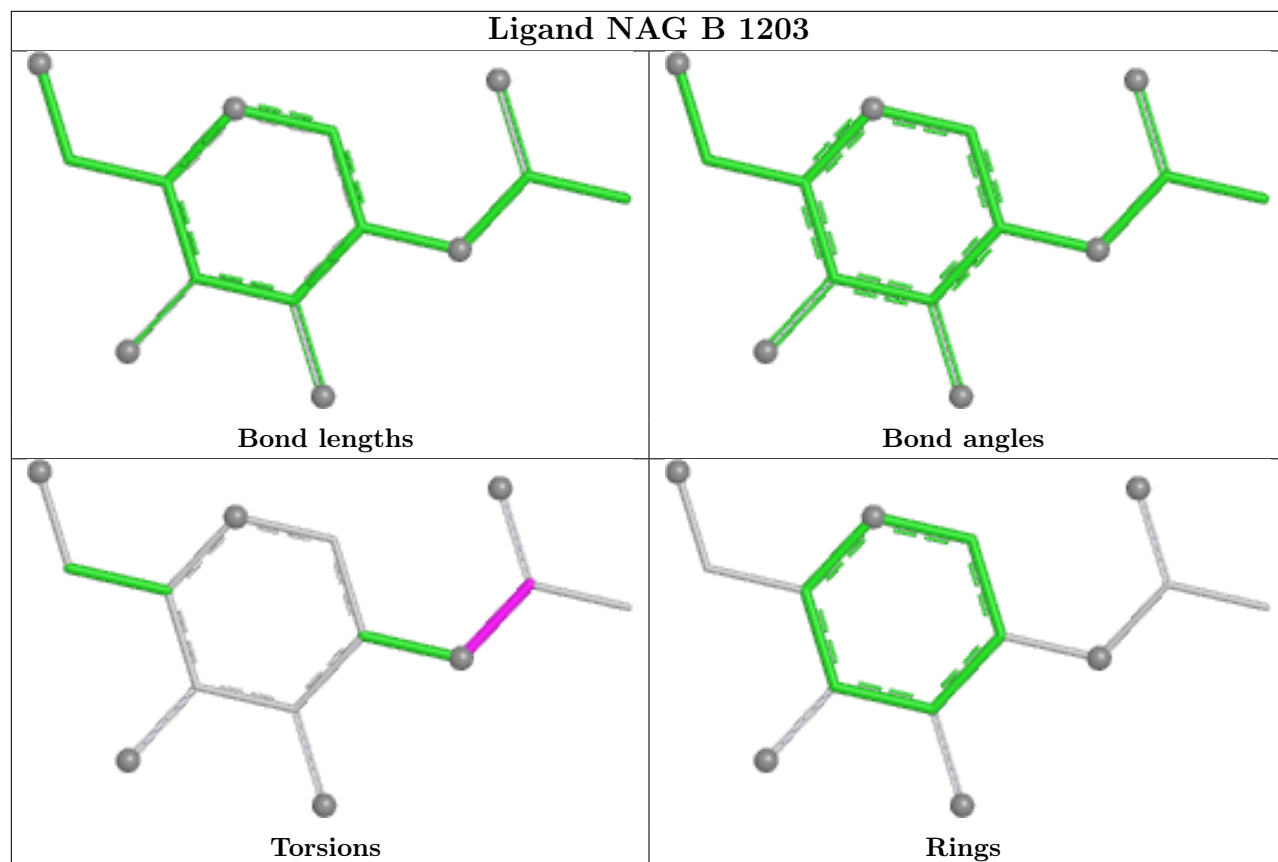
Ligand NAG C 1203

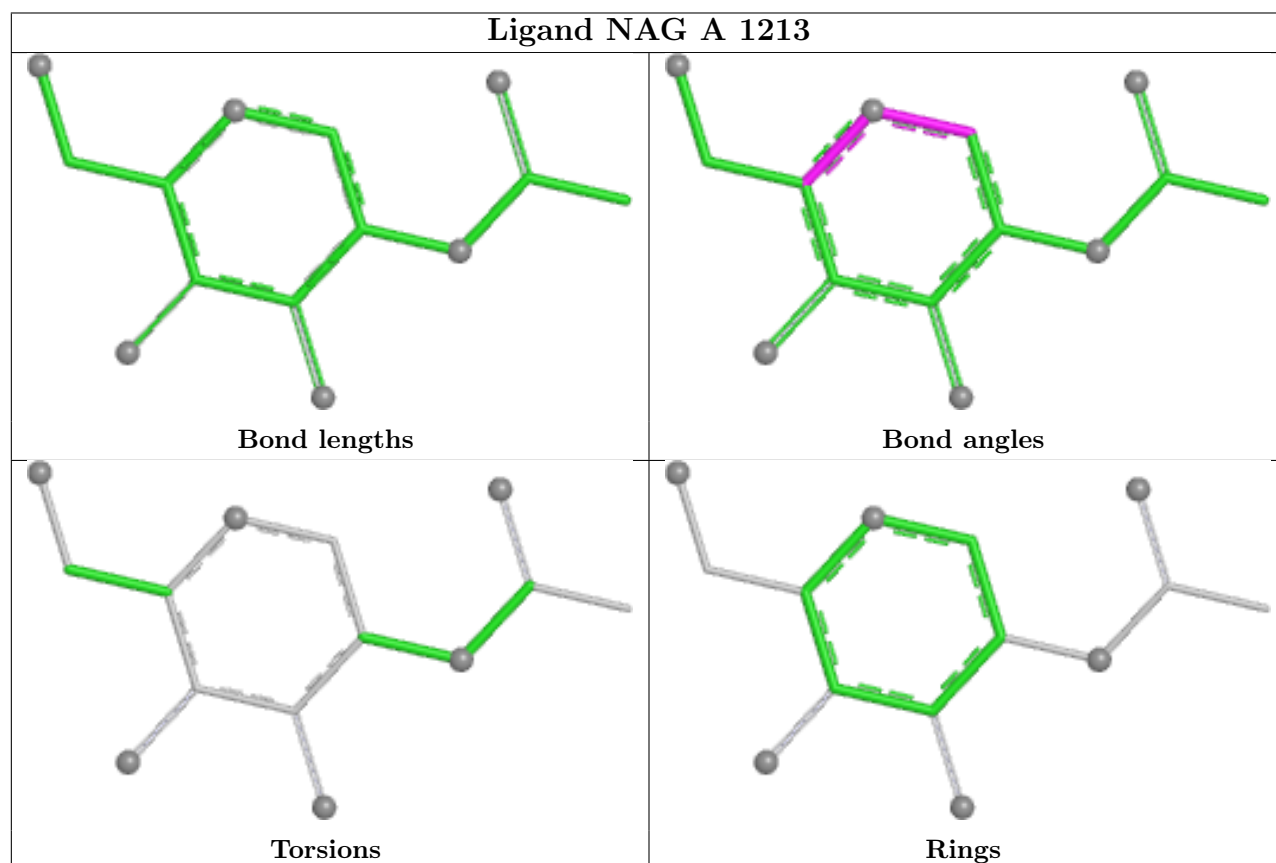
