



Full wwPDB EM Validation Report ⓘ

Aug 9, 2026 – 03:59 AM JST

PDB ID : 9MAO / pdb_00009mao
EMDB ID : EMD-63757
Title : SARS-CoV-2 spike-Crp5
Authors : Yang, Q.X.; Yang, Y.L.
Deposited on : 2025-03-14
Resolution : 3.09 Å(reported)

This is a Full wwPDB EM Validation 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 : 1.8.5 (274361), CSD as541be (2020)
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

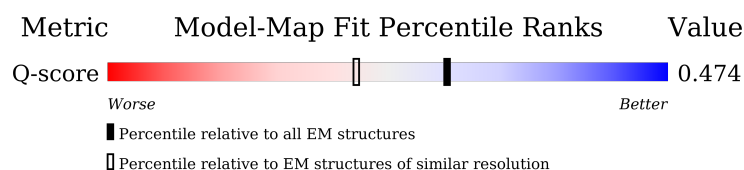
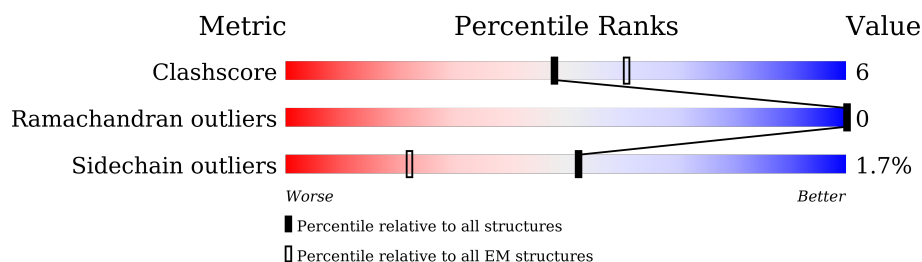
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	1273	 67% 13% 19%
1	B	1273	 67% 15% 18%
1	C	1273	 69% 12% 19%
2	D	36	 69% 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24741 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	C	1029	Total	C	N	O	S	0	0
			7922	5052	1316	1518	36		
1	B	1048	Total	C	N	O	S	0	0
			8116	5180	1347	1553	36		
1	A	1027	Total	C	N	O	S	0	0
			7968	5094	1315	1523	36		

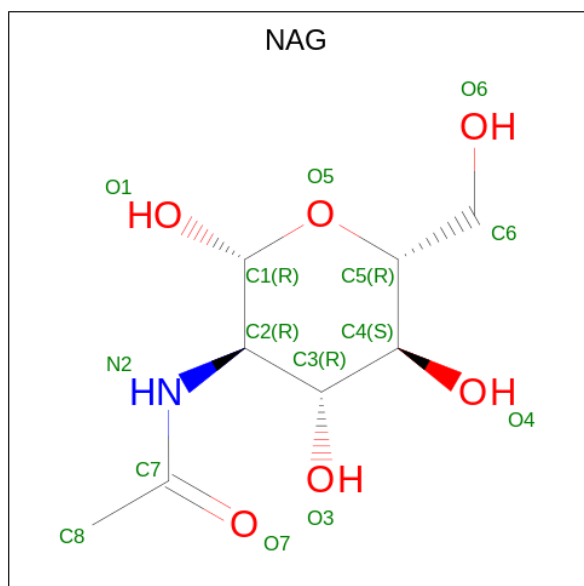
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Alpha-defensin 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	26	Total	C	N	O	S	0	0
			189	118	34	33	4		

- Molecule 3 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
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		
3	C	1	Total	C	N	O		0
			14	8	1	5		

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

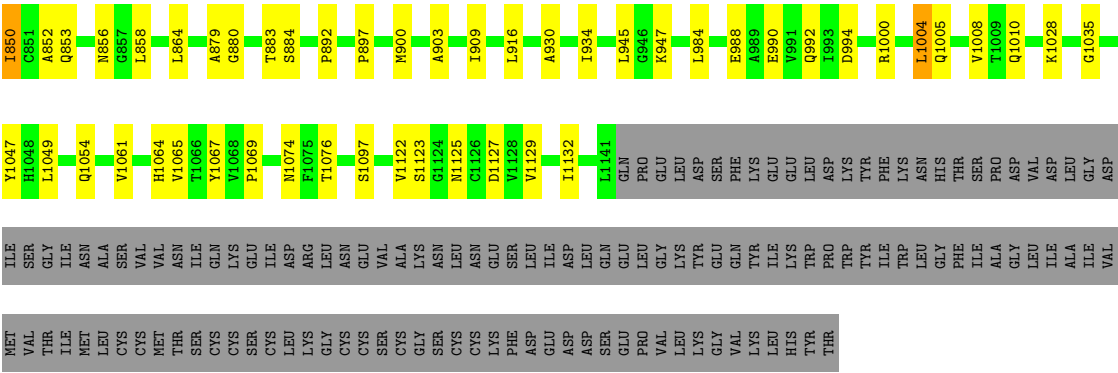
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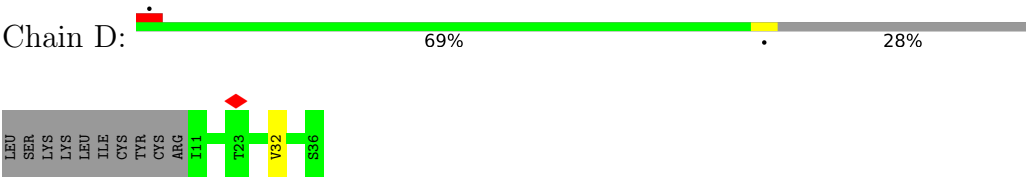
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	



I692	Q506	C336	F186	T95	MET
Y707	P507	V341	E191	GLU	PHE
P715	V511	F342	F192	LYS	VAL
V722	V512	K356	V193	SER	PHE
V725	L513	K356	I197	N99	LEU
E725	A522	C361	D198	I100	LEU
T523	T523	V362	F201	F106	PRO
V524	V524	C379	Y204	S112	VAL
C525	C525	L390	L223	L117	SER
T531	K335	T393	L229	V120	GLM
T742	N536	N394	P230	N121	CYS
T743	V395	V395	I231	N122	ASN
T747	V539	D405	R237	A123	LEU
T750	F559	I418	L242	I128	THR
L752	D571	N422	ALA	K129	ARG
Y756	R577	C432	HIS	V130	GLM
L763	G594	V433	LEU	C131	LEU
L765	V595	I434	ARG	E132	LEU
T770	S596	N439	SER	P139	PRO
A771	P600	K444	TYR	TYR	PRO
Q774	Q607	N448	THR	G142	ALA
K776	V608	L452	PRO	V143	ALA
L822	L611	V453	GLY	Y144	TYR
T827	N616	R454	ASP	HIS	R34
LEU	L455	L455	SER	LYS	Y41
ALA	V622	F456	SER	ASN	K41
ASP	R457	K458	SER	ASN	D53
ALA	C649	S459	THR	LYS	L54
GLY	Q675	I472	ALA	TRP	L54
PHE	Q677	C480	GLY	MET	S60
ILE	T676	N481	ALA	F154	S60
LYS	Q677	C488	L270	S155	F65
GLN	THR	Y489	K304	E156	HIS
TYR	ASN	F490	N317	F168	ALA
GLY	SER	ALA	F318	E169	ALA
ASP	PRO	ARG	R319	Y170	ILE
CYS	ARG	ALA	P322	P174	HIS
GLY	ARG	ALA	T323	THR	VAL
LEU	ALA	L492	LEU	ASP	SER
ASP	ARG	Q498	GLU	LEU	GLY
ILE	SER	N501	T326	GLU	THR
ALA	VAL	G502	V327	GLY	K77
ALA	ALA	S889	R328	GLN	L84
ARG	ARG	Q690	ASN	GLY	P85
ASP	ASP	S601	T326	ASN	F86
L840	L840	U502	T326	ASN	C96



• Molecule 2: Alpha-defensin 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42414	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	20.877	Depositor
Minimum map value	-0.184	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.530	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	335.52, 335.52, 335.52	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.08	0/8153	0.23	0/11111
1	B	0.08	0/8302	0.24	0/11318
1	C	0.08	0/8099	0.23	0/11040
2	D	0.11	0/191	0.38	0/254
All	All	0.08	0/24745	0.24	0/33723

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	7968	0	7712	101	0
1	B	8116	0	7855	110	0
1	C	7922	0	7650	92	0
2	D	189	0	170	0	0
3	A	168	0	156	0	0
3	B	196	0	182	0	0
3	C	182	0	169	1	0
All	All	24741	0	23894	286	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.

All (286) 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:A:498:GLN:HB2	1:A:501:ASN:HB2	1.73	0.70
1:C:740:MET:SD	1:B:319:ARG:NH1	2.65	0.68
1:B:290:ASP:HB3	1:B:293:LEU:HB2	1.75	0.67
1:B:95:THR:O	1:B:186:PHE:N	2.28	0.67
1:A:480:CYS:O	1:A:481:ASN:ND2	2.28	0.67
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.76	0.67
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.77	0.65
1:C:563:GLN:H	1:A:41:LYS:HB3	1.62	0.65
1:A:130:VAL:HG21	1:A:231:ILE:HG21	1.79	0.64
1:A:742:ILE:O	1:A:1000:ARG:NH2	2.29	0.64
1:B:213:VAL:HG13	1:B:215:ASP:H	1.64	0.62
1:B:852:ALA:O	1:B:856:ASN:ND2	2.32	0.62
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.64	0.61
1:B:409:GLN:HB3	1:B:419:ALA:HB2	1.82	0.61
1:C:977:LEU:HD11	1:C:993:ILE:HG12	1.82	0.60
1:B:616:ASN:HB3	1:B:619:GLU:HB2	1.82	0.60
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.34	0.60
1:B:393:THR:HA	1:B:522:ALA:HA	1.83	0.60
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.84	0.60
1:C:81:ASN:ND2	1:C:240:THR:O	2.35	0.59
1:C:786:LYS:HG2	1:C:787:GLN:HG3	1.84	0.59
1:A:112:SER:HA	1:A:132:GLU:HB2	1.85	0.59
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.68	0.59
1:B:1129:VAL:HB	1:B:1132:ILE:HB	1.85	0.59
1:C:786:LYS:H	1:C:786:LYS:HD2	1.68	0.58
1:B:101:ILE:HD13	1:B:242:LEU:HB3	1.85	0.58
1:B:206:LYS:HB2	1:B:223:LEU:HA	1.85	0.58
1:B:593:GLY:HA2	1:B:614:ASP:HB2	1.86	0.58
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.68	0.58
1:B:742:ILE:O	1:B:1000:ARG:NH2	2.36	0.58
1:A:452:LEU:HD23	1:A:492:LEU:HB3	1.86	0.57
1:A:559:PHE:HB3	1:A:577:ARG:HH11	1.69	0.57
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.86	0.57
1:C:409:GLN:HB3	1:C:416:GLY:HA3	1.86	0.57
1:A:852:ALA:O	1:A:856:ASN:ND2	2.38	0.57
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.85	0.57
1:B:1116:THR:OG1	1:B:1119:ASN:ND2	2.34	0.57
1:C:1069:PRO:HG2	1:A:892:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LYS:O	1:C:422:ASN:ND2	2.38	0.56
1:C:442:ASP:OD1	1:C:509:ARG:NH1	2.38	0.56
1:A:1125:ASN:ND2	1:A:1127:ASP:OD1	2.38	0.56
1:C:852:ALA:O	1:C:856:ASN:ND2	2.32	0.56
1:A:600:PRO:HG3	1:A:692:ILE:HD11	1.88	0.56
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.87	0.55
1:B:1086:LYS:HE2	1:B:1122:VAL:HG21	1.87	0.55
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.89	0.55
1:C:102:ARG:HG2	1:C:140:PHE:HD2	1.71	0.55
1:A:439:ASN:HD22	1:A:507:PRO:HD2	1.72	0.55
1:C:16:VAL:HA	3:C:1313:NAG:H82	1.87	0.55
1:B:914:ASN:ND2	1:A:1123:SER:OG	2.40	0.55
1:A:1054:GLN:HB2	1:A:1061:VAL:HB	1.89	0.55
1:C:188:ASN:HB2	1:C:207:HIS:HB3	1.89	0.55
1:A:328:ARG:NH2	1:A:531:THR:O	2.39	0.55
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.37	0.54
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.90	0.54
1:A:535:LYS:O	1:A:536:ASN:ND2	2.41	0.54
1:C:457:ARG:NH1	1:C:465:GLU:OE2	2.41	0.54
1:C:1006:THR:OG1	1:A:1005:GLN:NE2	2.41	0.54
1:B:77:LYS:HD3	1:B:253:ASP:HB2	1.89	0.54
1:C:117:LEU:HD23	1:C:130:VAL:HG13	1.90	0.53
1:B:273:ARG:HE	1:B:292:ALA:HB3	1.73	0.53
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.90	0.53
1:A:323:THR:H	1:A:539:VAL:HG12	1.72	0.53
1:A:472:ILE:HD12	1:A:488:CYS:HB3	1.90	0.53
1:C:432:CYS:HB2	1:C:513:LEU:HD12	1.91	0.53
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.31	0.53
1:C:94:SER:HB2	1:C:190:ARG:HB3	1.89	0.53
1:B:1125:ASN:ND2	1:B:1127:ASP:OD1	2.38	0.52
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.36	0.52
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.91	0.52
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.91	0.52
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.92	0.52
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.92	0.52
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	1.92	0.52
1:B:558:LYS:HD3	1:B:584:ILE:HD12	1.92	0.51
1:A:503:VAL:HA	1:A:506:GLN:HG3	1.92	0.51
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.91	0.51
1:B:379:CYS:HA	1:B:432:CYS:HA	1.92	0.51
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1126:CYS:HB2	1:C:1132:ILE:HG12	1.91	0.51
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.92	0.51
1:B:443:SER:HB3	1:B:499:PRO:HA	1.91	0.51
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.93	0.51
1:B:745:ASP:OD1	1:A:319:ARG:NH2	2.44	0.51
1:C:724:THR:HG23	1:C:934:ILE:HD12	1.93	0.50
1:B:674:TYR:OH	1:B:690:GLN:NE2	2.41	0.50
1:A:379:CYS:HA	1:A:432:CYS:HA	1.92	0.50
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.92	0.50
1:B:68:ILE:HB	1:B:78:ARG:H	1.76	0.50
1:B:94:SER:HA	1:B:264:ALA:HB3	1.92	0.50
1:A:457:ARG:NH2	1:A:459:SER:O	2.43	0.50
1:C:424:LYS:NZ	1:C:425:LEU:O	2.42	0.50
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.93	0.50
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.93	0.50
1:C:730:SER:OG	1:C:778:THR:OG1	2.30	0.49
1:C:1035:GLY:HA3	1:B:1040:VAL:HG21	1.94	0.49
1:A:393:THR:HA	1:A:522:ALA:HA	1.95	0.49
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.93	0.49
1:C:1082:CYS:HB2	1:C:1132:ILE:HD11	1.94	0.49
1:B:600:PRO:HD2	1:B:608:VAL:HG12	1.95	0.49
1:A:31:SER:HB2	1:A:60:SER:H	1.78	0.49
1:C:1040:VAL:HG21	1:A:1035:GLY:HA3	1.95	0.49
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.94	0.49
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.95	0.49
1:A:726:ILE:O	1:A:947:LYS:NZ	2.37	0.49
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.25	0.48
1:B:597:VAL:HG13	1:B:610:VAL:HG12	1.94	0.48
1:A:101:ILE:HG13	1:A:242:LEU:HB2	1.94	0.48
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.94	0.48
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.95	0.48
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.94	0.48
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.95	0.48
1:A:393:THR:O	1:A:523:THR:OG1	2.25	0.48
1:C:95:THR:HG22	1:C:186:PHE:HD2	1.78	0.48
1:A:1129:VAL:HB	1:A:1132:ILE:HB	1.93	0.48
1:B:322:PRO:HB3	1:B:539:VAL:HA	1.95	0.48
1:A:326:ILE:HD13	1:A:539:VAL:HG21	1.95	0.48
1:C:138:ASP:OD1	1:C:138:ASP:N	2.45	0.48
1:B:138:ASP:OD1	1:B:138:ASP:N	2.47	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:LEU:O	1:A:853:GLN:NE2	2.41	0.48
1:B:880:GLY:O	1:B:884:SER:OG	2.27	0.48
1:A:336:CYS:HA	1:A:361:CYS:HB2	1.95	0.48
1:B:53:ASP:OD1	1:B:54:LEU:N	2.42	0.47
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.47
1:A:122:ASN:OD1	1:A:123:ALA:N	2.47	0.47
1:C:187:LYS:HE2	1:C:209:PRO:HB2	1.96	0.47
1:C:892:PRO:HD2	1:B:1069:PRO:HG2	1.96	0.47
1:B:472:ILE:HA	1:B:491:PRO:HD3	1.96	0.47
1:A:65:PHE:HE2	1:A:84:LEU:HD21	1.80	0.47
1:C:91:TYR:N	1:C:268:GLY:O	2.39	0.47
1:C:457:ARG:NH2	1:C:469:SER:OG	2.47	0.47
1:C:502:GLY:O	1:C:506:GLN:NE2	2.48	0.47
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.79	0.47
1:A:341:VAL:HG22	1:A:356:LYS:HD3	1.96	0.47
1:A:201:PHE:O	1:A:229:LEU:N	2.45	0.47
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.96	0.47
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.96	0.47
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.96	0.47
1:B:421:TYR:HD1	1:B:457:ARG:HB3	1.80	0.46
1:B:853:GLN:HG2	1:B:963:VAL:HG21	1.96	0.46
1:A:715:PRO:HB3	1:A:1069:PRO:HB3	1.95	0.46
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.96	0.46
1:B:902:MET:HE3	1:B:1049:LEU:HD13	1.98	0.46
1:C:457:ARG:HG2	1:C:461:LEU:HD23	1.98	0.46
1:B:452:LEU:HD13	1:B:492:LEU:HD13	1.96	0.46
1:A:607:GLN:HE22	1:A:691:SER:HA	1.81	0.46
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.97	0.46
1:B:94:SER:HG	1:B:263:ALA:N	2.12	0.46
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.32	0.46
1:A:498:GLN:OE1	1:A:501:ASN:ND2	2.39	0.46
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.98	0.46
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.98	0.46
1:B:909:ILE:HD13	1:B:1049:LEU:HD21	1.98	0.46
1:B:600:PRO:HG3	1:B:692:ILE:HD11	1.98	0.46
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.97	0.46
1:B:454:ARG:NH1	1:B:469:SER:O	2.48	0.46
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.32	0.46
1:B:895:GLN:NE2	1:A:1074:ASN:OD1	2.49	0.46
1:C:106:PHE:HB3	1:C:235:ILE:HG23	1.98	0.45
1:B:556:ASN:HB2	1:B:584:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.97	0.45
1:B:94:SER:OG	1:B:263:ALA:N	2.49	0.45
1:C:745:ASP:H	1:B:319:ARG:NH1	2.14	0.45
1:B:50:SER:OG	1:B:304:LYS:NZ	2.50	0.45
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.98	0.45
1:A:342:PHE:HZ	1:A:513:LEU:HD21	1.81	0.45
1:A:439:ASN:HA	1:A:507:PRO:HG2	1.99	0.45
1:A:747:THR:O	1:A:751:ASN:ND2	2.50	0.45
1:C:326:ILE:HA	1:C:531:THR:HG21	1.99	0.45
1:C:1129:VAL:HB	1:C:1132:ILE:HB	1.99	0.45
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.99	0.45
1:B:326:ILE:HD11	1:B:534:VAL:HG22	1.99	0.45
1:A:86:PHE:H	1:A:237:ARG:HA	1.81	0.45
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.98	0.45
1:C:187:LYS:HD2	1:C:211:ASN:HB2	1.99	0.45
1:B:373:SER:OG	1:A:405:ASP:OD2	2.34	0.45
1:B:975:SER:OG	1:A:571:ASP:OD2	2.24	0.45
1:C:16:VAL:N	1:C:138:ASP:OD2	2.50	0.45
1:C:294:ASP:OD1	1:C:294:ASP:N	2.47	0.45
1:A:142:GLY:O	1:A:155:SER:N	2.50	0.45
1:C:902:MET:HE3	1:C:1049:LEU:HD13	1.99	0.44
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.99	0.44
1:B:743:CYS:SG	1:B:750:SER:N	2.90	0.44
1:B:334:ASN:O	1:B:334:ASN:ND2	2.49	0.44
1:B:1054:GLN:HB2	1:B:1061:VAL:HB	2.00	0.44
1:C:501:ASN:HB3	1:C:505:TYR:HB2	1.99	0.44
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.99	0.44
1:A:675:GLN:HG2	1:A:676:THR:H	1.81	0.44
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.99	0.44
1:B:439:ASN:O	1:B:443:SER:OG	2.28	0.44
1:C:563:GLN:HG3	1:C:564:GLN:H	1.83	0.44
1:C:1141:LEU:HD13	1:B:1141:LEU:HD21	2.00	0.44
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.99	0.44
1:B:188:ASN:HD22	1:B:207:HIS:HB3	1.82	0.43
1:B:624:ILE:O	1:B:625:HIS:ND1	2.50	0.43
1:A:117:LEU:HD23	1:A:130:VAL:HG22	1.98	0.43
1:C:669:GLY:N	1:A:864:LEU:O	2.47	0.43
1:C:981:LEU:HD21	1:C:993:ILE:HD11	1.98	0.43
1:C:54:LEU:H	1:C:54:LEU:HD23	1.84	0.43
1:C:743:CYS:SG	1:C:750:SER:N	2.91	0.43
1:A:453:TYR:HE2	1:A:455:LEU:HD13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HA	1:A:491:PRO:HD3	2.00	0.43
1:A:763:LEU:HD13	1:A:1004:LEU:HD22	2.00	0.43
1:A:850:ILE:H	1:A:850:ILE:HG13	1.55	0.43
1:A:879:ALA:O	1:A:883:THR:OG1	2.34	0.43
1:A:434:ILE:HB	1:A:511:VAL:HG13	2.00	0.43
1:A:1028:LYS:HE3	1:A:1028:LYS:HB2	1.84	0.43
1:A:332:ILE:HD11	1:A:525:CYS:HB2	2.01	0.43
1:A:444:LYS:NZ	1:A:448:ASN:OD1	2.51	0.43
1:B:716:THR:HG21	1:B:1073:LYS:HD3	2.01	0.43
1:B:981:LEU:HD21	1:B:993:ILE:HD11	2.00	0.43
1:A:743:CYS:SG	1:A:750:SER:N	2.92	0.43
1:B:462:LYS:HG2	1:B:465:GLU:CD	2.44	0.42
1:B:770:ILE:O	1:B:774:GLN:HG2	2.19	0.42
1:B:1054:GLN:N	1:B:1061:VAL:O	2.52	0.42
1:C:96:GLU:O	1:C:186:PHE:N	2.53	0.42
1:C:986:PRO:N	1:C:987:PRO:HD2	2.34	0.42
1:B:930:ALA:O	1:B:934:ILE:HG12	2.19	0.42
1:A:53:ASP:OD1	1:A:54:LEU:N	2.45	0.42
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.01	0.42
1:C:503:VAL:HA	1:C:506:GLN:HE22	1.85	0.42
1:C:1054:GLN:N	1:C:1061:VAL:O	2.52	0.42
1:A:106:PHE:HB2	1:A:117:LEU:HB3	2.00	0.42
1:A:596:SER:O	1:A:611:LEU:N	2.49	0.42
1:A:930:ALA:O	1:A:934:ILE:HG12	2.19	0.42
1:C:403:ARG:HE	1:C:495:TYR:HD1	1.67	0.42
1:C:903:ALA:HB2	1:C:916:LEU:HD22	2.00	0.42
1:B:110:LEU:H	1:B:114:THR:HG21	1.85	0.42
1:B:188:ASN:HA	1:B:208:THR:H	1.83	0.42
1:B:293:LEU:HG	1:B:294:ASP:H	1.84	0.42
1:B:438:SER:OG	1:B:442:ASP:OD2	2.32	0.42
1:B:792:PRO:HG2	1:A:707:TYR:HB3	2.01	0.42
1:A:770:ILE:O	1:A:774:GLN:HG2	2.20	0.42
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.54	0.42
1:C:410:ILE:HG23	1:C:425:LEU:HD21	2.01	0.42
1:C:661:GLU:O	1:C:695:TYR:OH	2.37	0.42
1:B:119:ILE:HG12	1:B:128:ILE:HG12	2.00	0.42
1:B:420:ASP:OD1	1:B:424:LYS:NZ	2.52	0.42
1:B:982:SER:HB3	1:A:390:LEU:HD21	2.02	0.42
1:A:897:PRO:HD2	1:A:900:MET:HE2	2.02	0.42
1:C:55:PHE:HB2	1:C:275:PHE:CE1	2.55	0.42
1:A:139:PRO:HB3	1:A:156:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG22	1:A:490:PHE:HA	2.02	0.42
1:A:880:GLY:O	1:A:884:SER:OG	2.30	0.42
1:A:988:GLU:O	1:A:992:GLN:HG2	2.19	0.42
1:A:89:GLY:HA3	1:A:270:LEU:HB2	2.01	0.42
1:B:108:THR:OG1	1:B:234:ASN:O	2.38	0.42
1:B:623:ALA:HB3	1:B:627:ASP:HB3	2.01	0.42
1:C:934:ILE:HD13	1:C:934:ILE:HA	1.93	0.41
1:C:278:LYS:HE2	1:C:278:LYS:HB3	1.97	0.41
1:C:1028:LYS:HG2	1:C:1042:PHE:CZ	2.55	0.41
1:B:347:PHE:HD2	1:B:347:PHE:HA	1.68	0.41
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.95	0.41
1:B:773:GLU:HG2	1:B:1019:ARG:HD2	2.02	0.41
1:C:328:ARG:NH2	1:C:531:THR:O	2.52	0.41
1:B:188:ASN:ND2	1:B:207:HIS:HB3	2.36	0.41
1:A:733:LYS:HD2	1:A:771:ALA:HB1	2.02	0.41
1:C:201:PHE:HD2	1:C:229:LEU:HD12	1.85	0.41
1:C:210:ILE:HG23	1:C:211:ASN:H	1.84	0.41
1:B:724:THR:HG23	1:B:934:ILE:HD12	2.02	0.41
1:B:882:ILE:HG13	1:B:883:THR:HG23	2.02	0.41
1:A:197:ILE:HG22	1:A:198:ASP:H	1.86	0.41
1:B:736:VAL:HG11	1:B:1004:LEU:HD11	2.03	0.41
1:B:93:ALA:HB3	1:B:266:TYR:HB2	2.03	0.41
1:B:645:THR:OG1	1:B:648:GLY:O	2.36	0.41
1:C:81:ASN:HB2	1:C:242:LEU:HD12	2.03	0.41
1:C:424:LYS:HB3	1:C:463:PRO:HA	2.03	0.41
1:C:882:ILE:HG13	1:C:883:THR:HG23	2.03	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.53	0.41
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	2.02	0.41
1:B:66:HIS:CG	1:B:67:ALA:H	2.39	0.41
1:B:188:ASN:C	1:B:190:ARG:H	2.29	0.41
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.56	0.41
1:A:191:GLU:HB3	1:A:223:LEU:HD11	2.03	0.41
1:B:392:PHE:N	1:B:524:VAL:O	2.47	0.40
1:B:624:ILE:H	1:B:624:ILE:HG13	1.55	0.40
1:B:746:SER:HB2	1:B:749:CYS:HB3	2.03	0.40
1:C:421:TYR:HB3	1:C:458:LYS:HA	2.03	0.40
1:C:979:ASP:HB3	1:C:983:ARG:NH2	2.36	0.40
1:B:353:TRP:HB2	1:B:466:ARG:HH11	1.87	0.40
1:B:708:SER:HB3	1:B:711:SER:HB3	2.02	0.40
1:A:361:CYS:SG	1:A:362:VAL:N	2.95	0.40
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ARG:HA	1:C:573:THR:HA	2.01	0.40
1:B:82:PRO:HG2	1:B:84:LEU:HD21	2.03	0.40