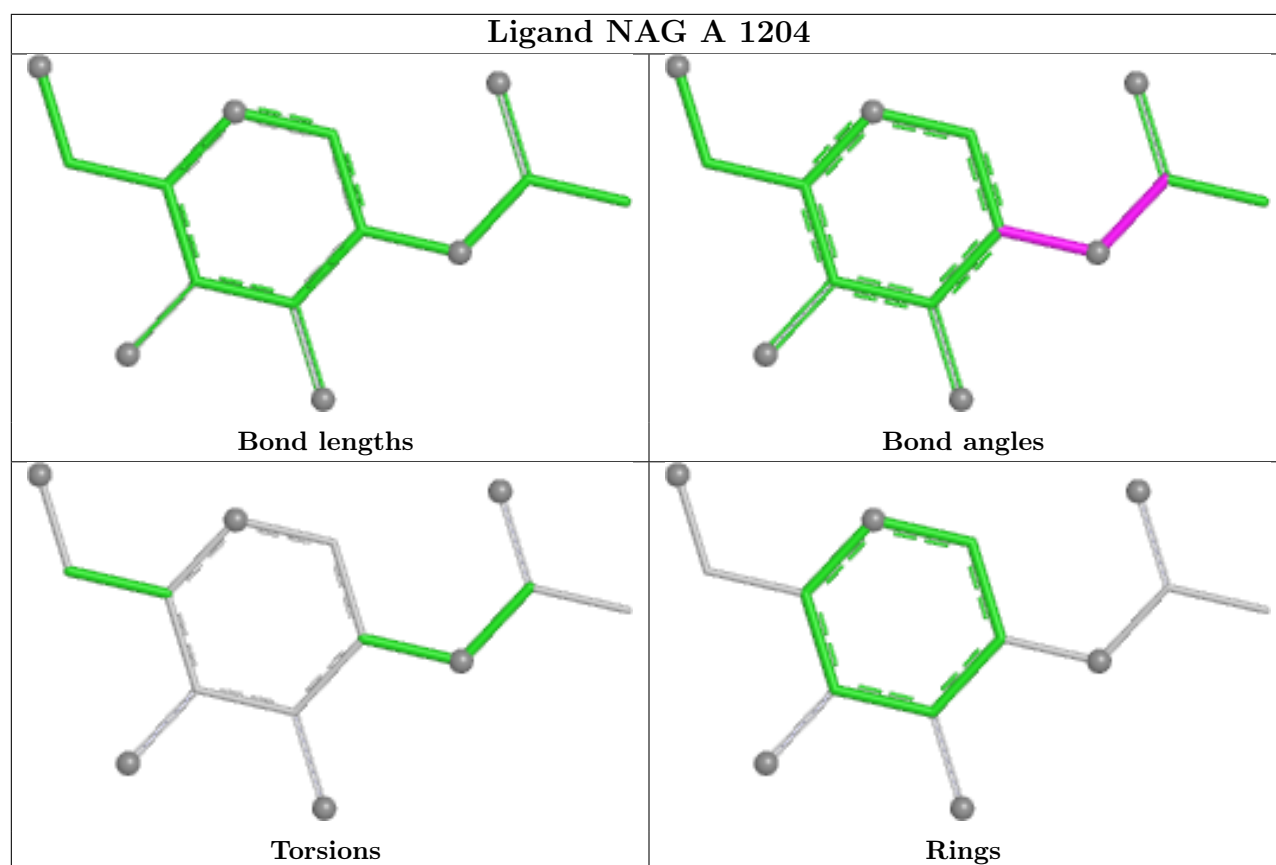


Ligand NAG B 1212









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.

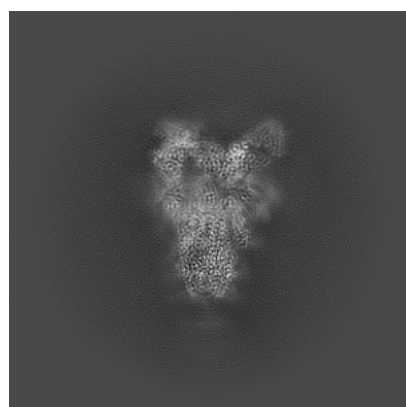
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49372. These allow visual inspection of the internal detail of the map and identification of artifacts.

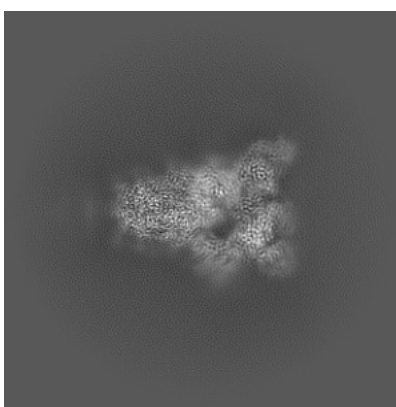
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

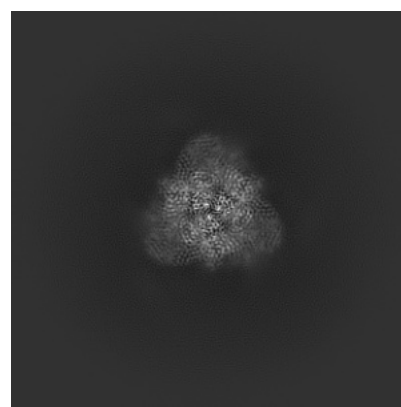
6.1.1 Primary map



X



Y

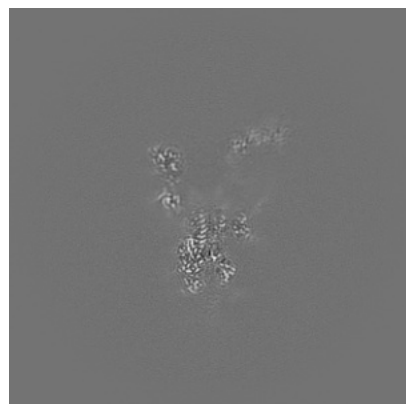


Z

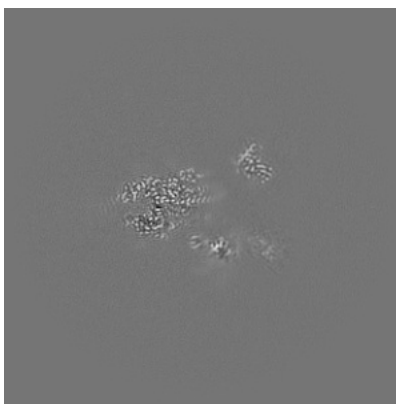
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

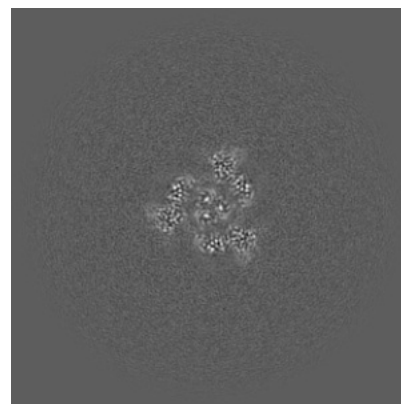
6.2.1 Primary map



X Index: 294



Y Index: 294

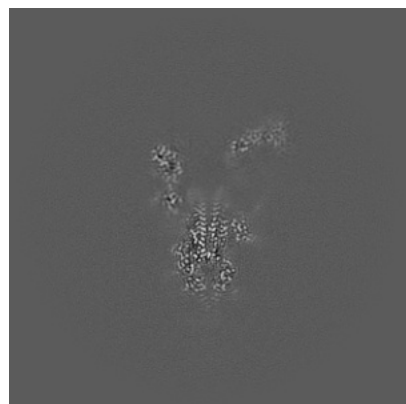


Z Index: 294

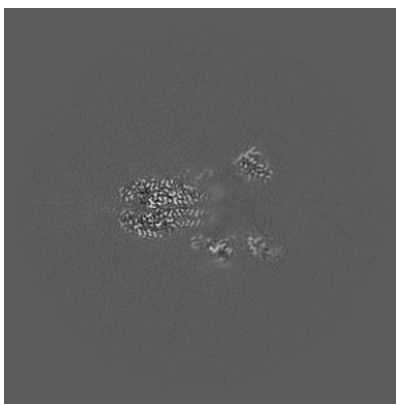
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