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	1011/1273 (79%)	957 (95%)	54 (5%)	0	100	100
1	B	1032/1273 (81%)	975 (94%)	57 (6%)	0	100	100
1	C	1013/1273 (80%)	951 (94%)	62 (6%)	0	100	100
2	D	24/36 (67%)	20 (83%)	4 (17%)	0	100	100
All	All	3080/3855 (80%)	2903 (94%)	177 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	888/1115 (80%)	870 (98%)	18 (2%)	48	72
1	B	904/1115 (81%)	891 (99%)	13 (1%)	59	76
1	C	878/1115 (79%)	863 (98%)	15 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	19/34 (56%)	18 (95%)	1 (5%)	20	51
All	All	2689/3379 (80%)	2642 (98%)	47 (2%)	52	74

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	101	ILE
1	C	113	LYS
1	C	130	VAL
1	C	166	CYS
1	C	267	VAL
1	C	296	LEU
1	C	320	VAL
1	C	332	ILE
1	C	533	LEU
1	C	624	ILE
1	C	642	VAL
1	C	676	THR
1	C	786	LYS
1	C	849	LEU
1	C	1004	LEU
1	B	236	THR
1	B	312	ILE
1	B	347	PHE
1	B	395	VAL
1	B	500	THR
1	B	533	LEU
1	B	535	LYS
1	B	538	CYS
1	B	554	GLU
1	B	620	VAL
1	B	622	VAL
1	B	624	ILE
1	B	642	VAL
1	A	120	VAL
1	A	304	LYS
1	A	327	VAL
1	A	336	CYS
1	A	361	CYS
1	A	395	VAL
1	A	481	ASN
1	A	559	PHE

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Mol	Chain	Res	Type
1	A	608	VAL
1	A	616	ASN
1	A	622	VAL
1	A	649	CYS
1	A	676	THR
1	A	776	LYS
1	A	850	ILE
1	A	1004	LEU
1	A	1010	GLN
1	A	1122	VAL
2	D	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	ASN
1	C	121	ASN
1	C	321	GLN
1	C	563	GLN
1	C	607	GLN
1	C	658	ASN
1	C	677	GLN
1	C	755	GLN
1	C	853	GLN
1	C	907	ASN
1	C	957	GLN
1	C	1002	GLN
1	C	1011	GLN
1	C	1071	GLN
1	C	1106	GLN
1	C	1135	ASN
1	B	69	HIS
1	B	134	GLN
1	B	188	ASN
1	B	317	ASN
1	B	370	ASN
1	B	388	ASN
1	B	437	ASN
1	B	493	GLN
1	B	506	GLN
1	B	540	ASN
1	B	580	GLN

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Mol	Chain	Res	Type
1	B	628	GLN
1	B	655	HIS
1	B	675	GLN
1	B	690	GLN
1	B	755	GLN
1	B	762	GLN
1	B	853	GLN
1	B	913	GLN
1	B	955	ASN
1	B	957	GLN
1	B	1011	GLN
1	B	1071	GLN
1	B	1113	GLN
1	B	1135	ASN
1	A	137	ASN
1	A	321	GLN
1	A	409	GLN
1	A	439	ASN
1	A	536	ASN
1	A	540	ASN
1	A	564	GLN
1	A	628	GLN
1	A	644	GLN
1	A	677	GLN
1	A	703	ASN
1	A	755	GLN
1	A	762	GLN
1	A	853	GLN
1	A	913	GLN
1	A	955	ASN
1	A	969	ASN
1	A	978	ASN
1	A	1005	GLN
1	A	1011	GLN
1	A	1071	GLN

5.3.3 RNA ⓘ

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	$\# Z > 2$
3	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	B	1308	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1307	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	1313	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	C	1304	1	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	A	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	B	1309	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	B	1314	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1304	1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.54	0
3	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	C	1313	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1311	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1312	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	C	1311	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	1312	1	14,14,15	0.23	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1305	NAG	O5-C5-C6-O6
3	C	1312	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	C	1313	NAG	C4-C5-C6-O6
3	B	1313	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1307	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	A	1312	NAG	C4-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6
3	C	1312	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	B	1313	NAG	C4-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	C	1313	NAG	O5-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1312	NAG	O5-C5-C6-O6
3	B	1312	NAG	C4-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1304	NAG	C3-C2-N2-C7
3	C	1308	NAG	C3-C2-N2-C7
3	A	1301	NAG	C3-C2-N2-C7
3	A	1304	NAG	C3-C2-N2-C7

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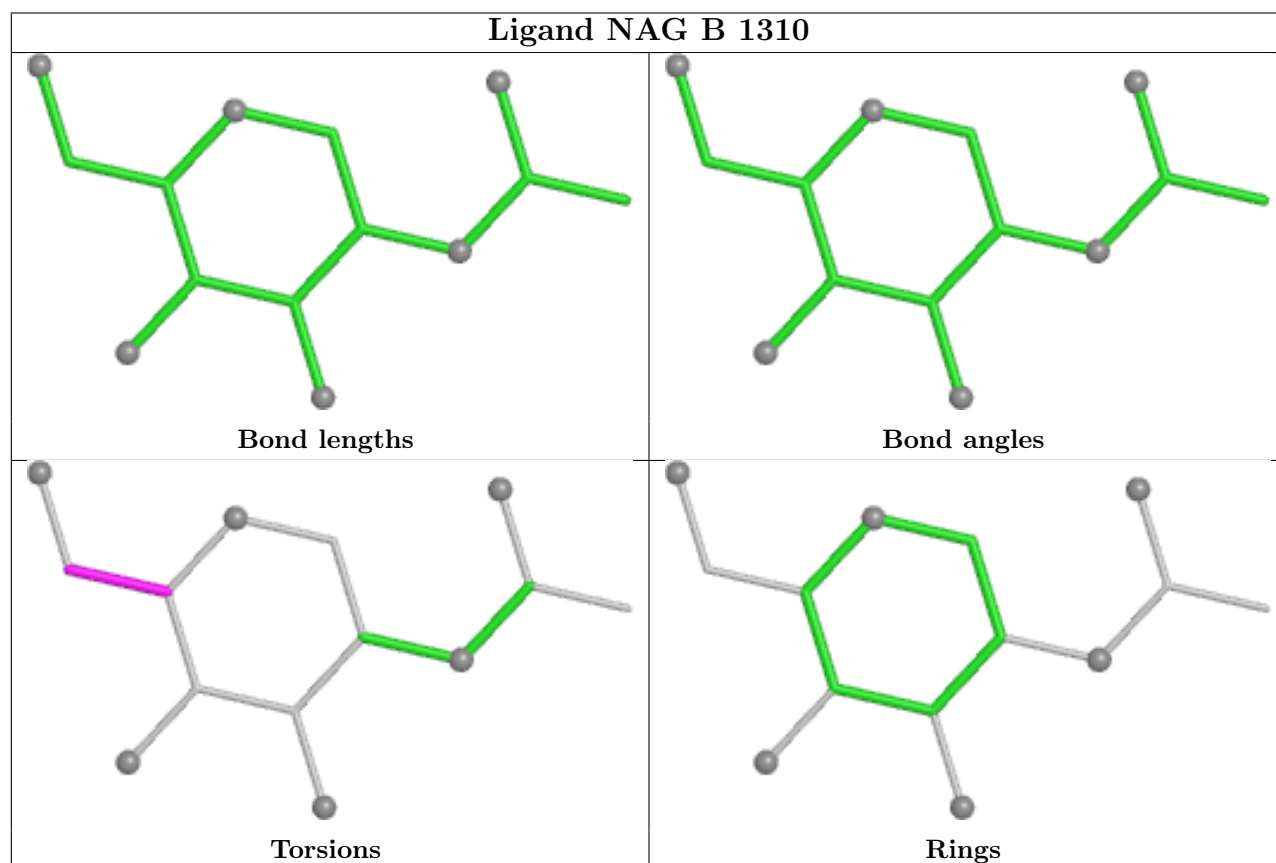
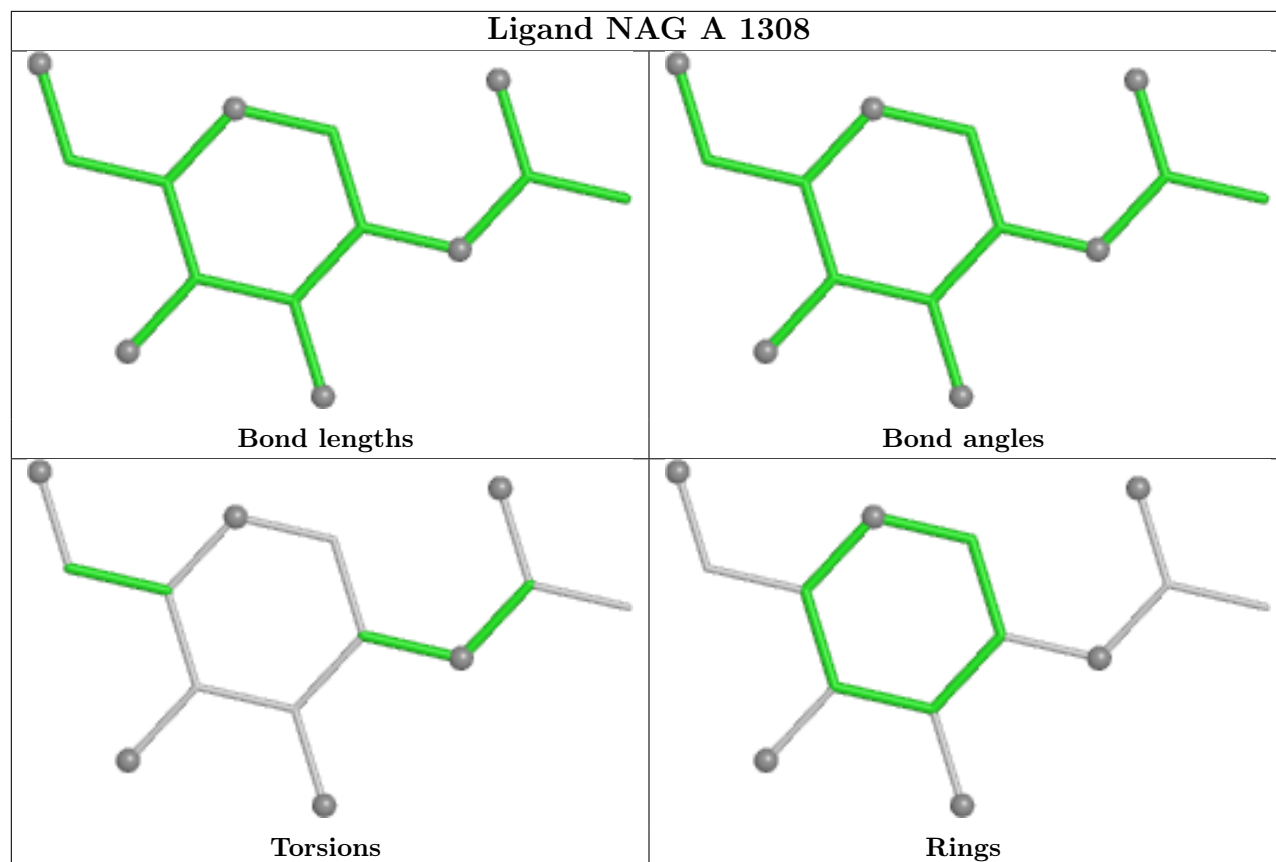
Mol	Chain	Res	Type	Atoms
3	A	1301	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6

There are no ring outliers.