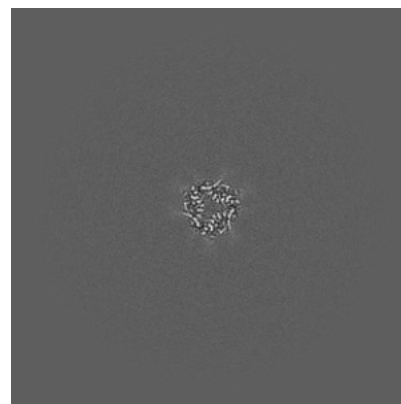
6.3.1 Primary map



X Index: 290



Y Index: 300

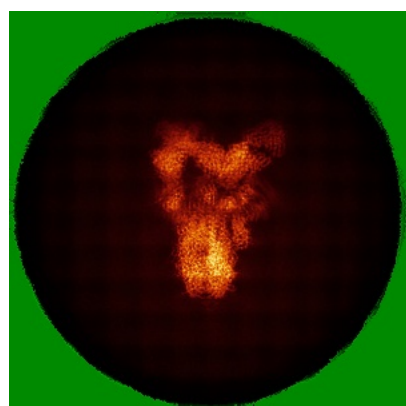


Z Index: 200

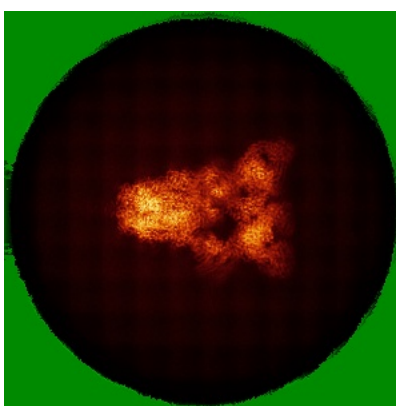
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

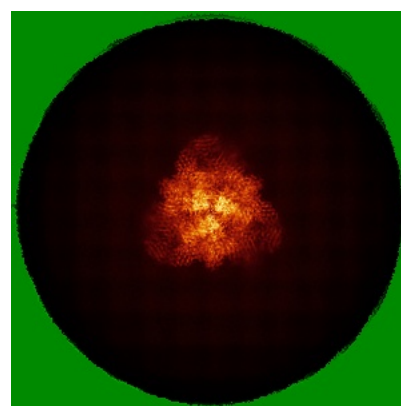
6.4.1 Primary map



X



Y

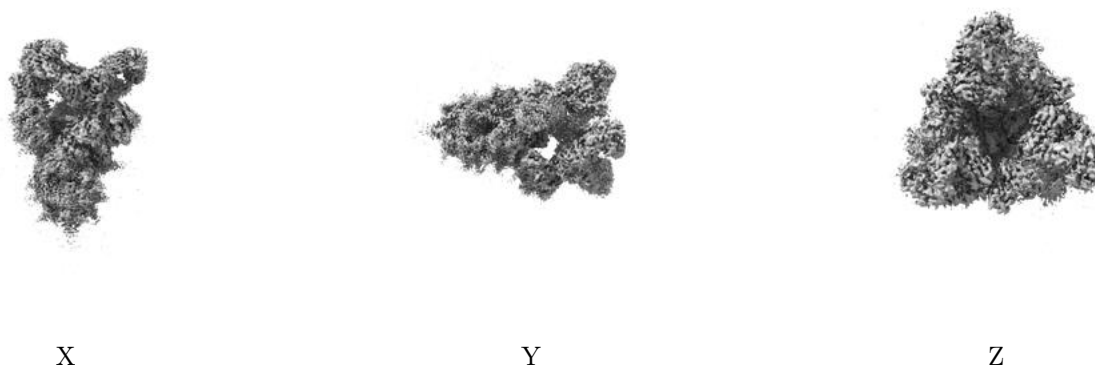


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

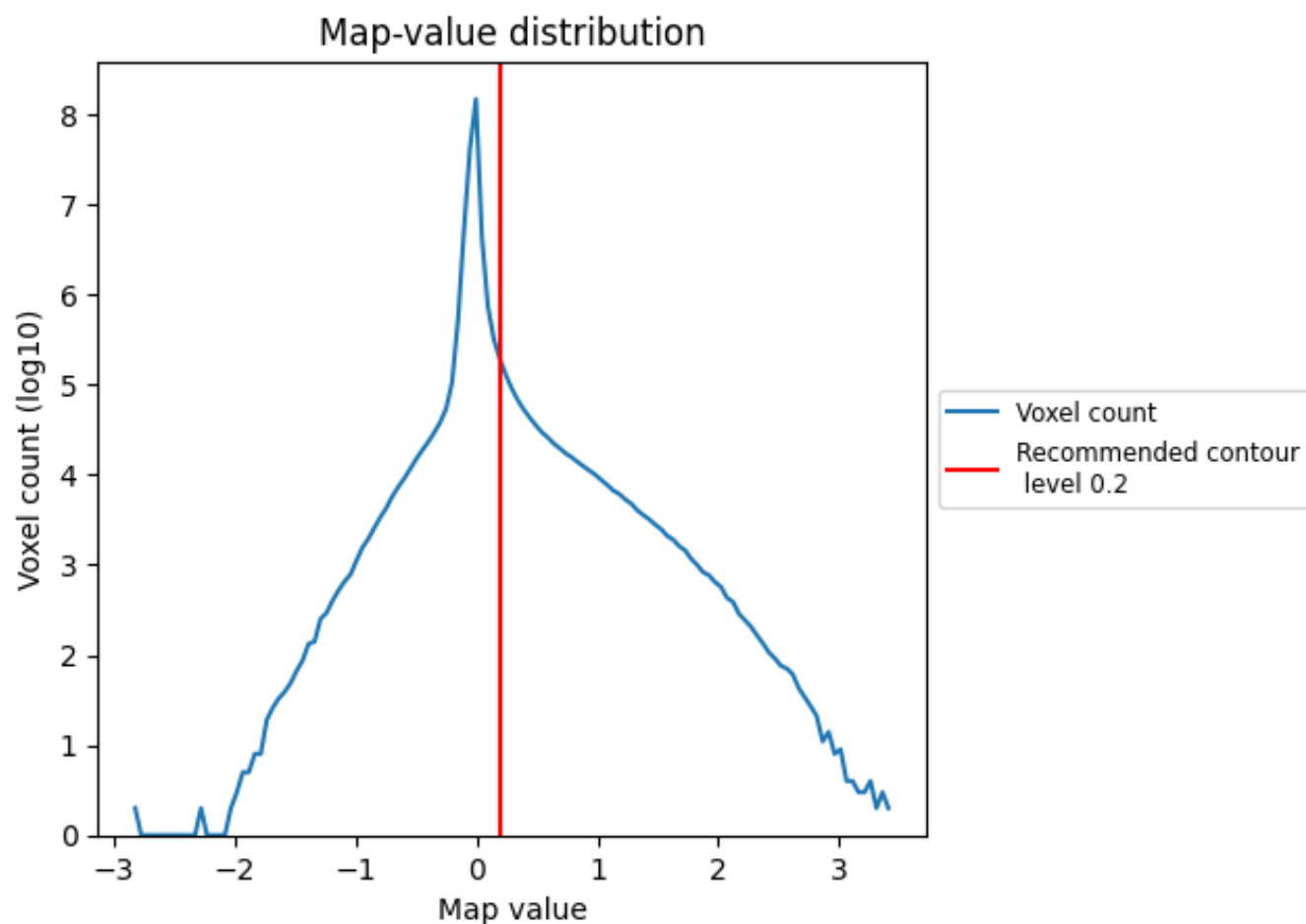
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

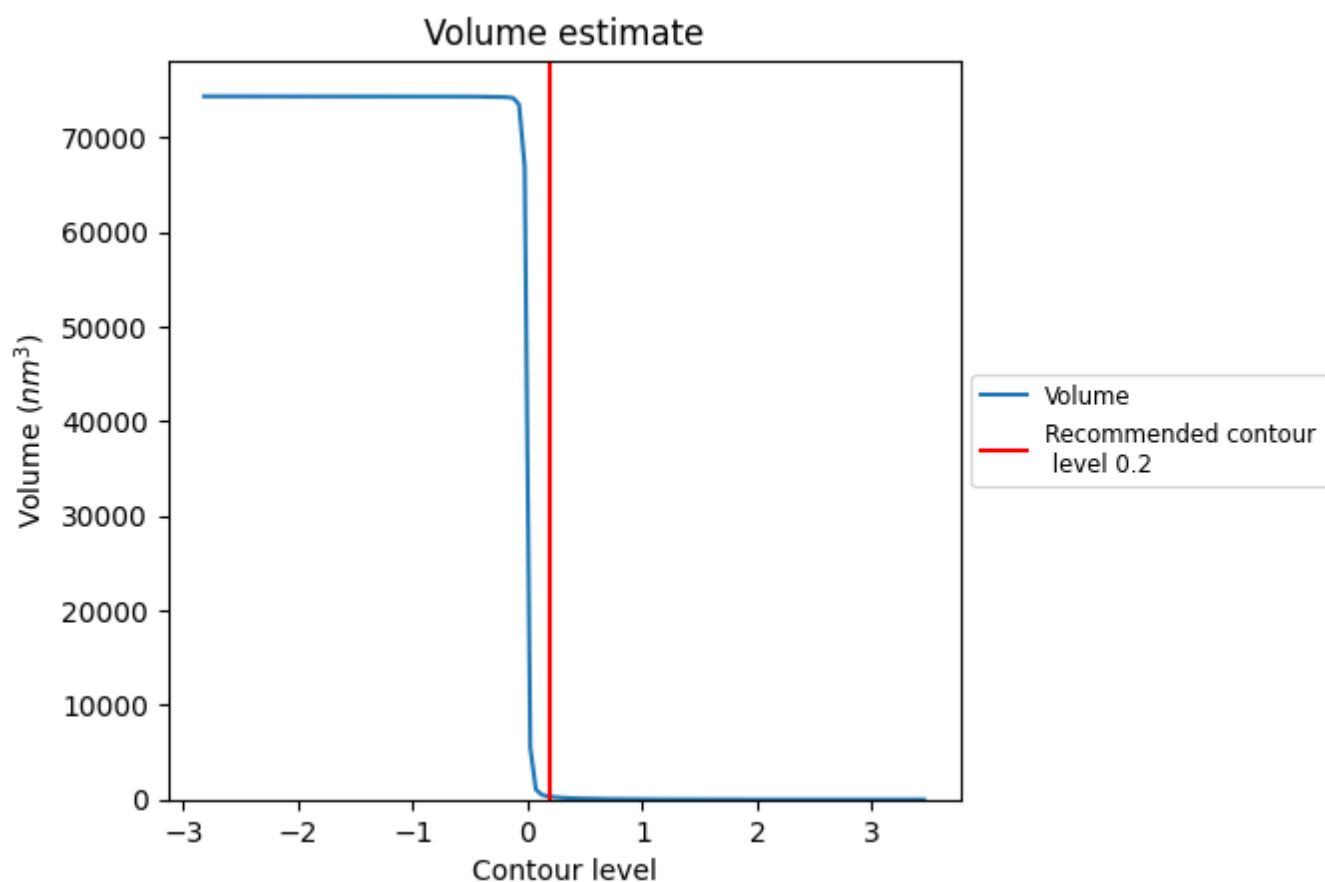
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