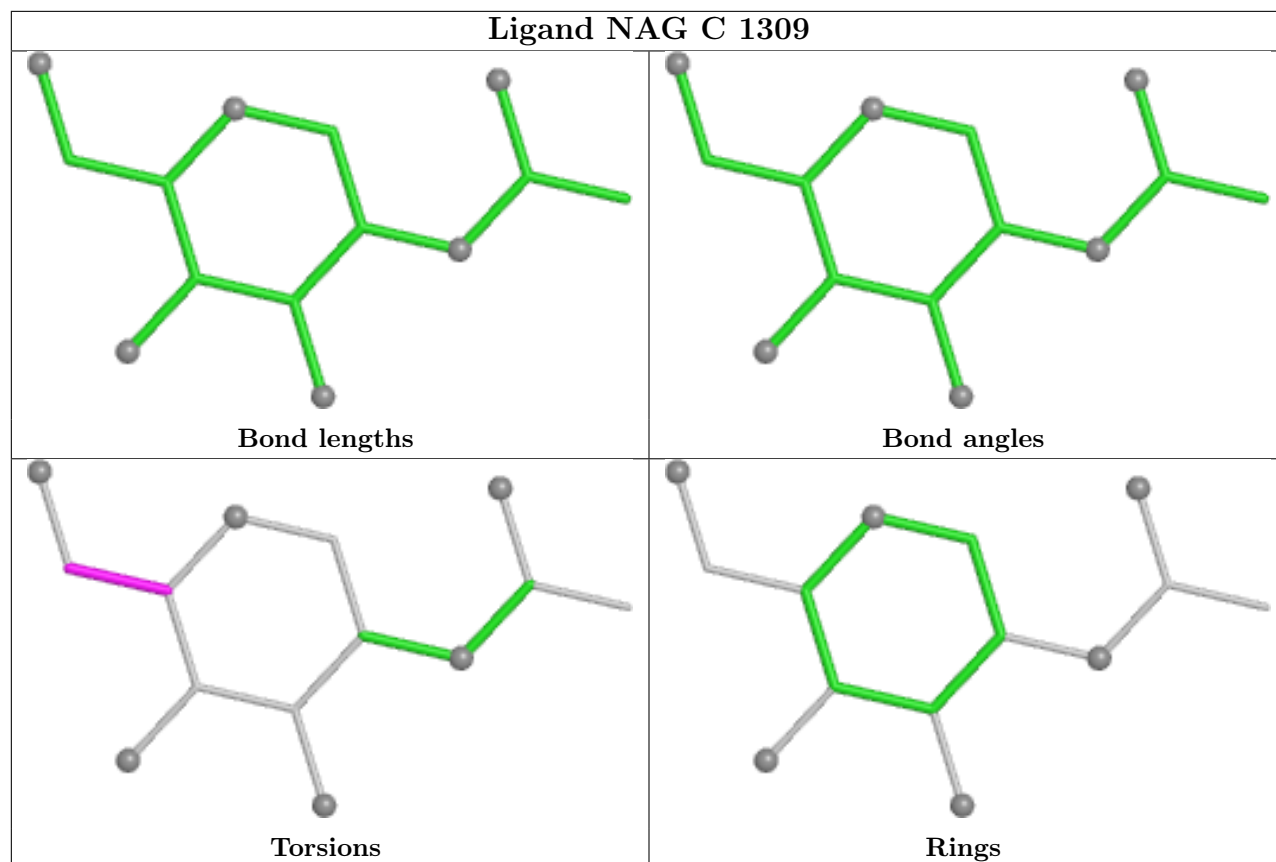
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1313	NAG	1	0

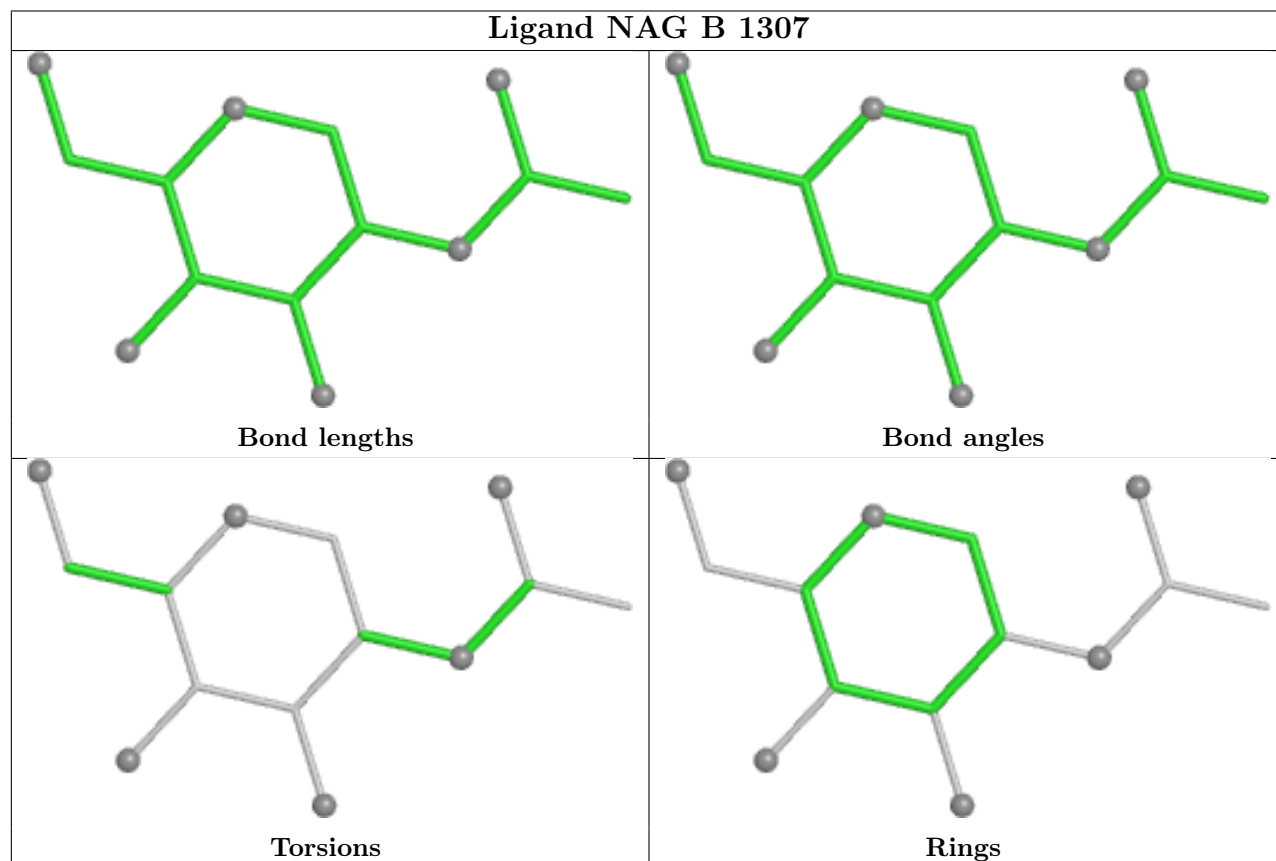
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

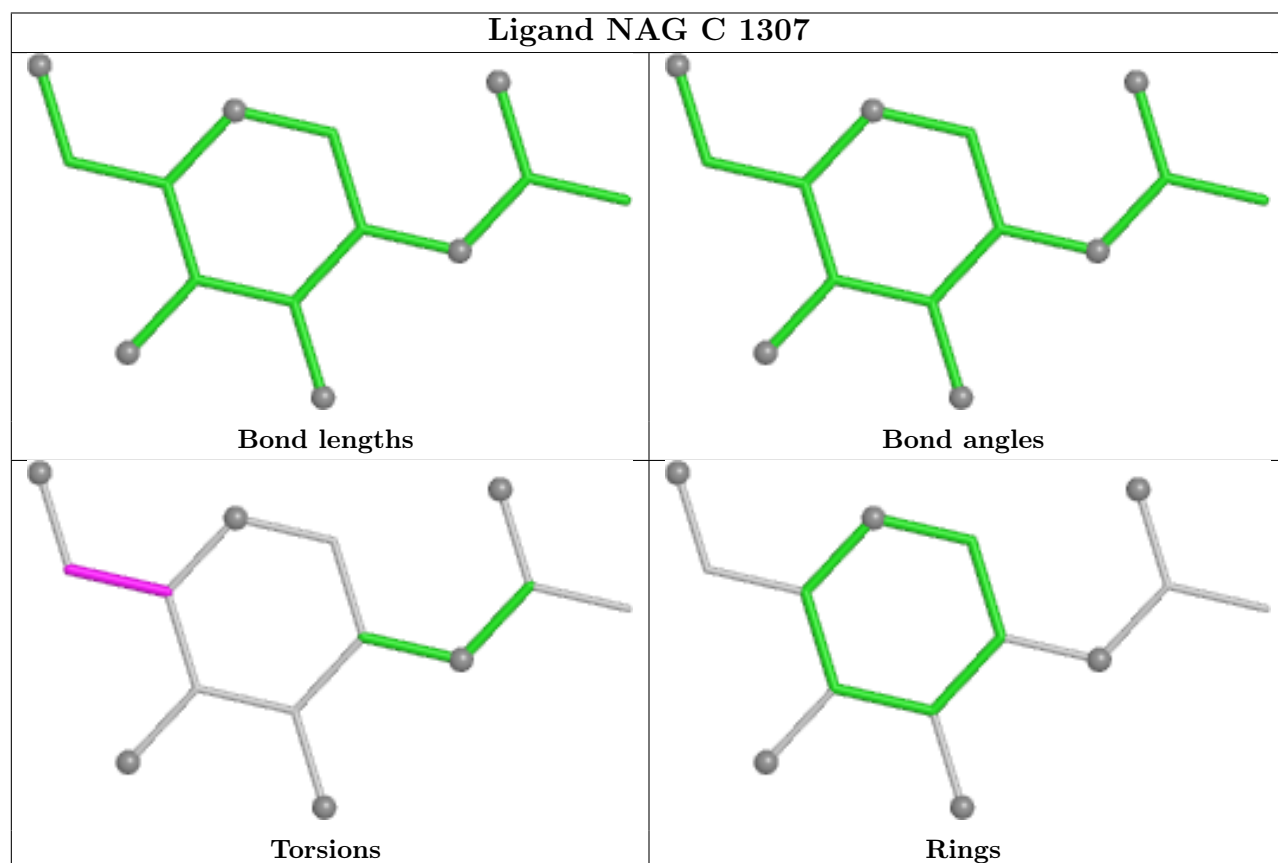
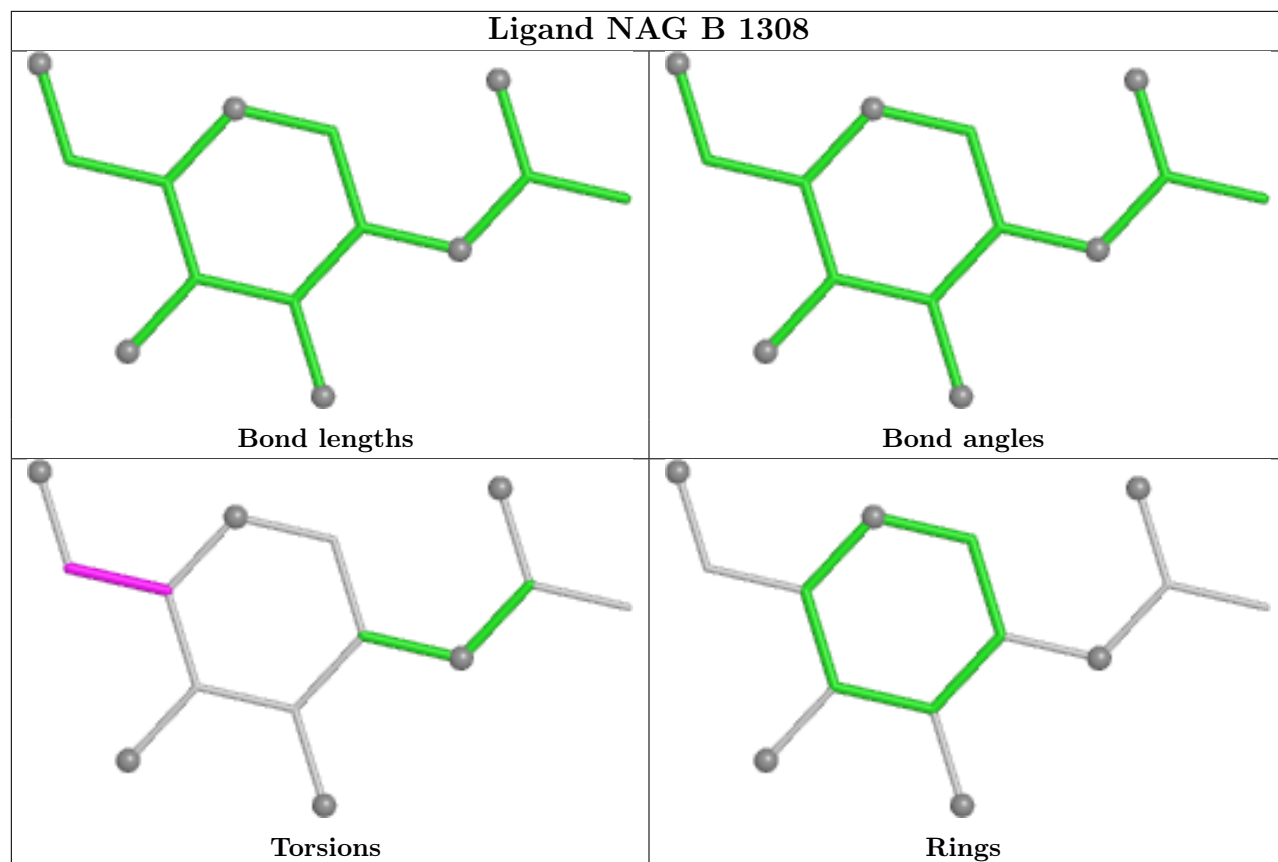


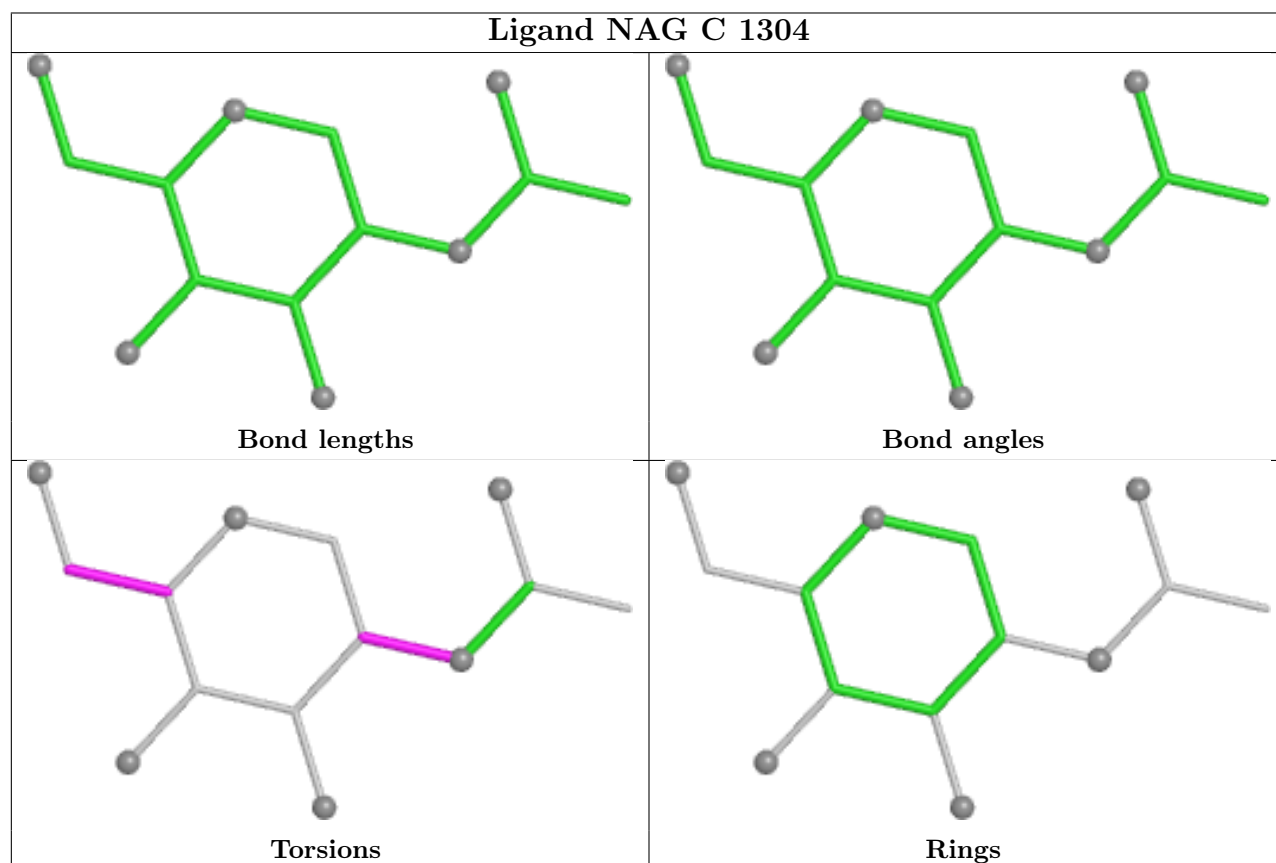
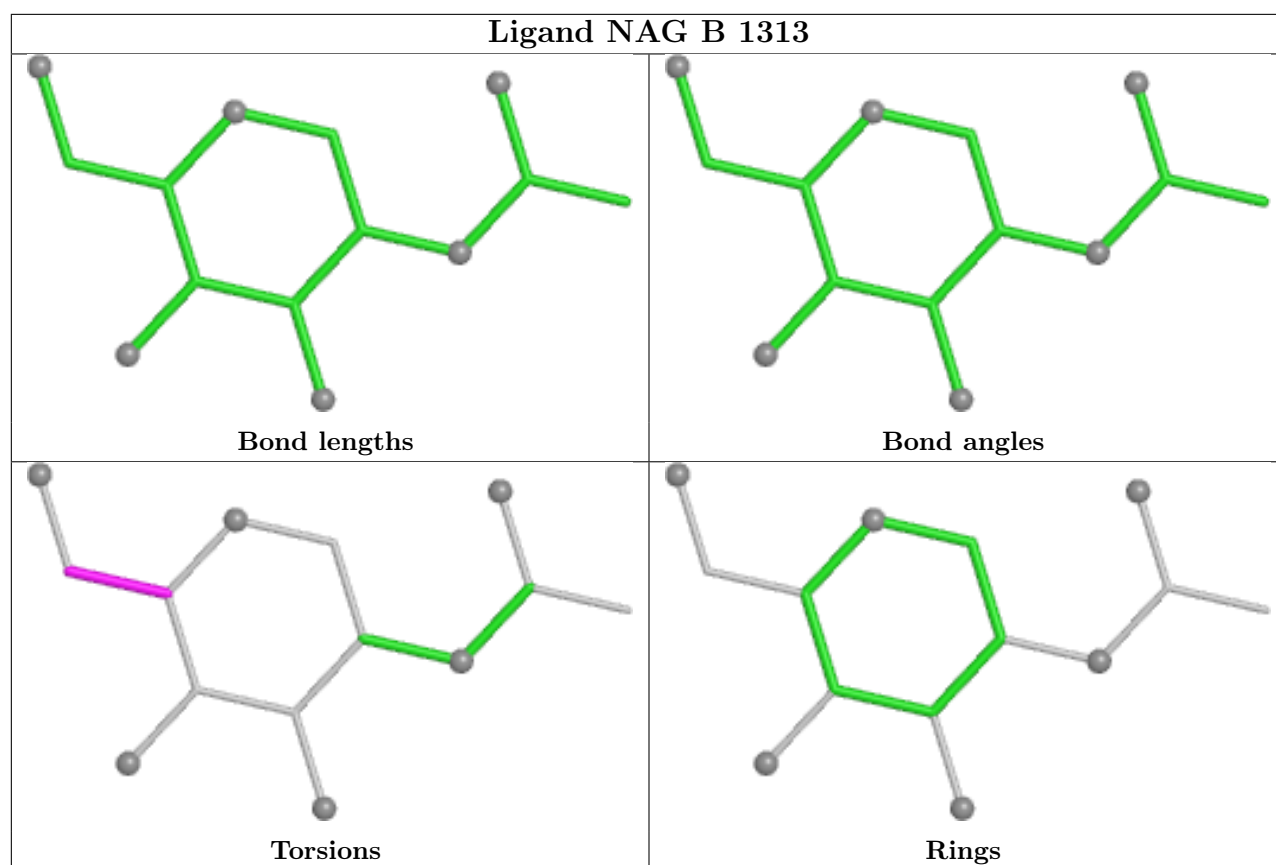
Ligand NAG C 1309



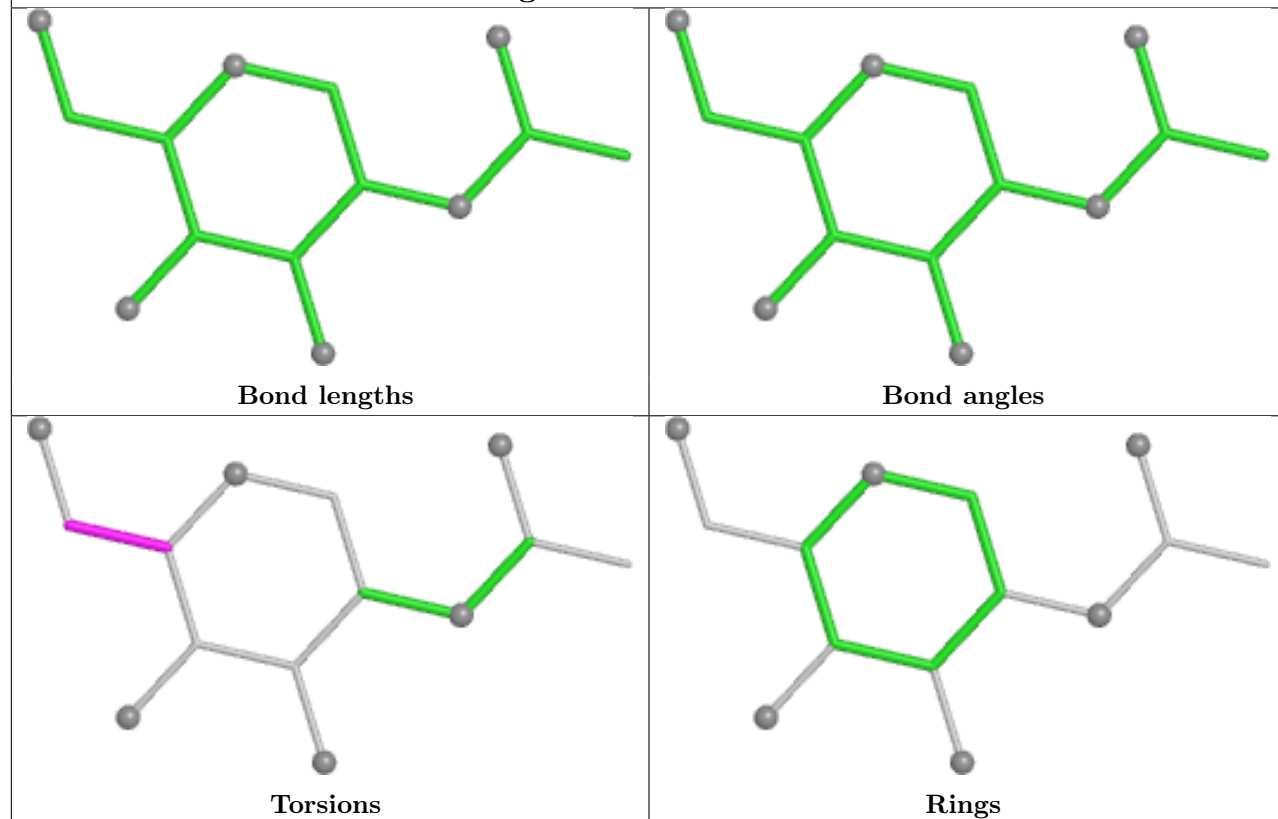
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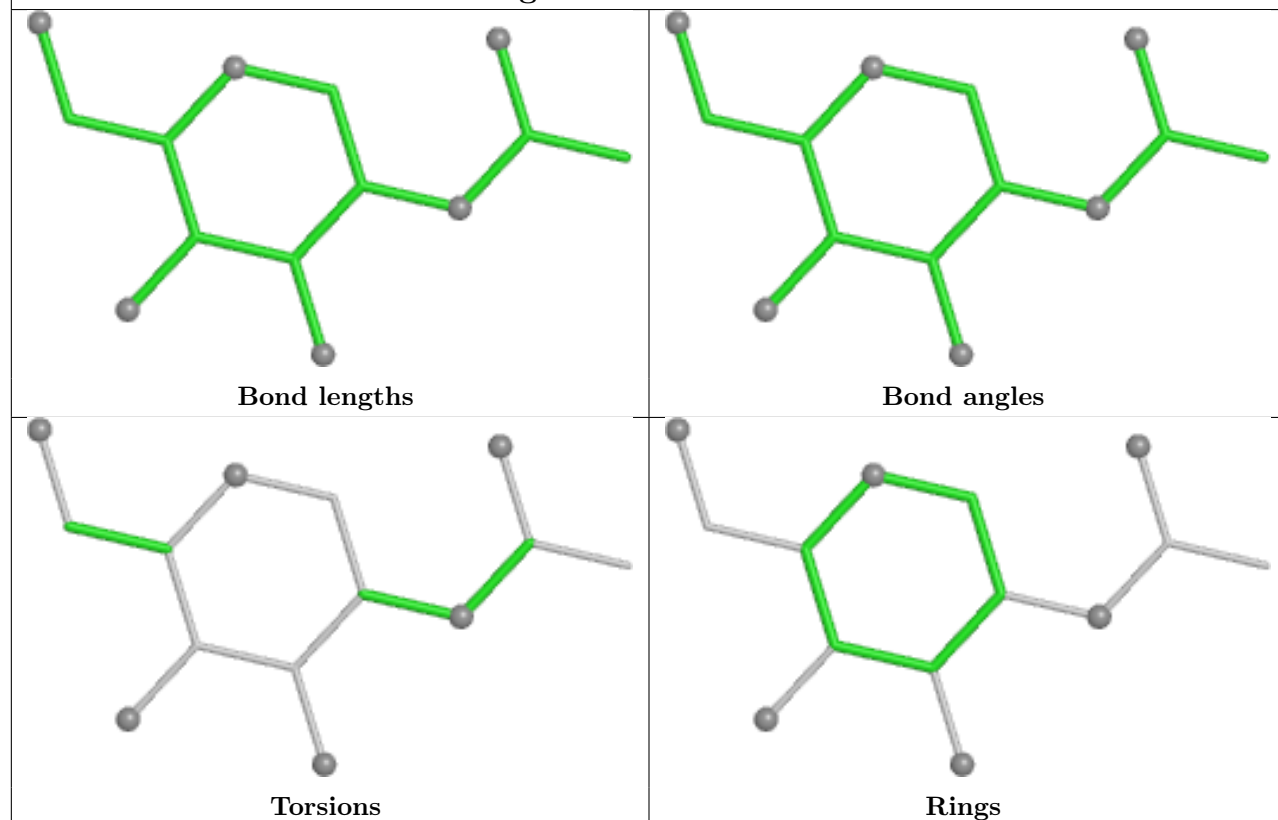




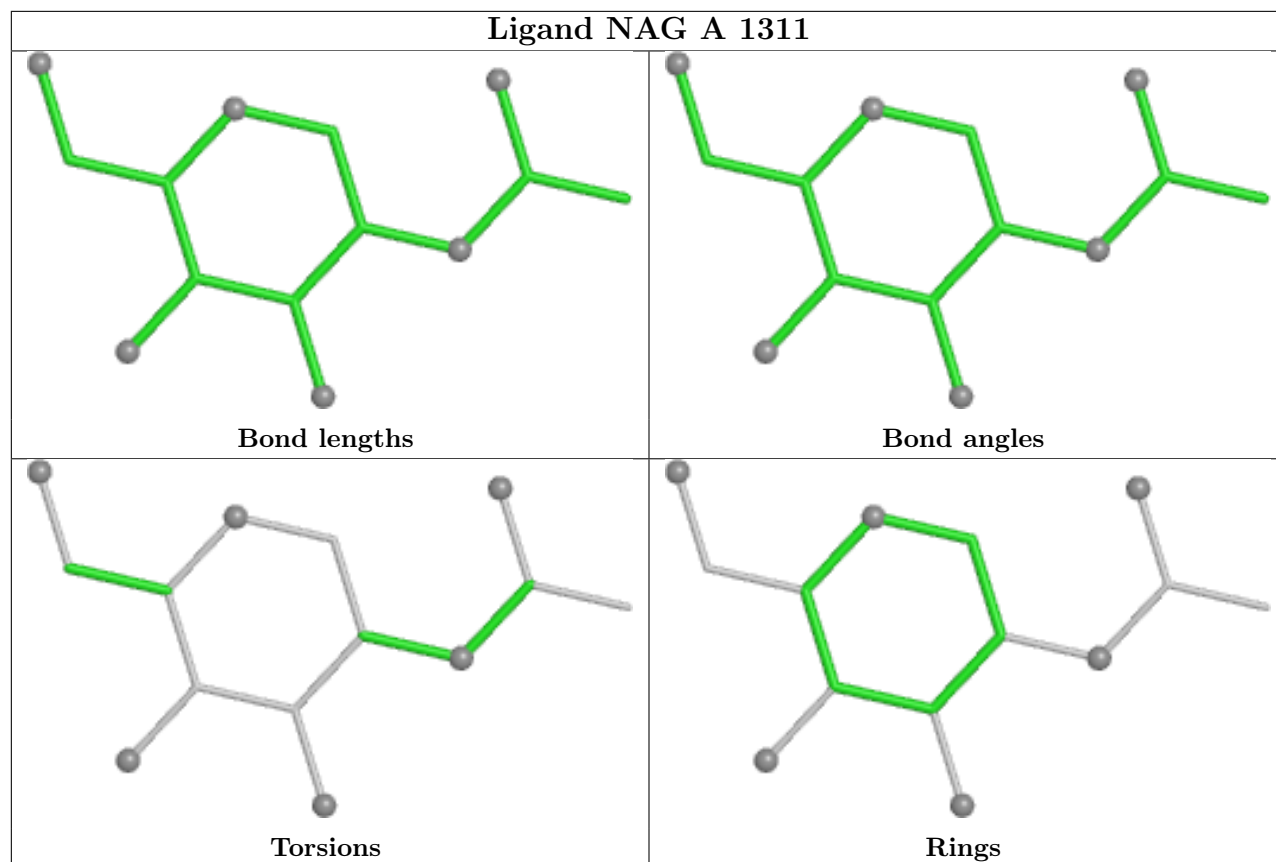
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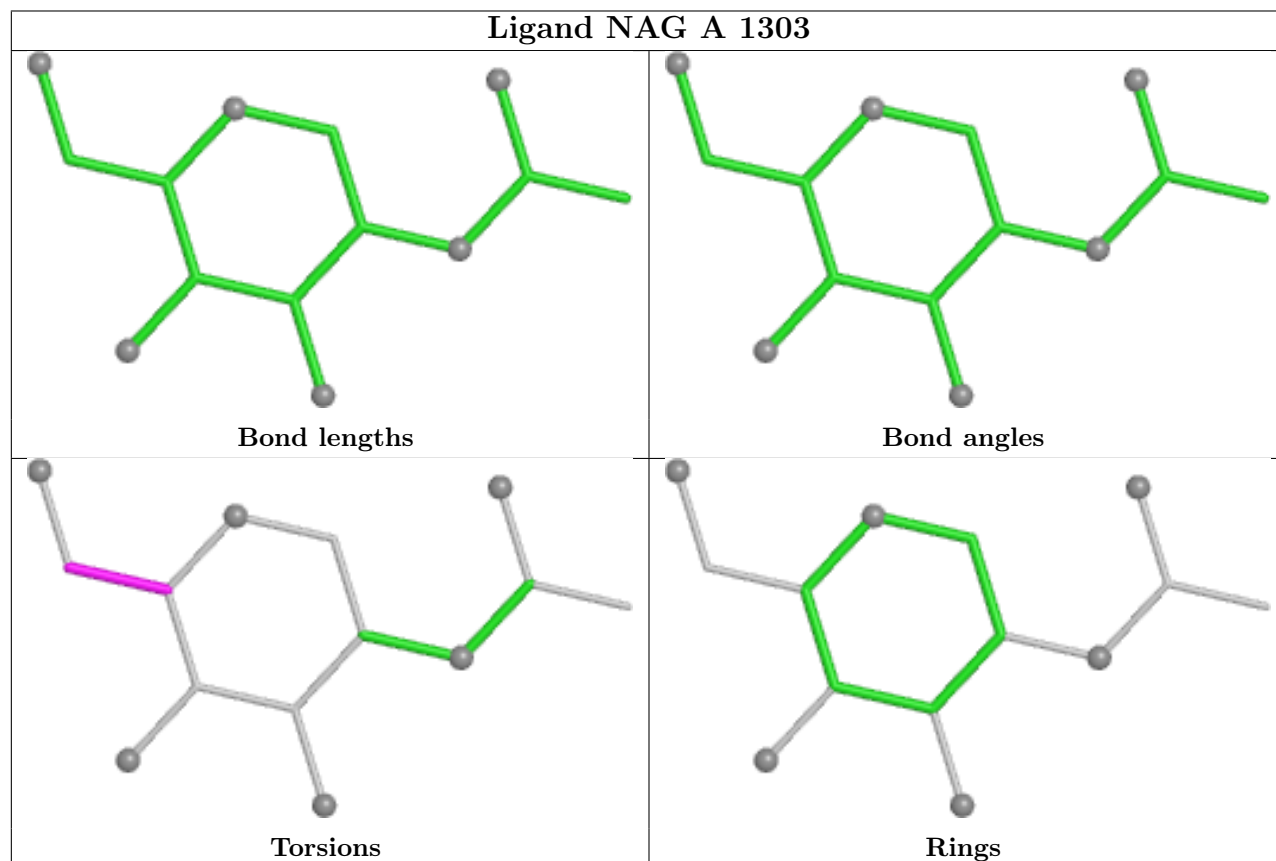
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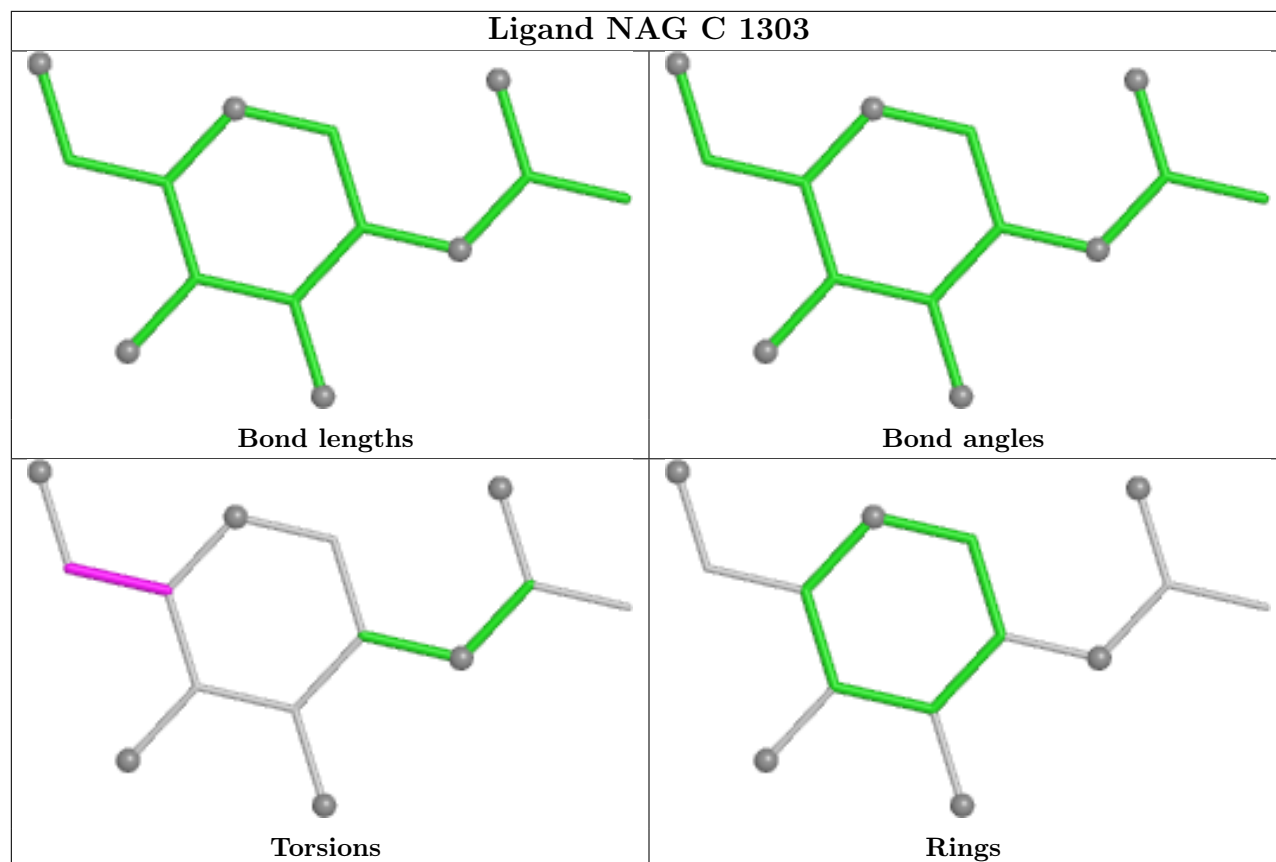
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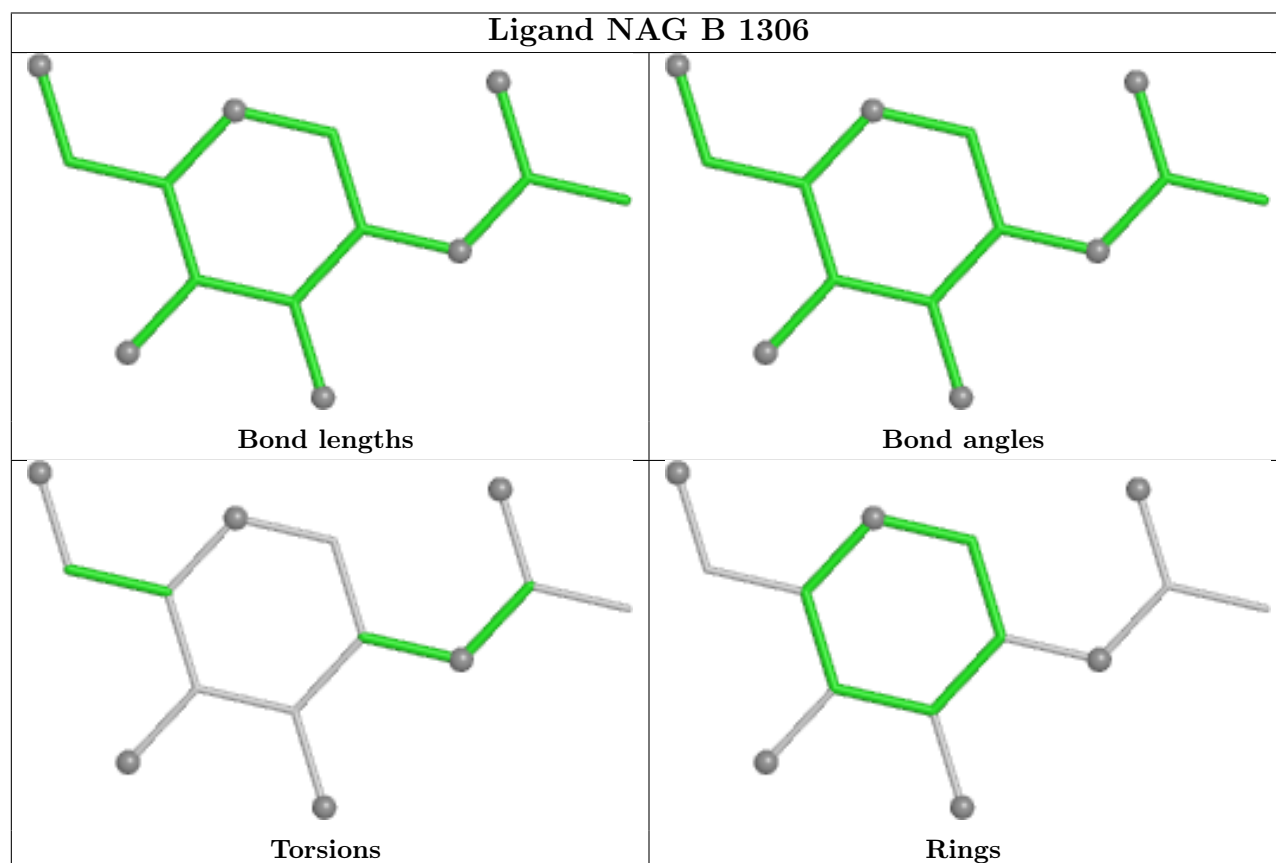
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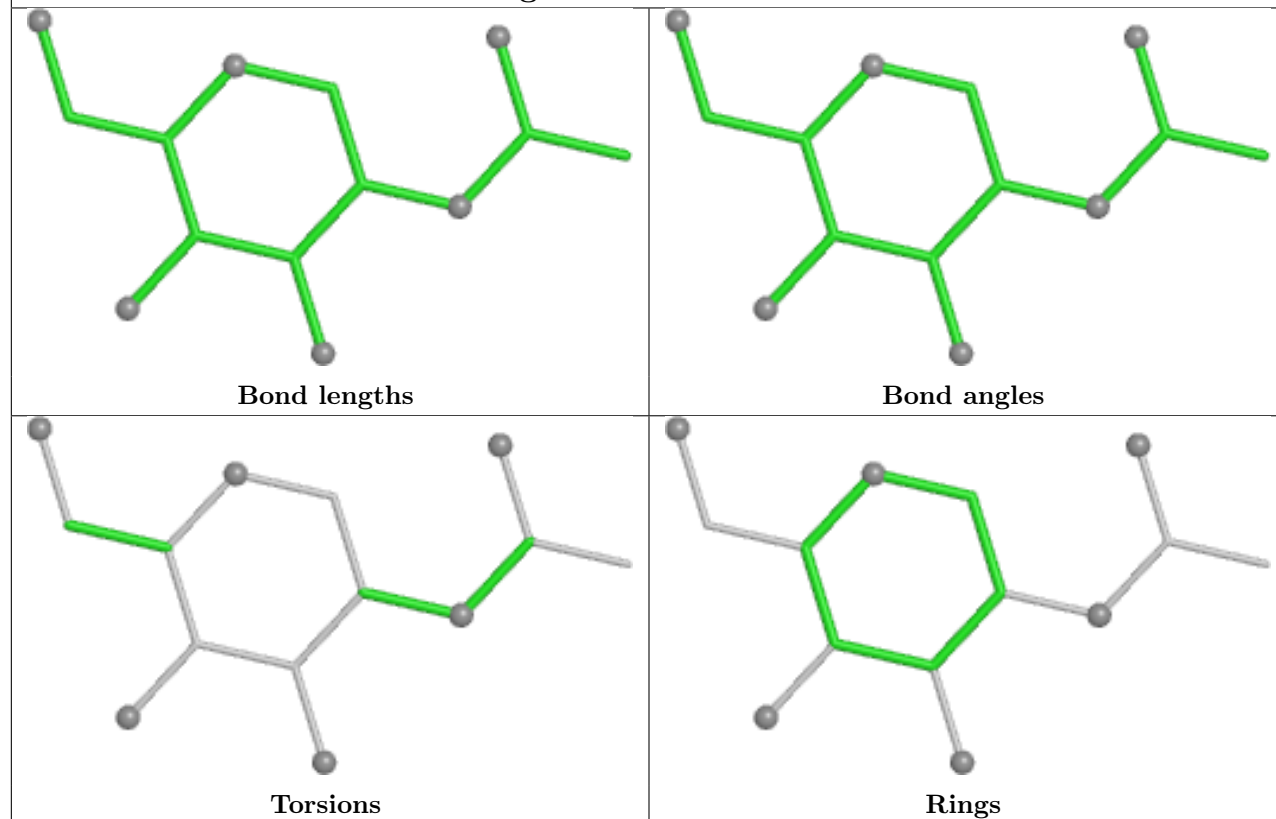
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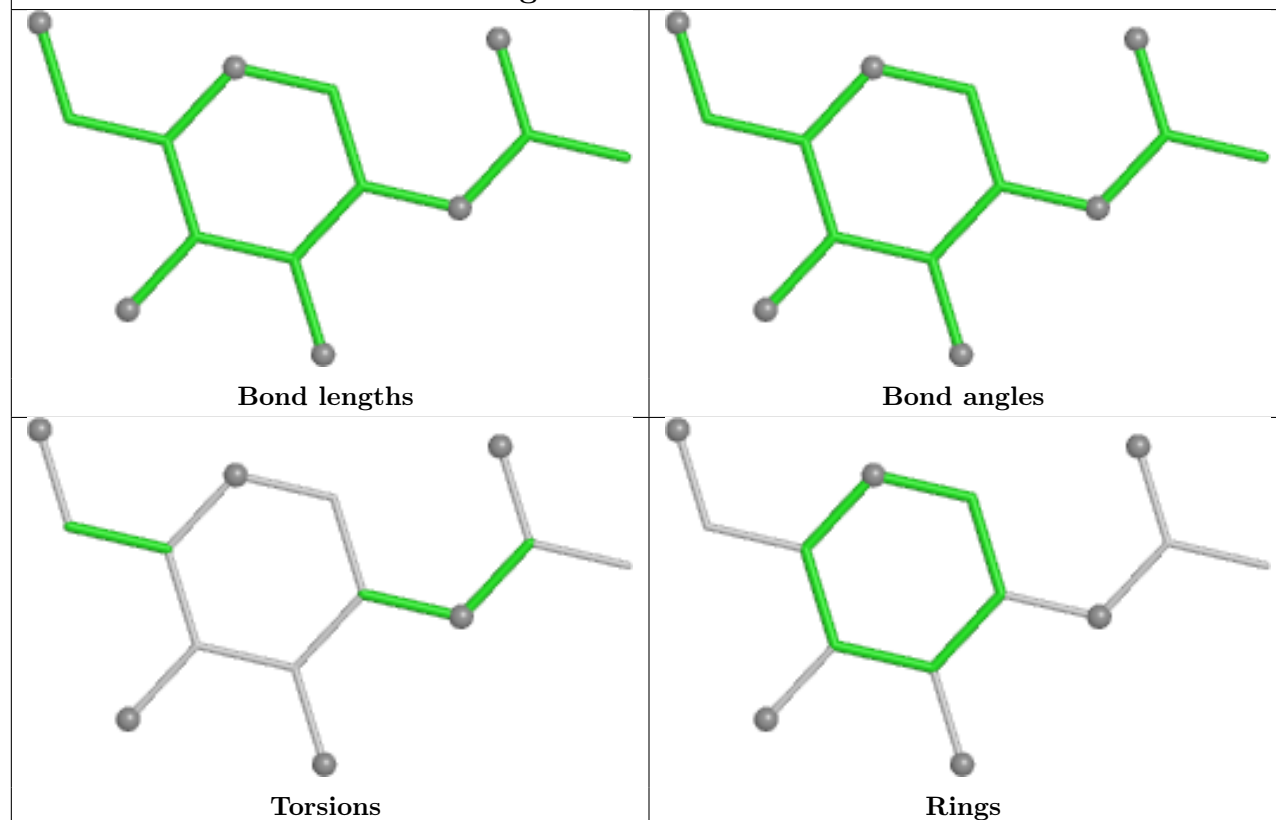
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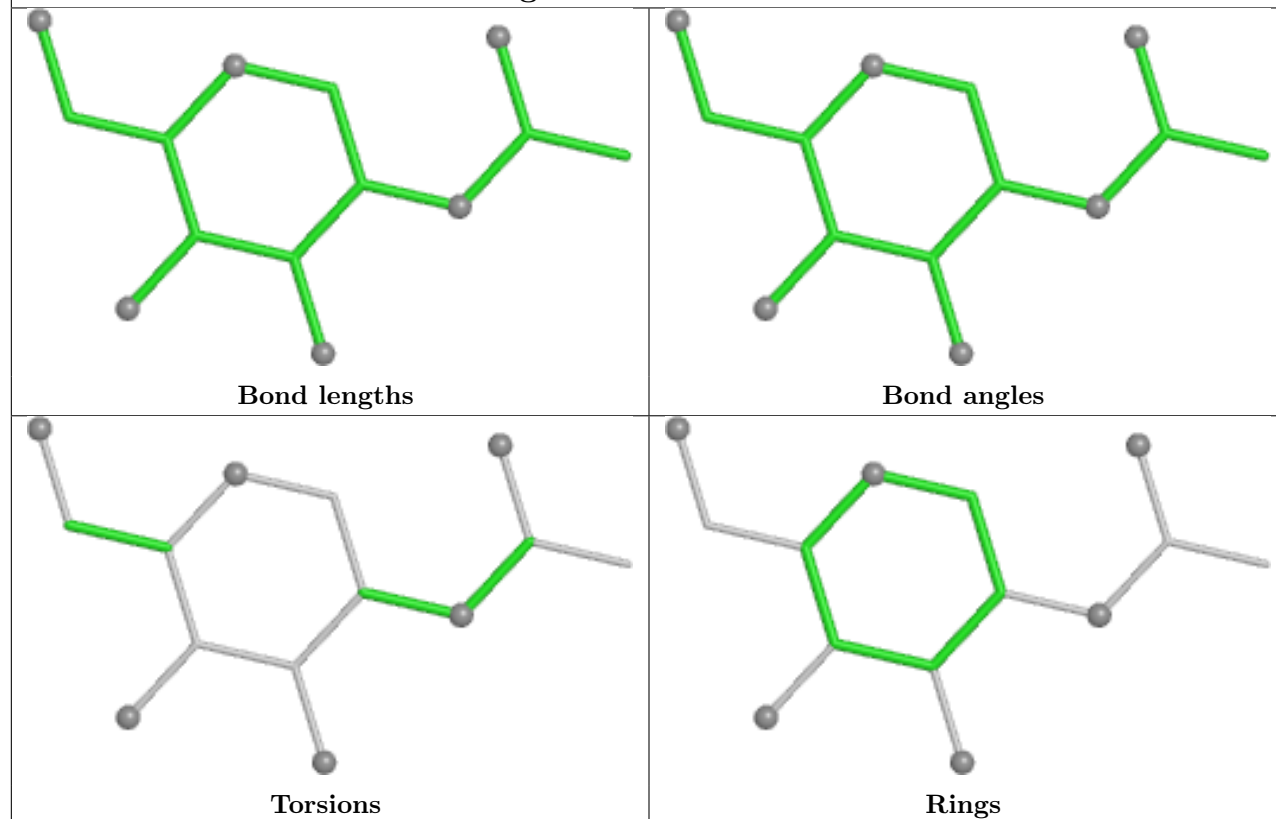
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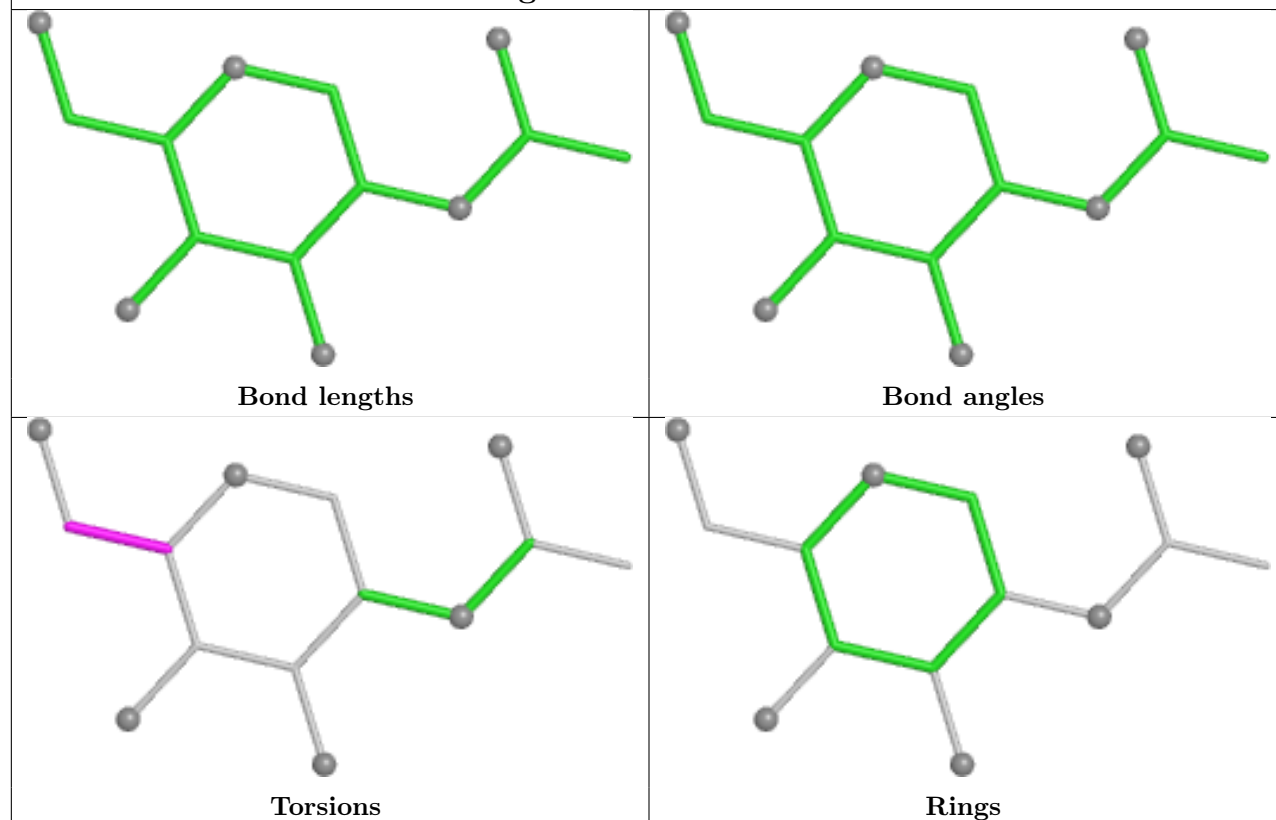
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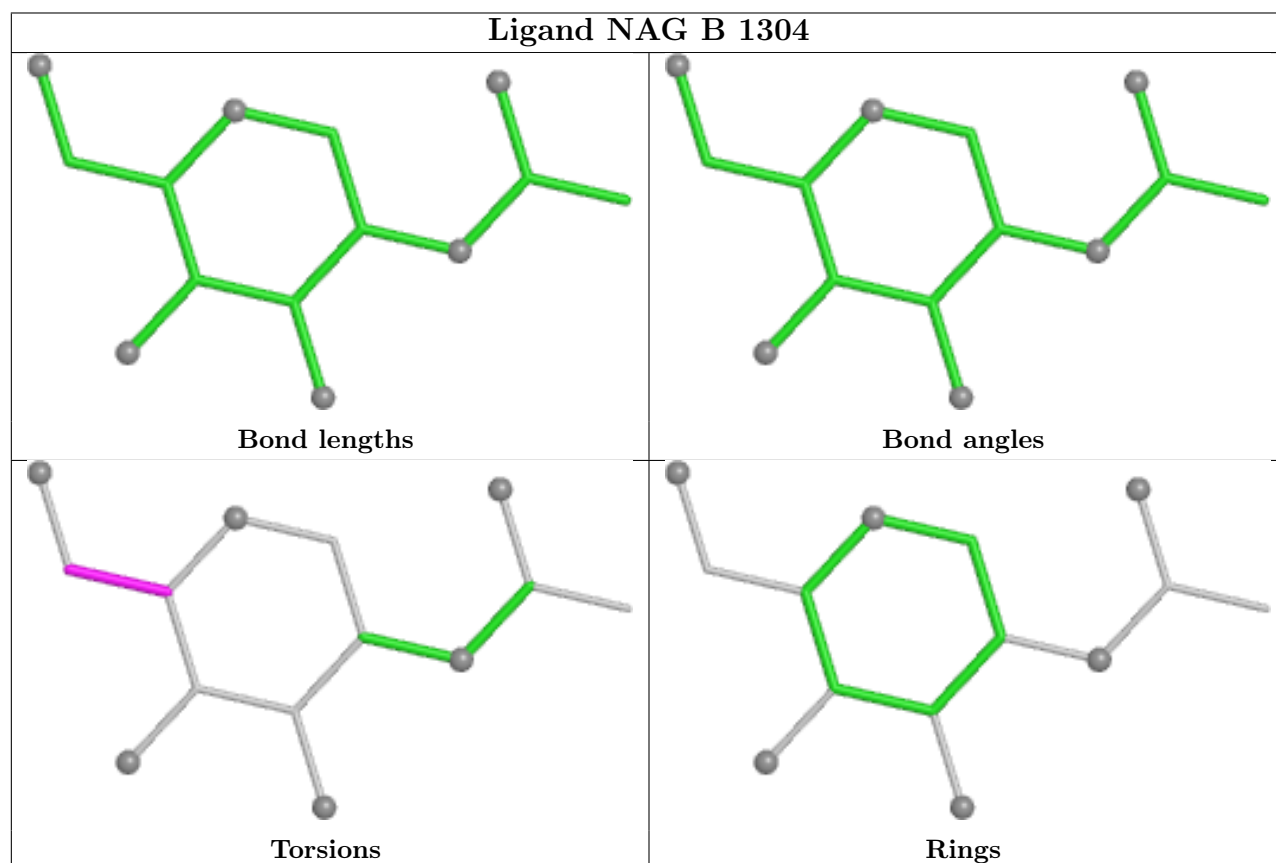
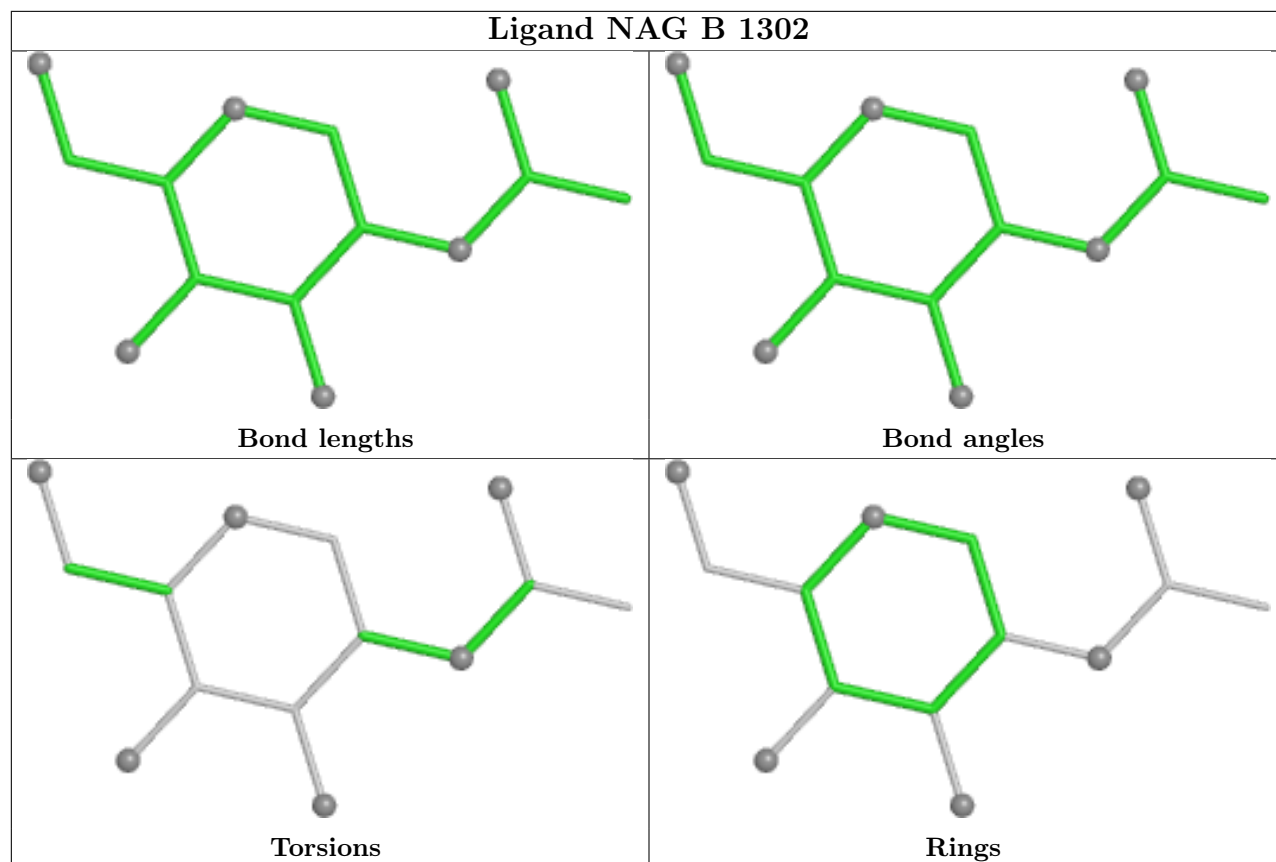