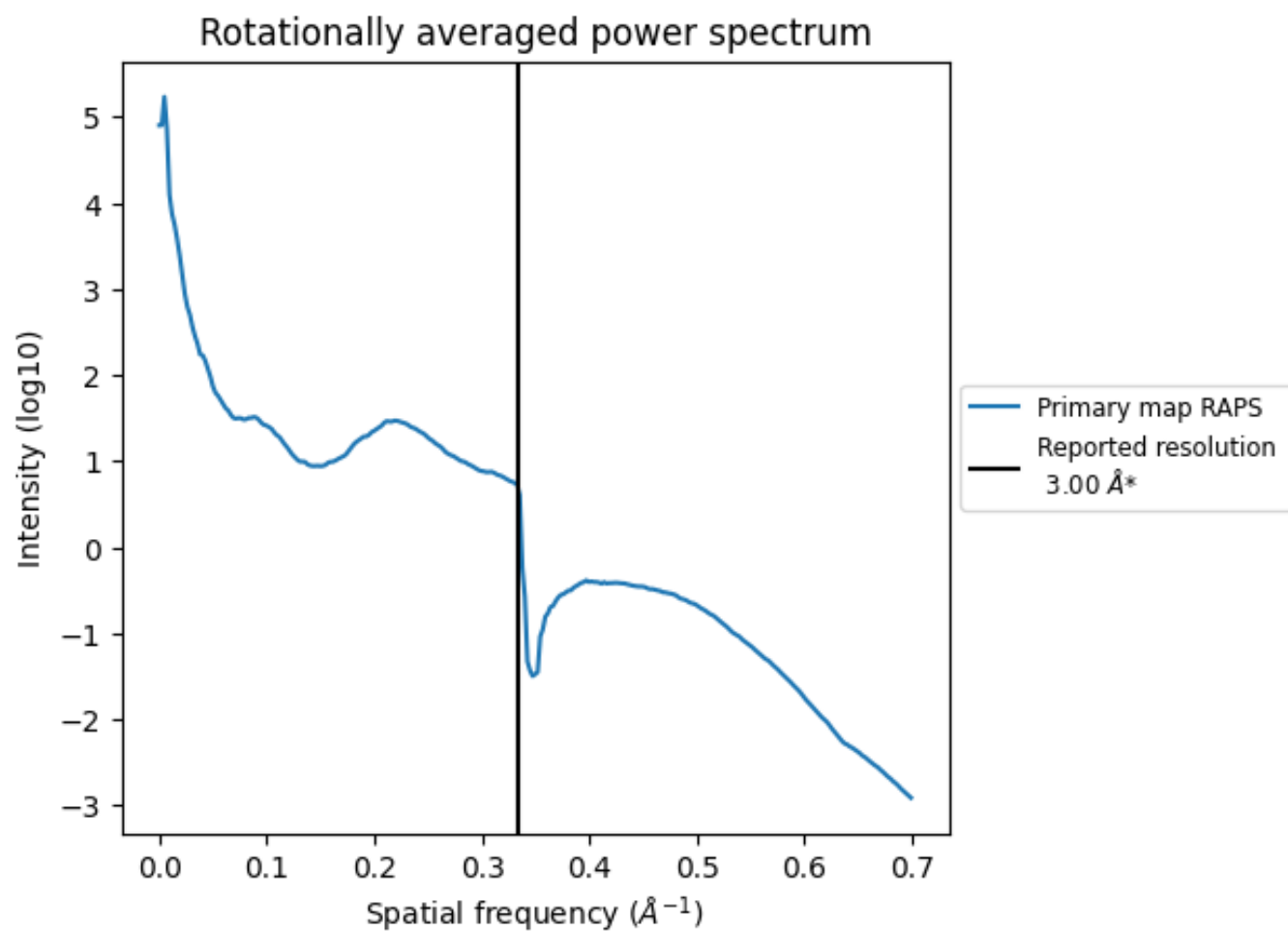
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm³; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