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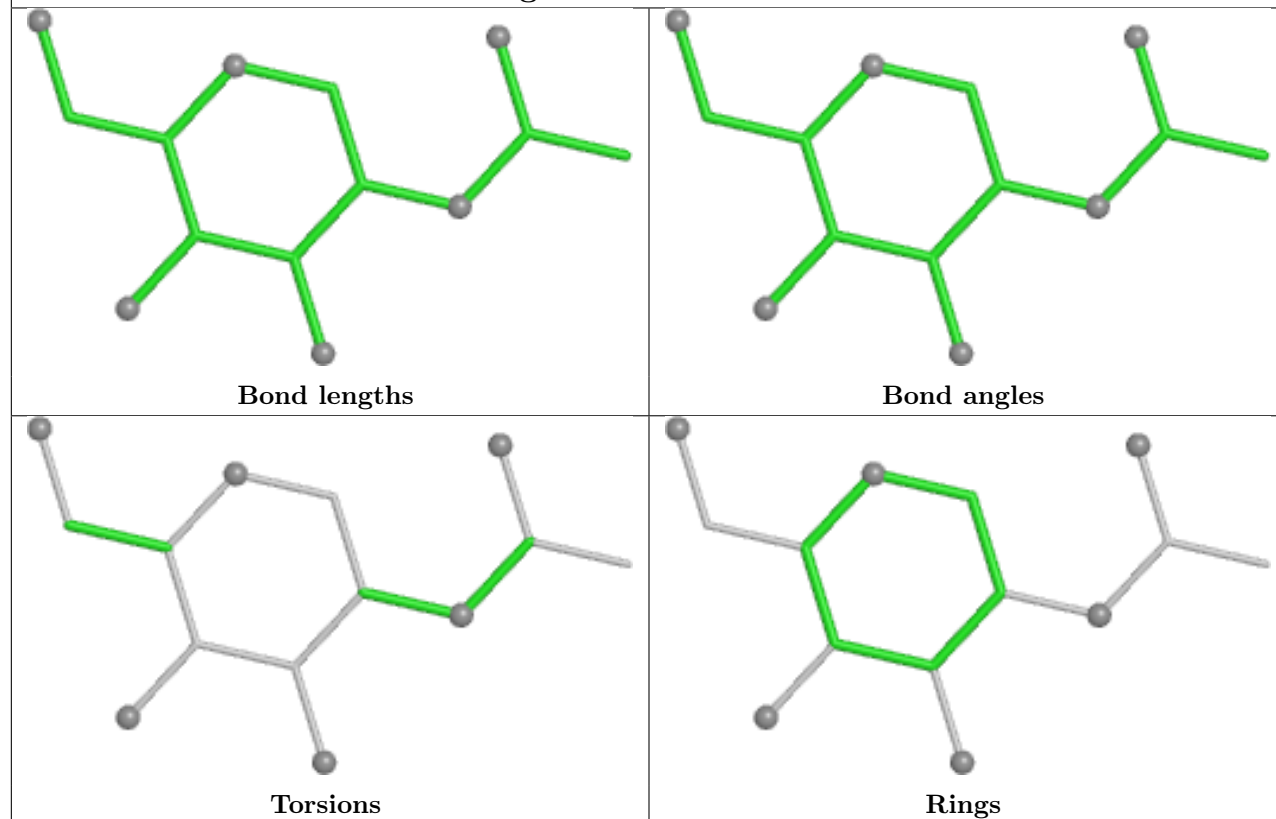