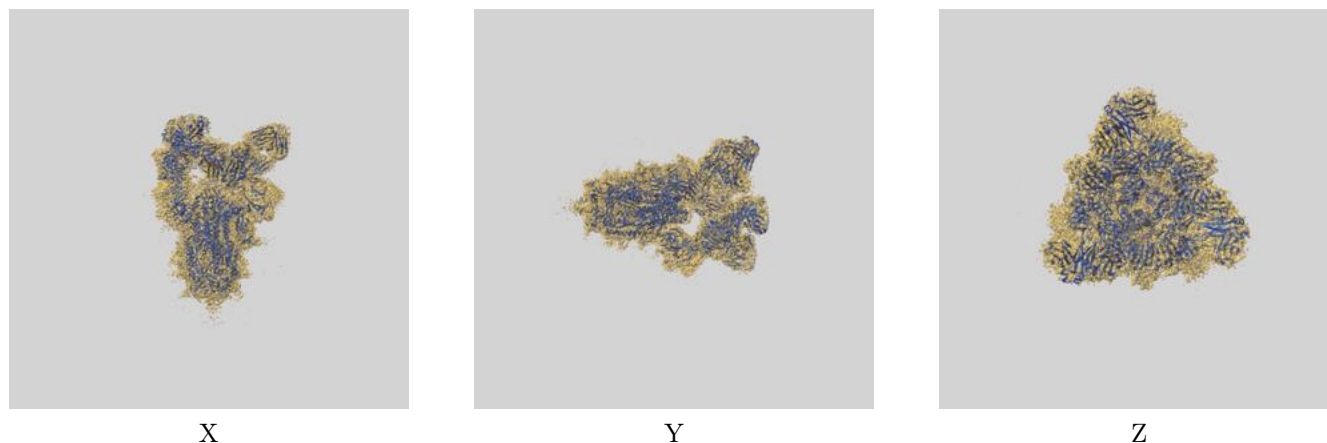
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

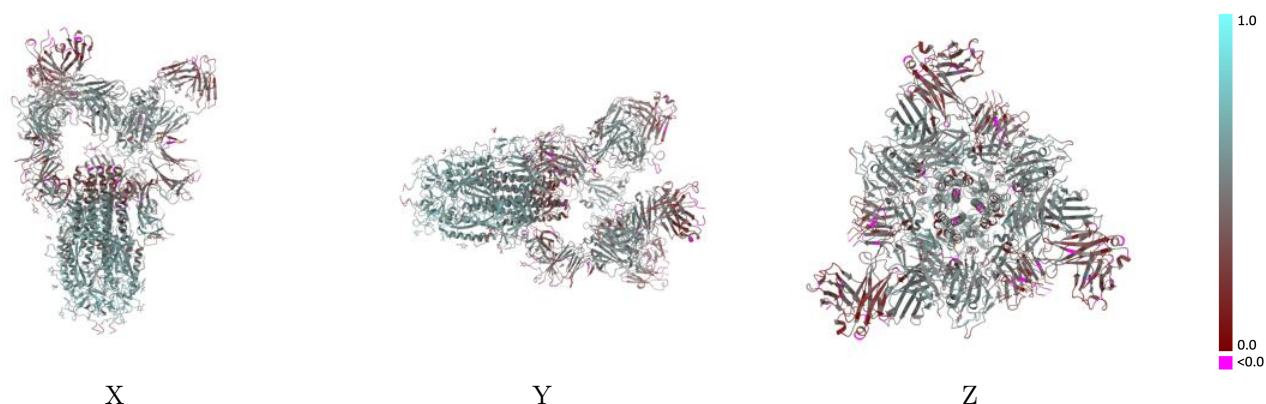
This section contains information regarding the fit between EMDB map EMD-49372 and PDB model 9NFT. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