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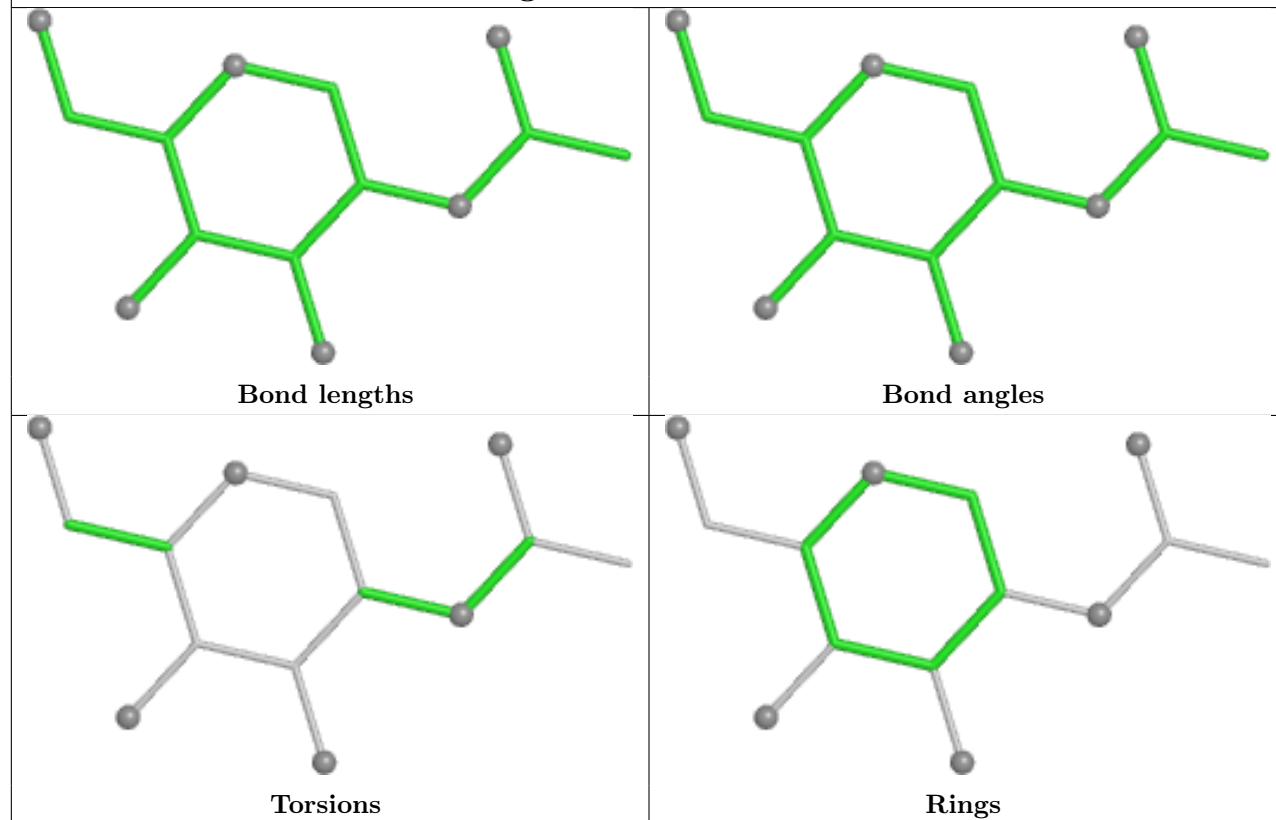




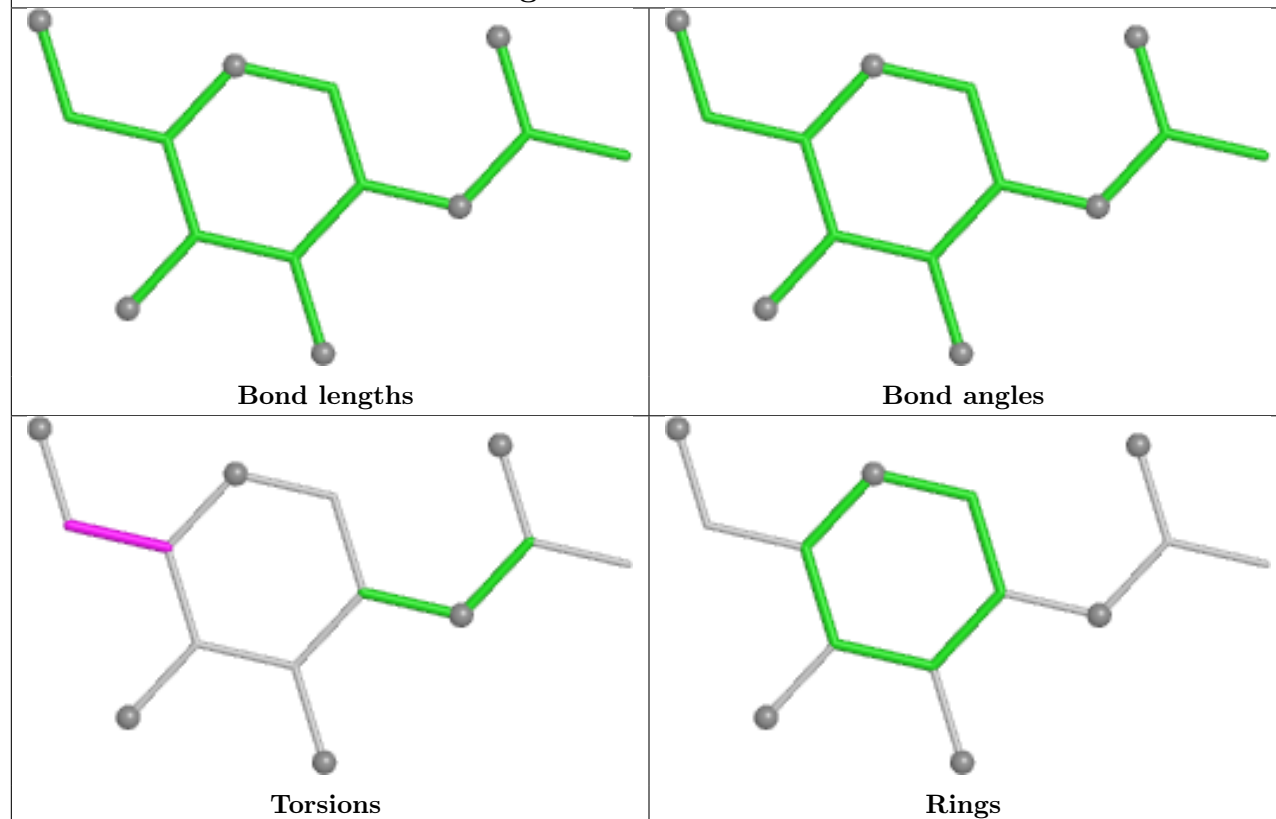
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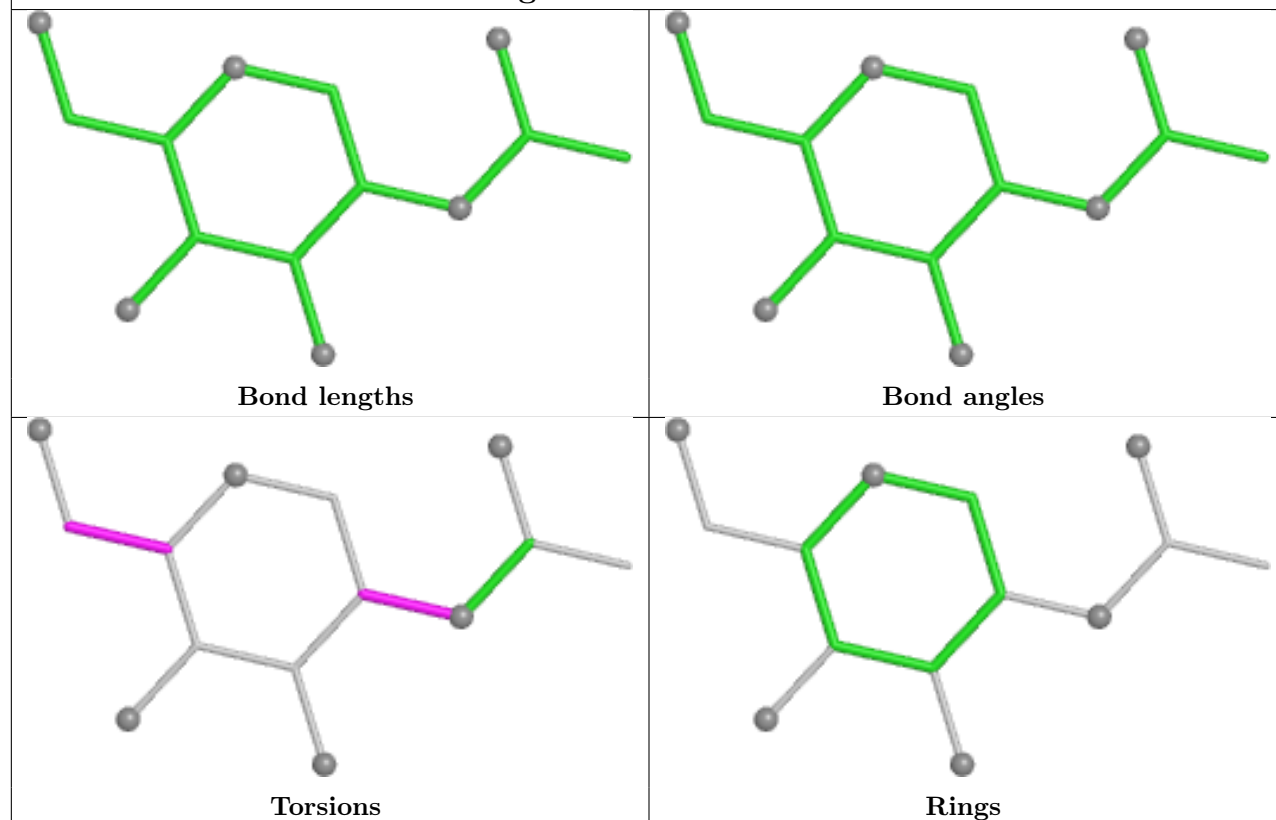
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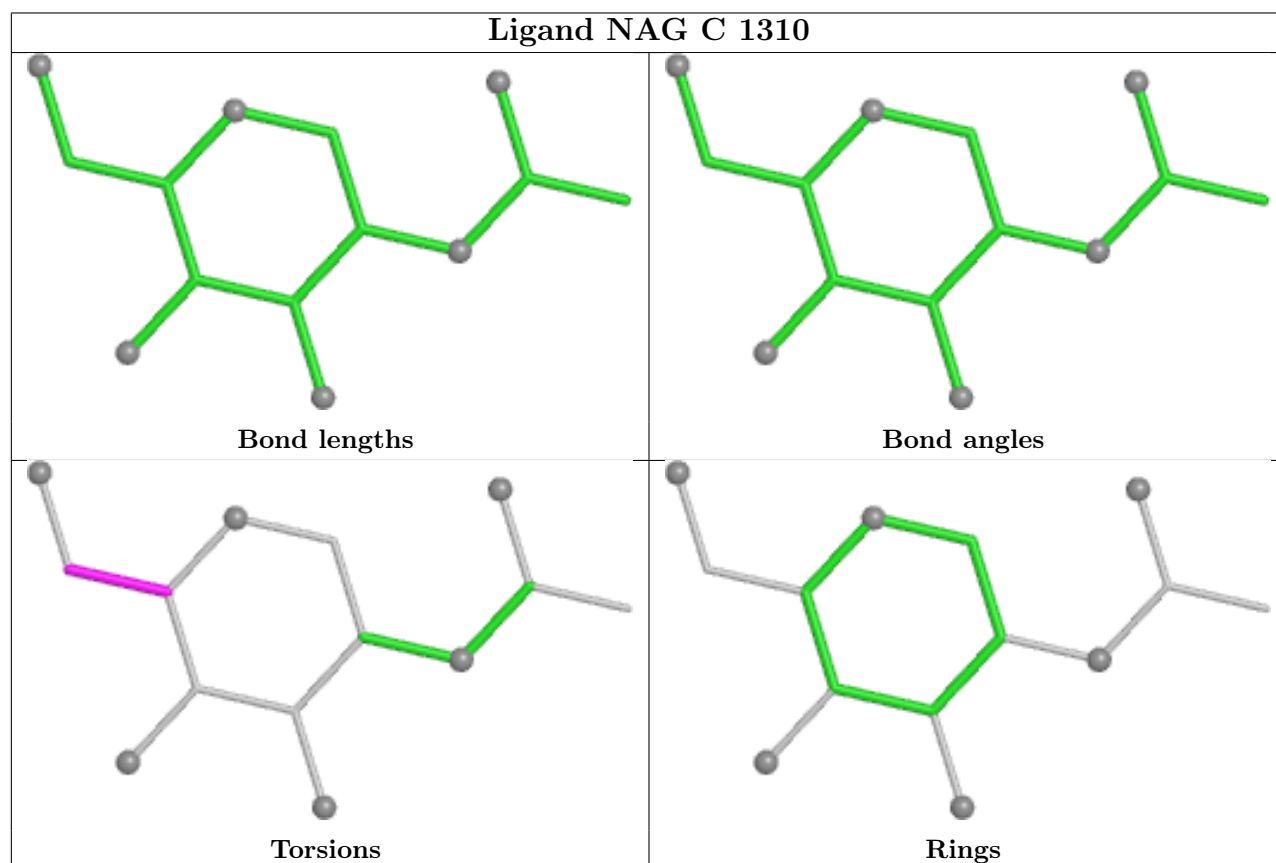
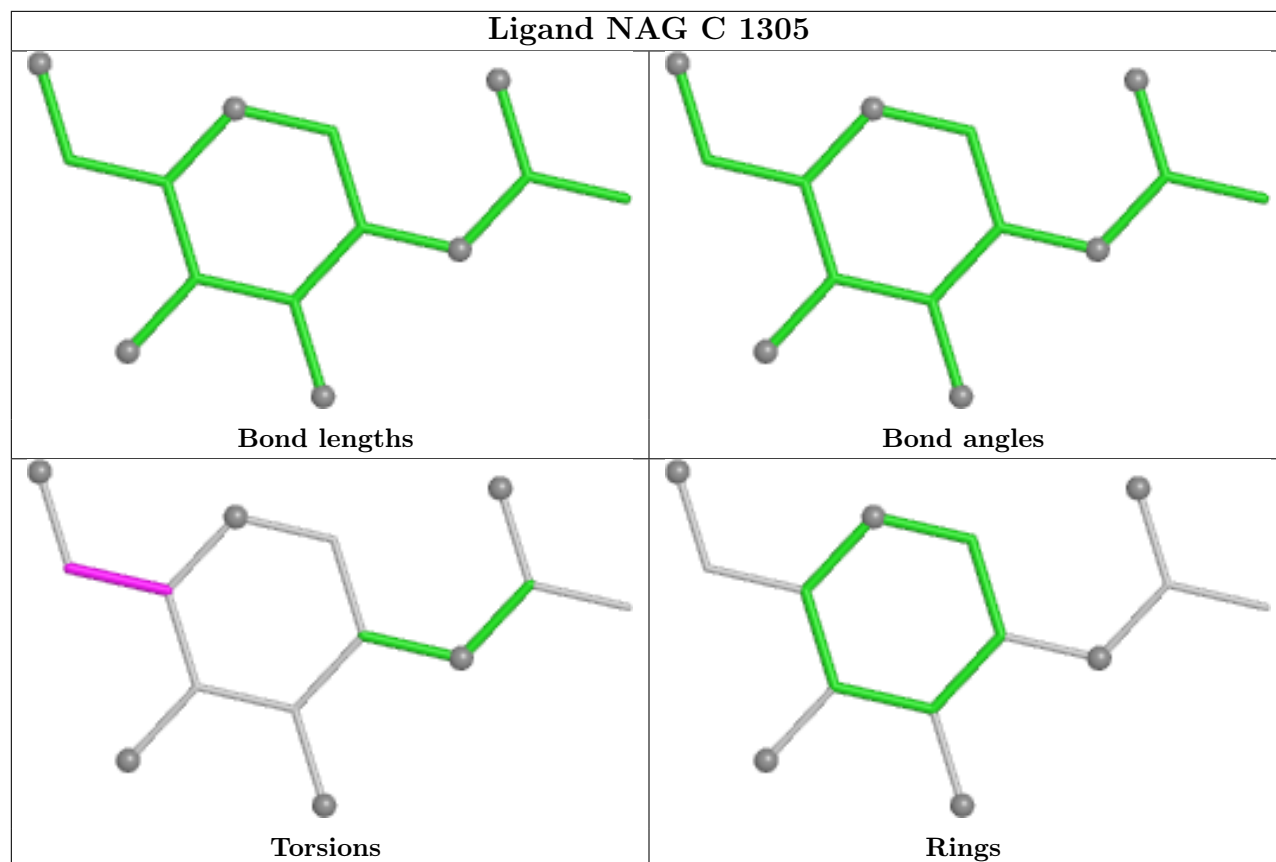


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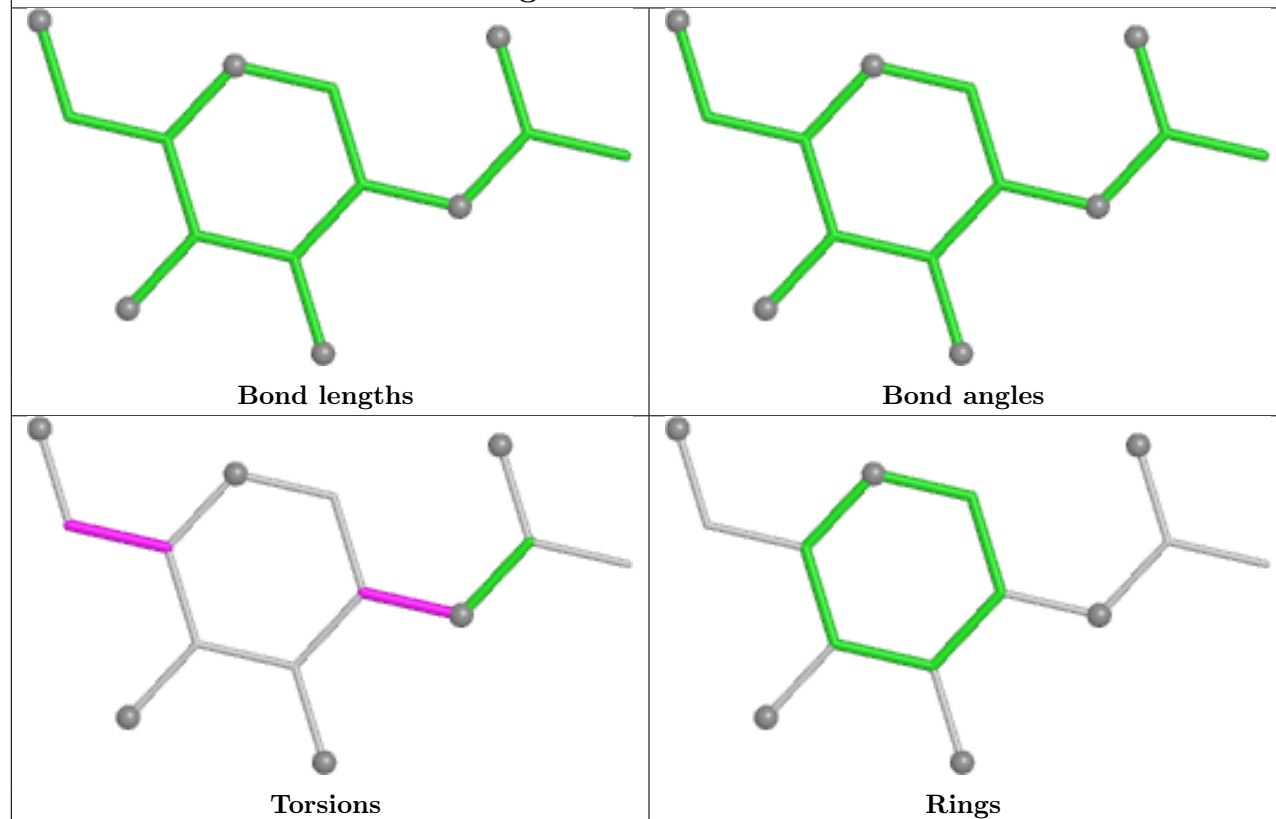


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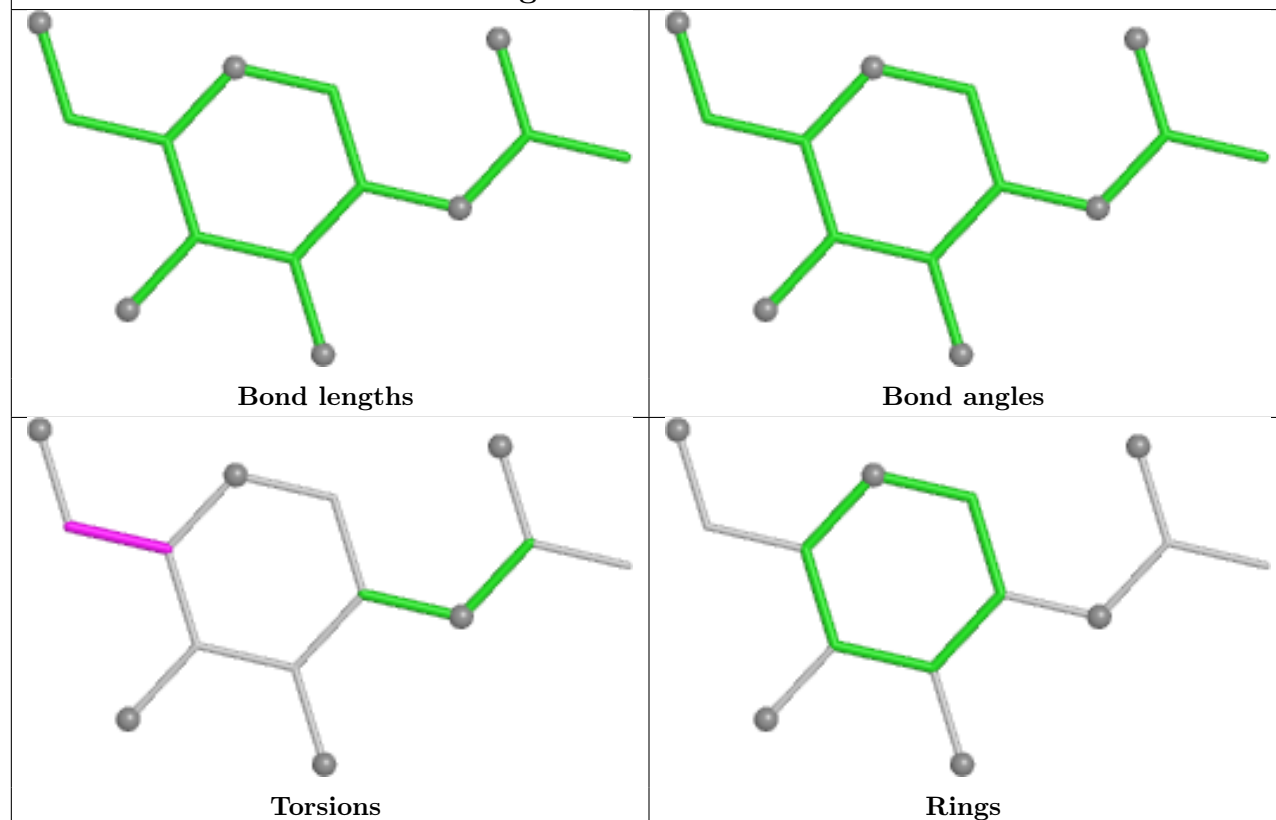




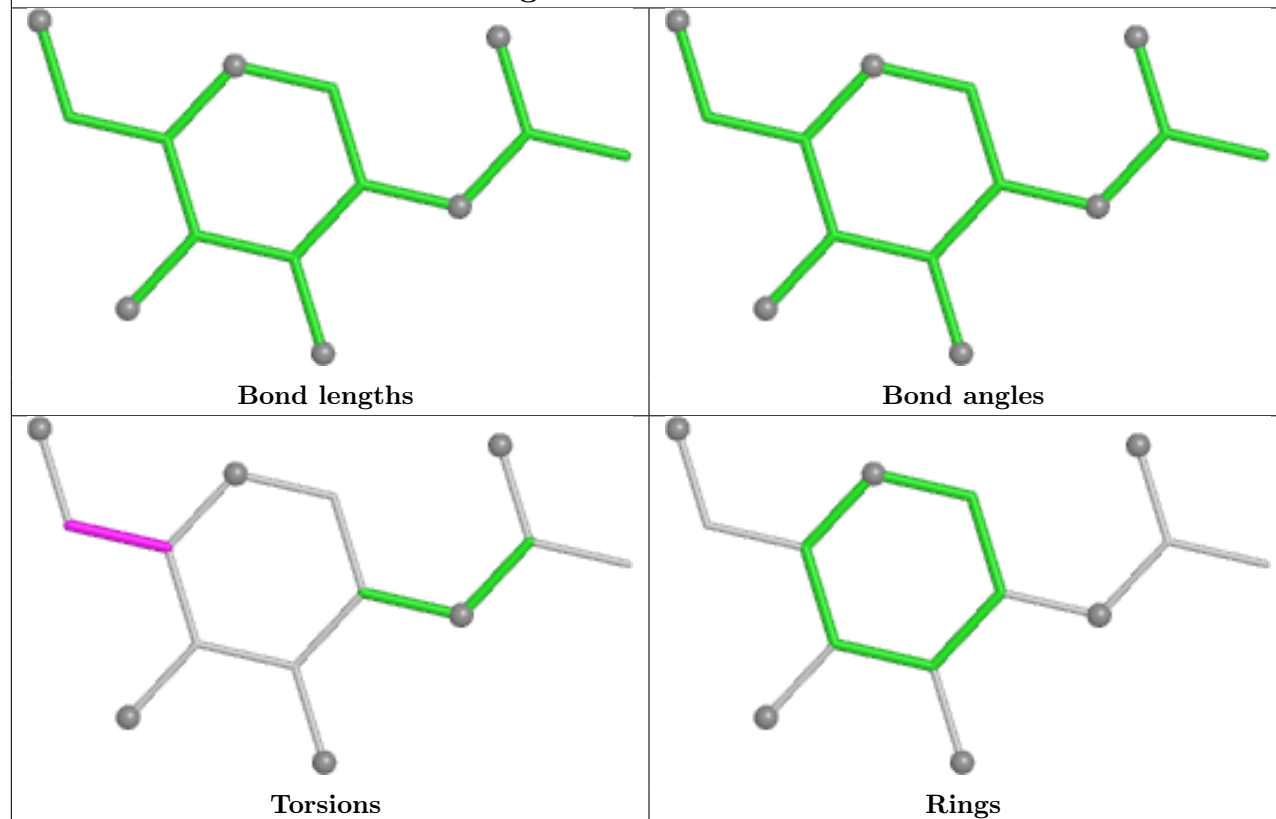
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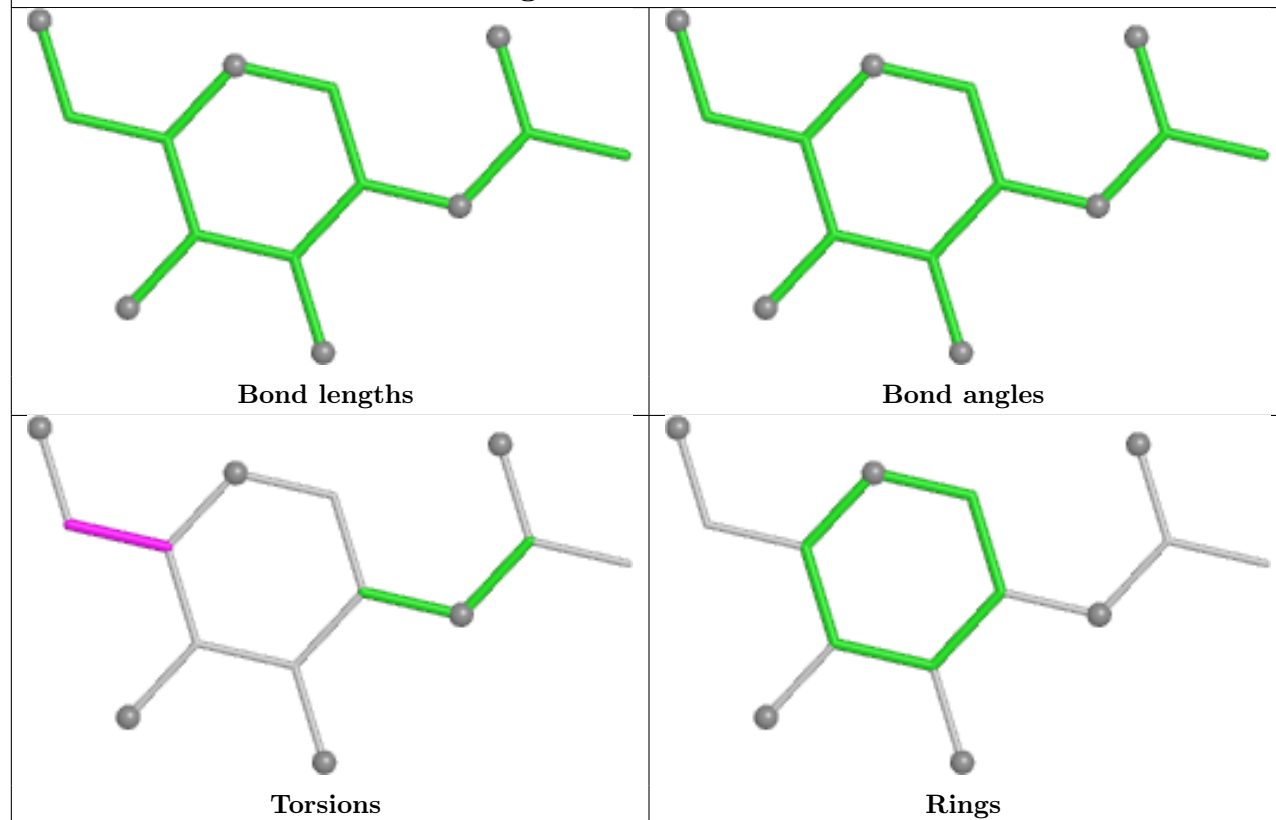
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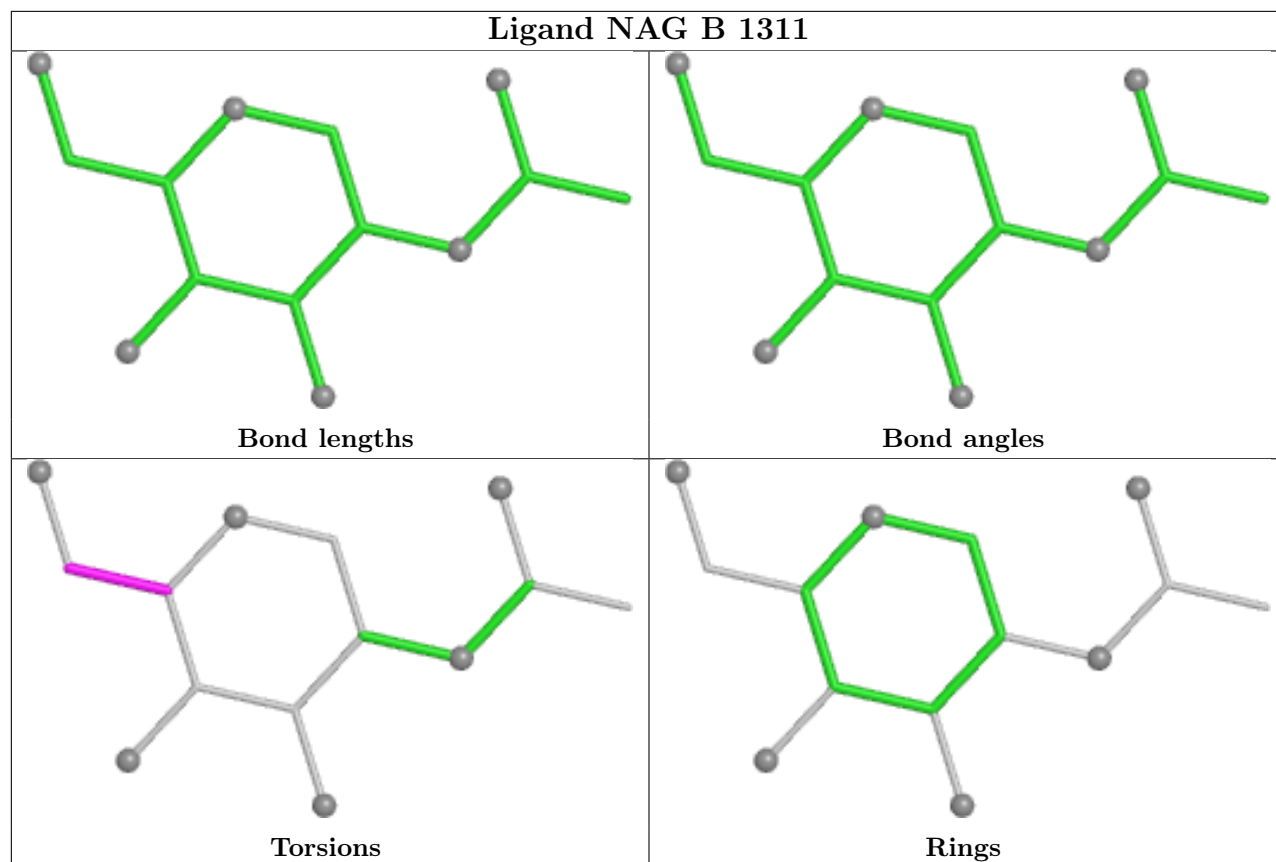
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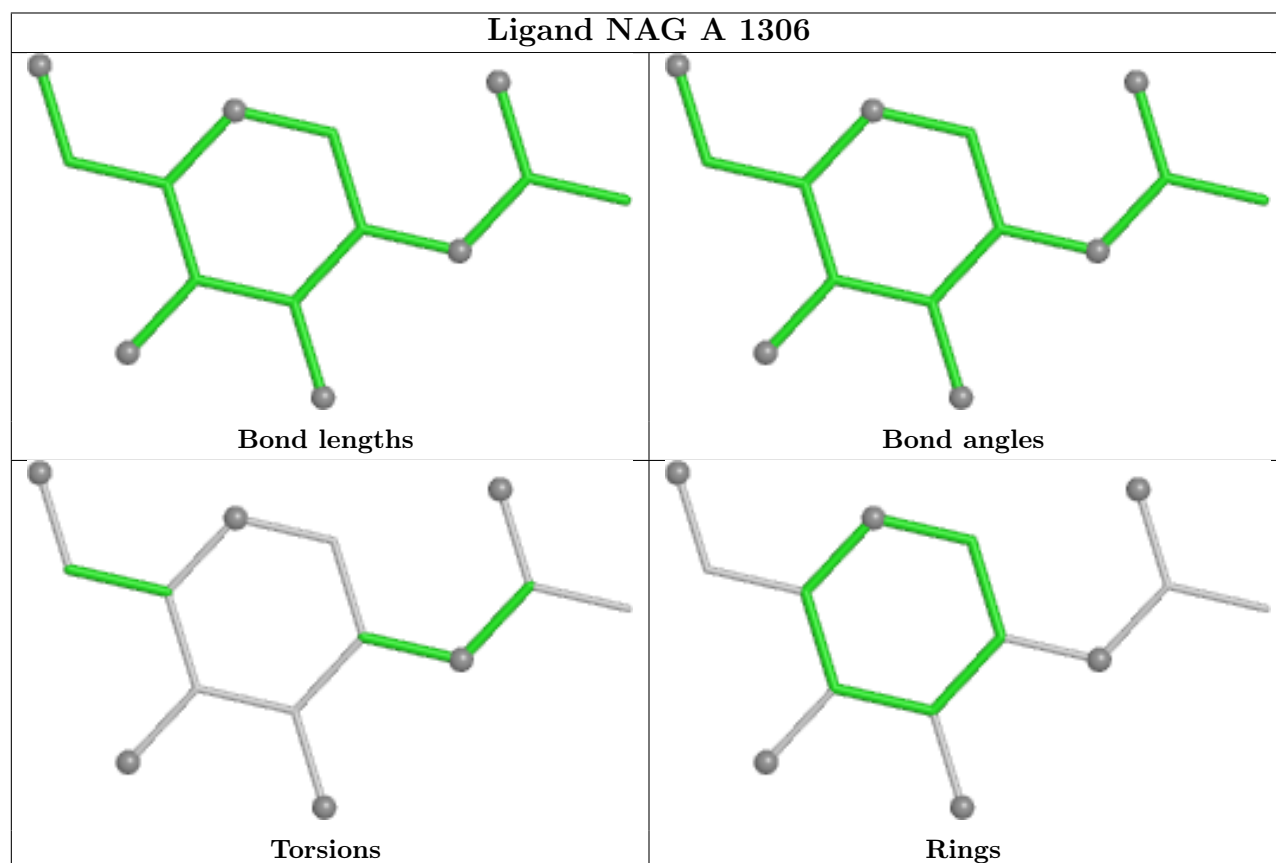
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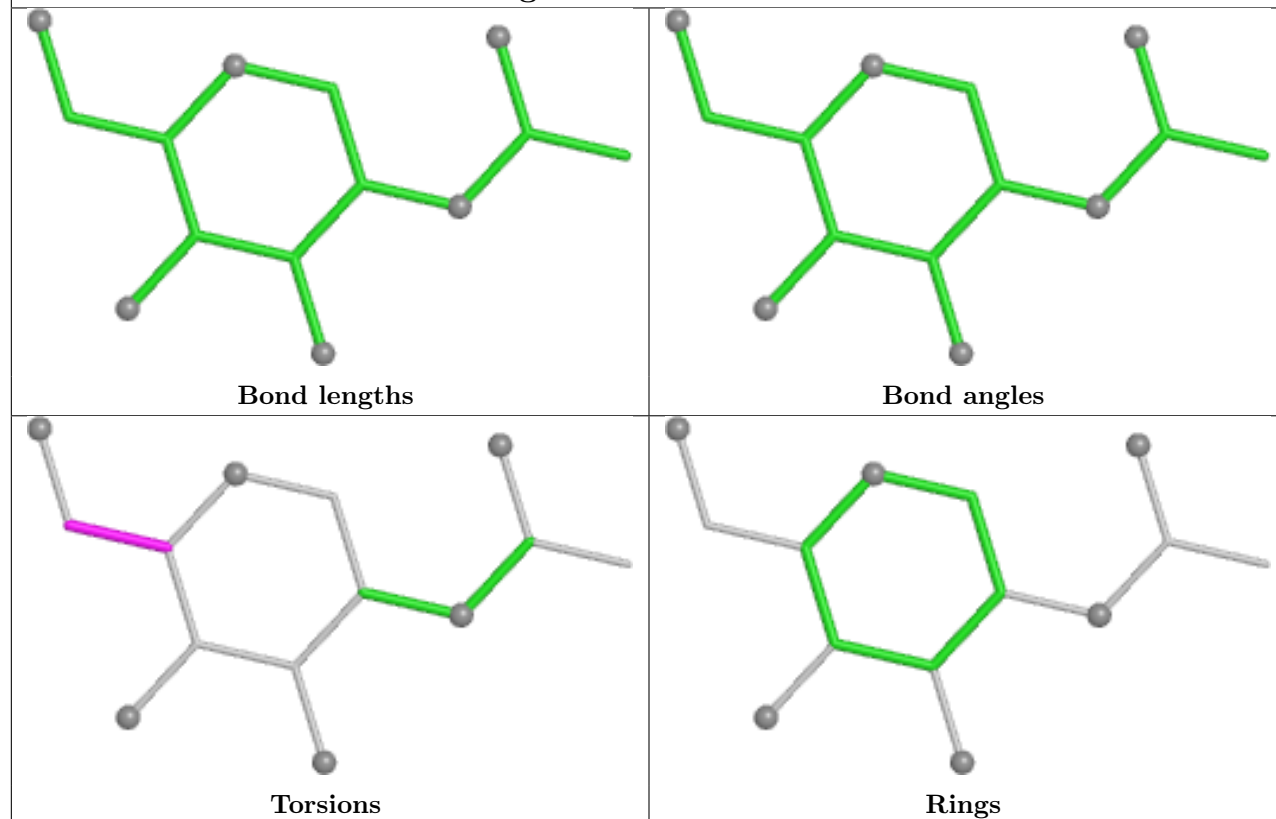
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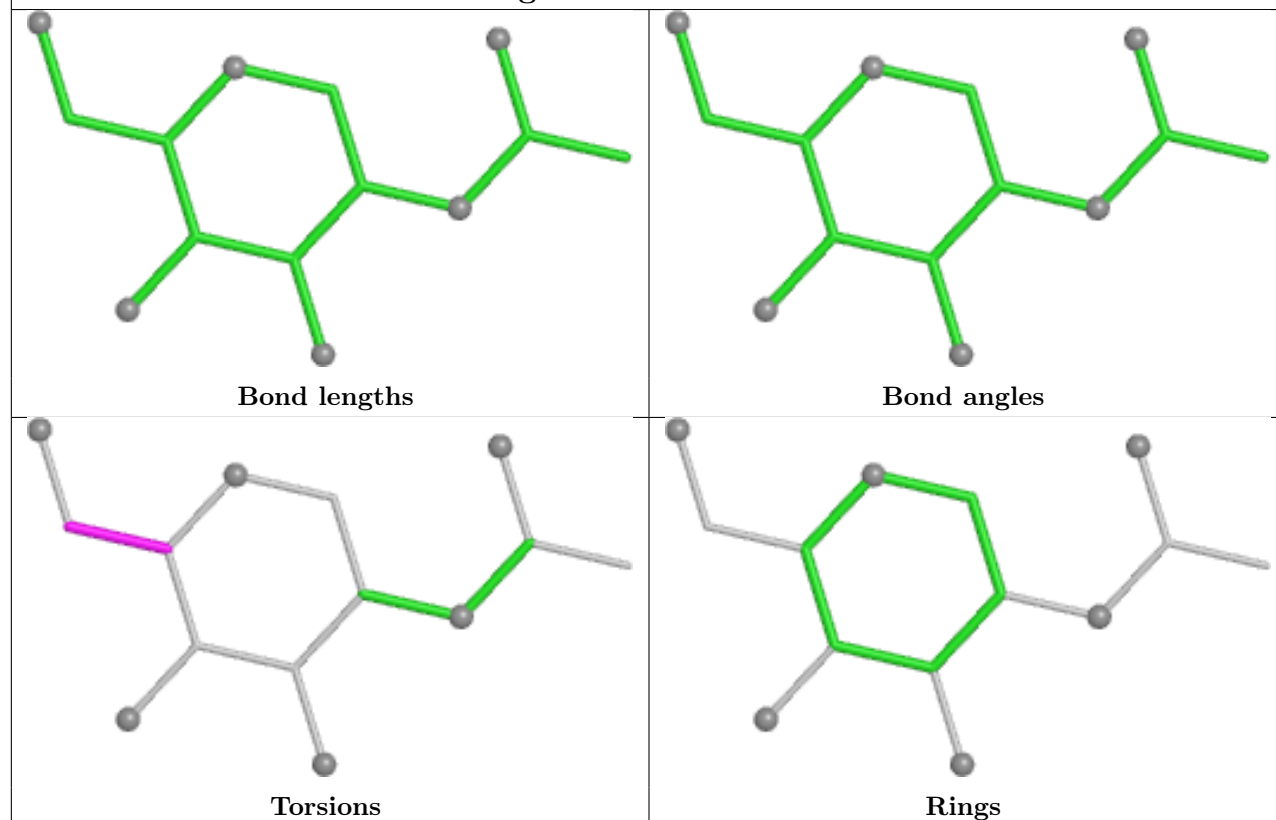
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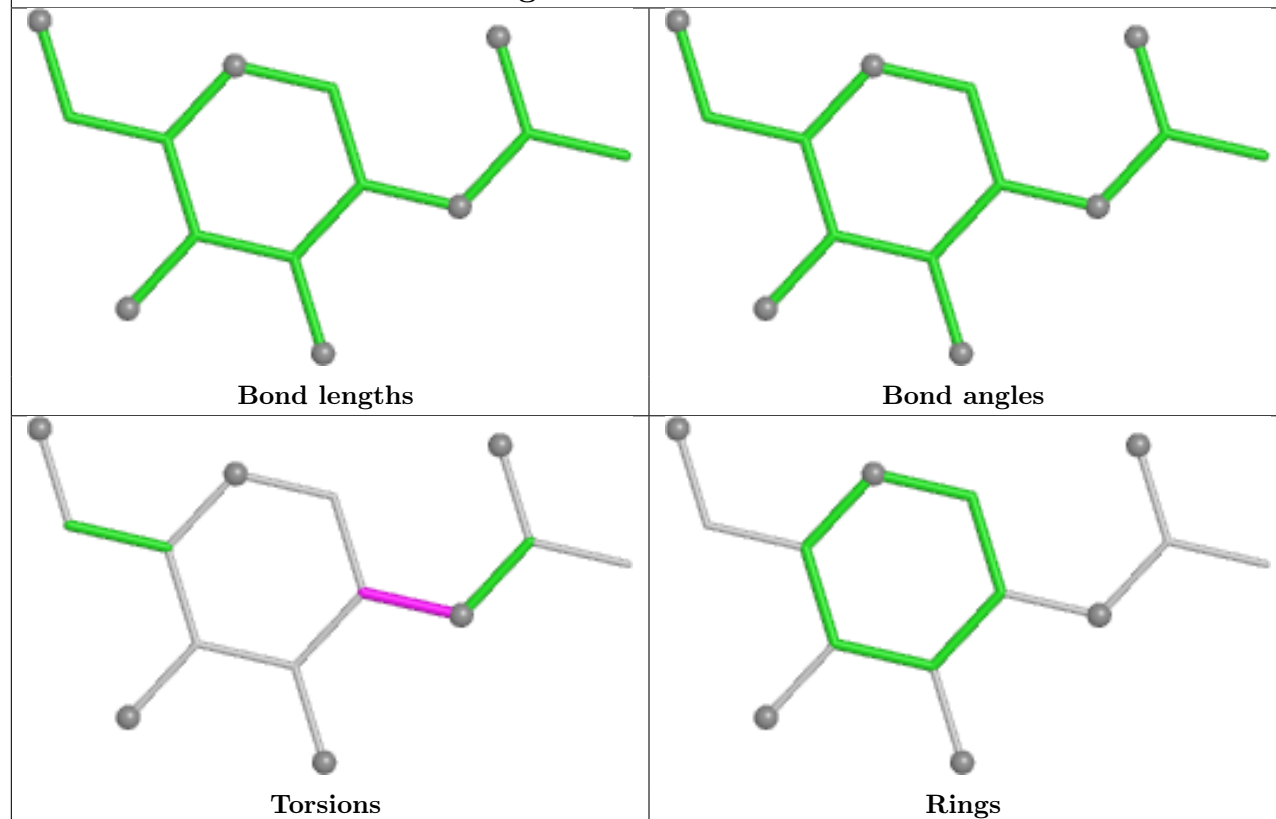
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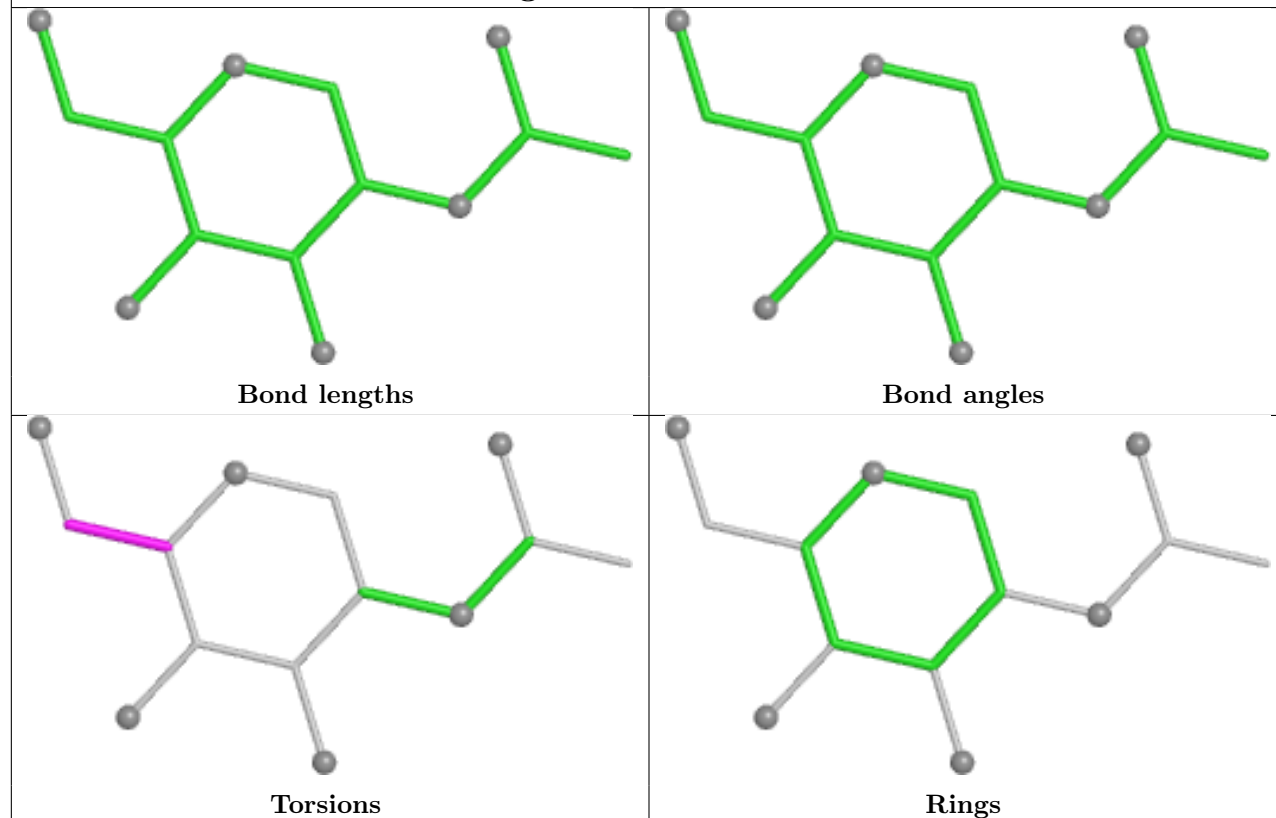
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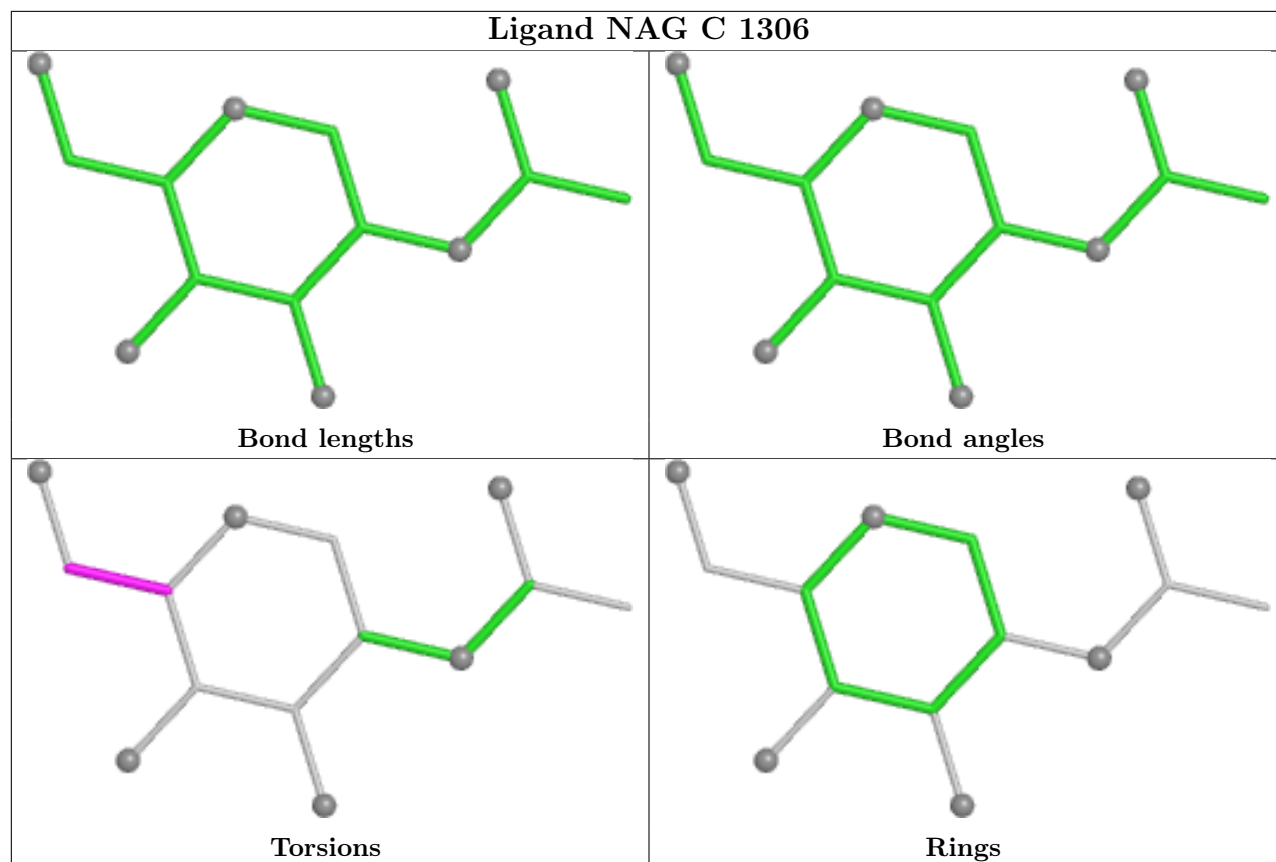
Ligand NAG A 1304