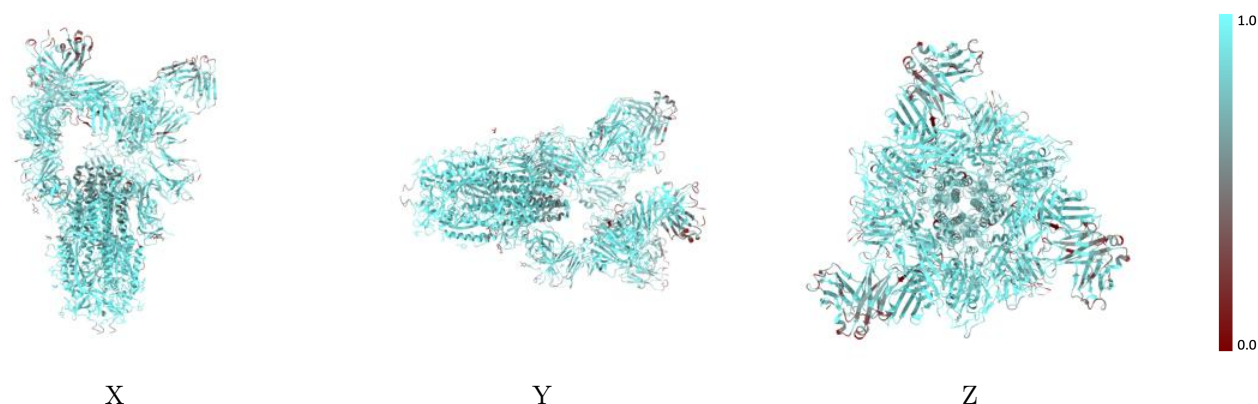
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



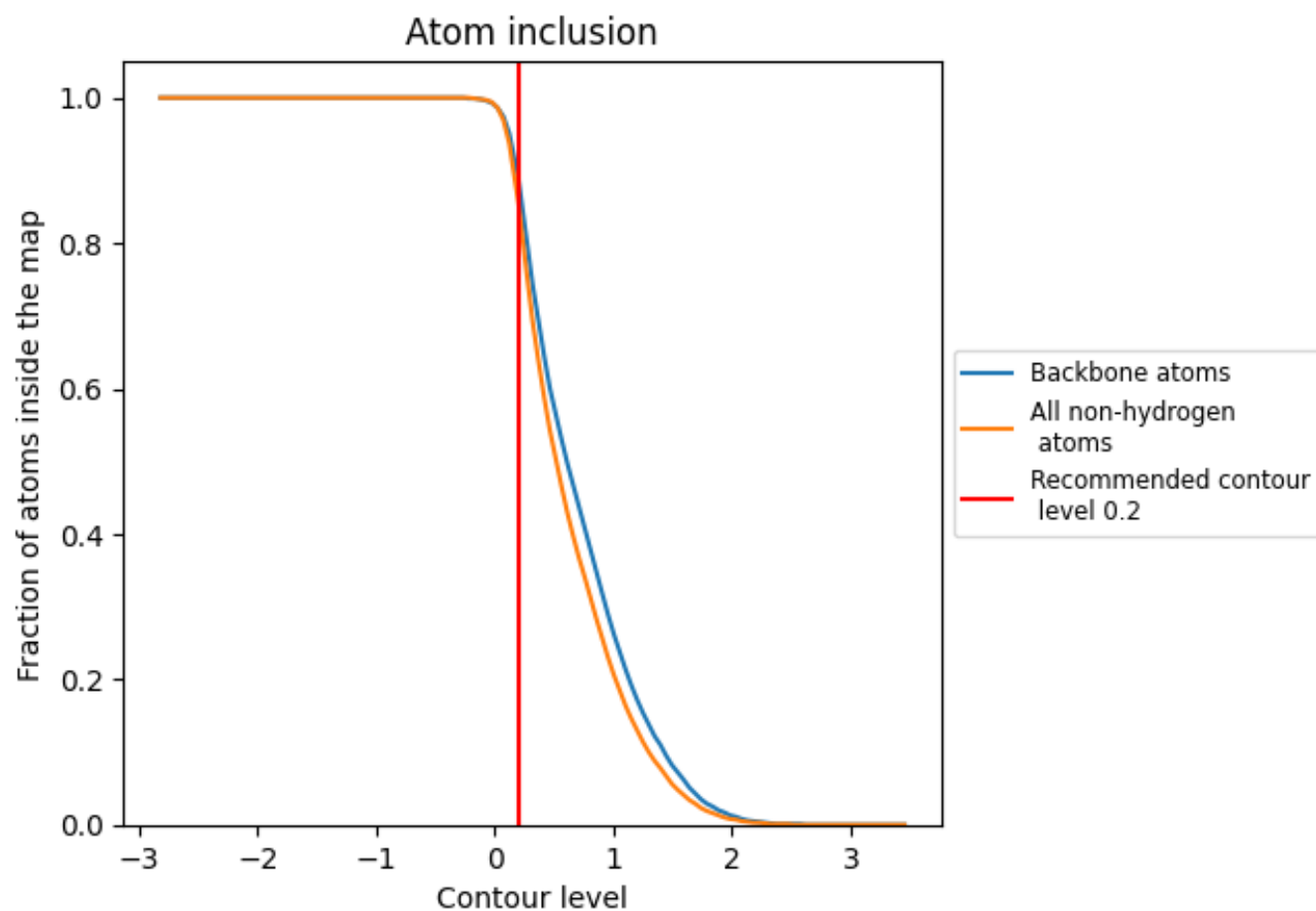
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.4660
A	0.8870	0.4910
B	0.8840	0.4870
C	0.8840	0.4870
D	0.7560	0.3990
E	0.7920	0.4150
F	0.7610	0.4050
G	0.7940	0.4190
H	0.7730	0.4150
I	0.7960	0.4190

1.0

0.0

<0.0