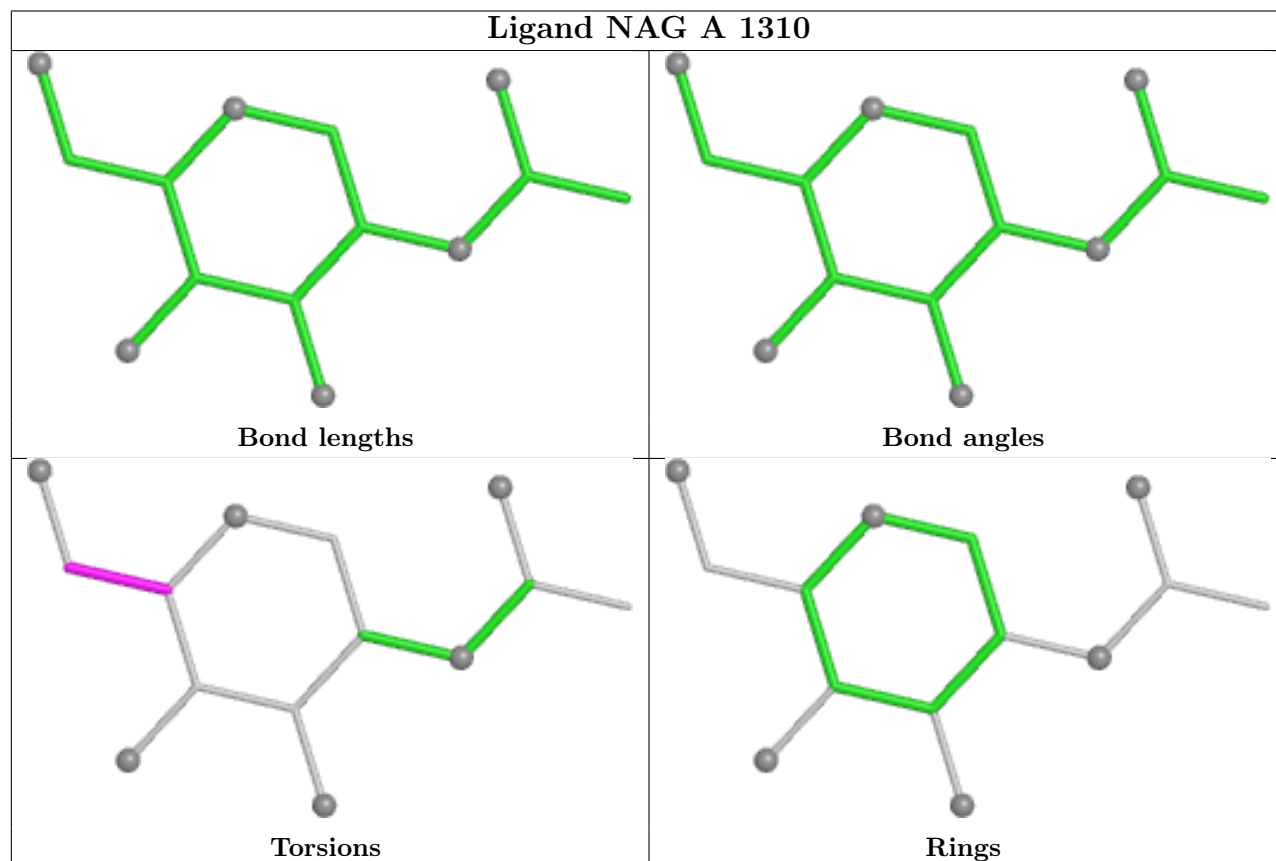
Ligand NAG C 1311

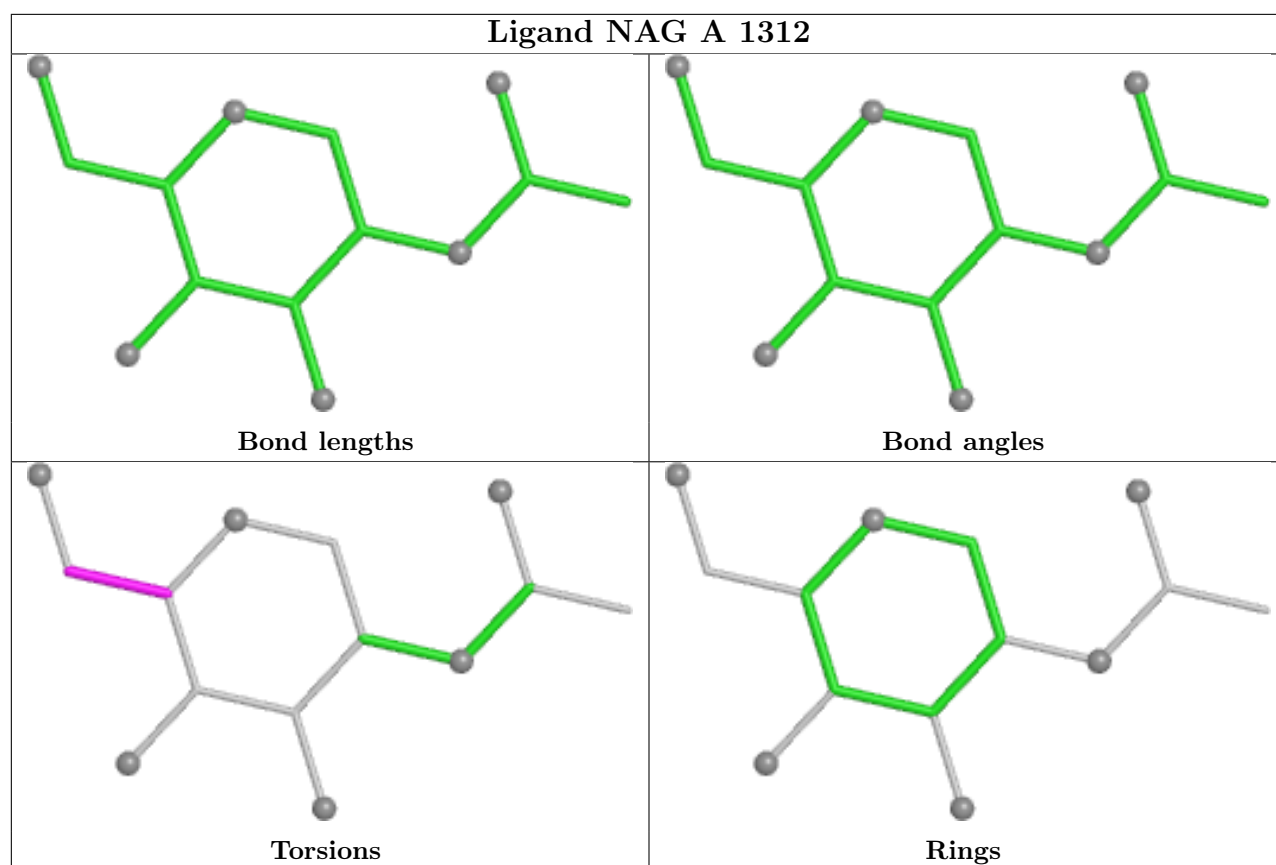


Ligand NAG C 1306



Ligand NAG A 1310





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.

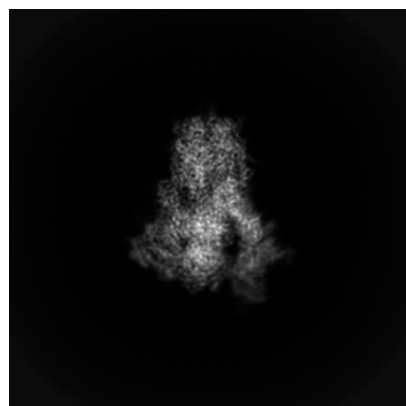
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63757. These allow visual inspection of the internal detail of the map and identification of artifacts.

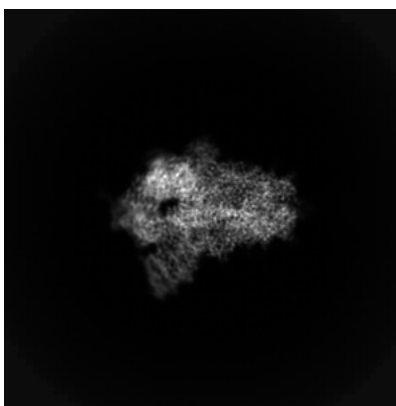
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

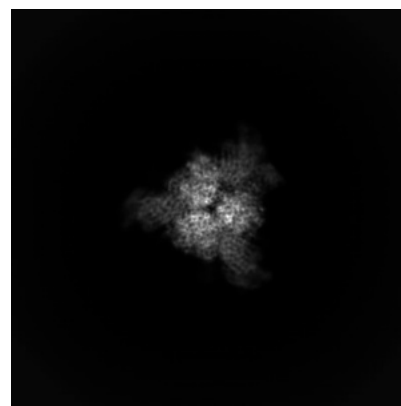
6.1.1 Primary map



X

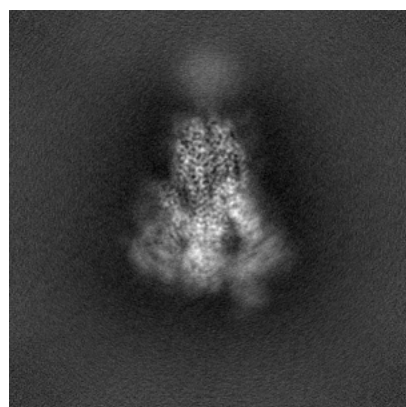


Y

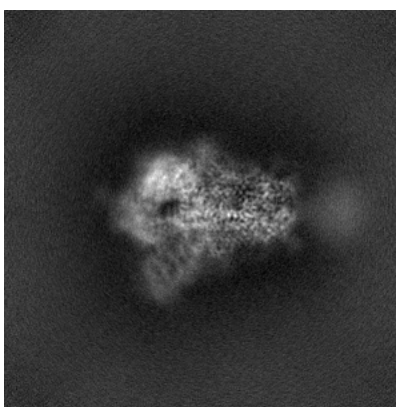


Z

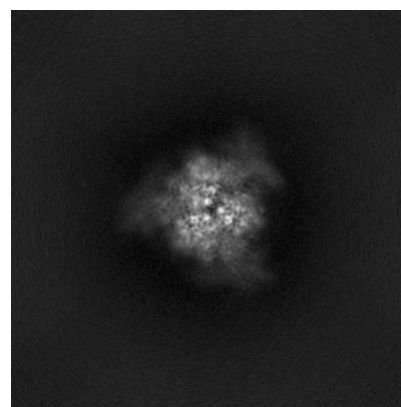
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

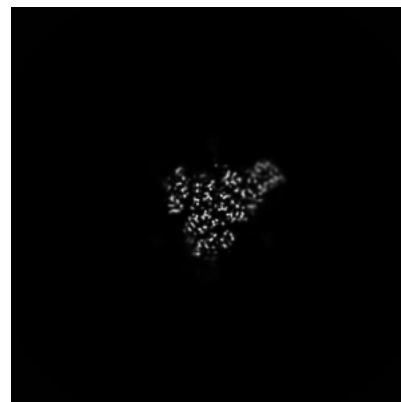
6.2.1 Primary map



X Index: 180

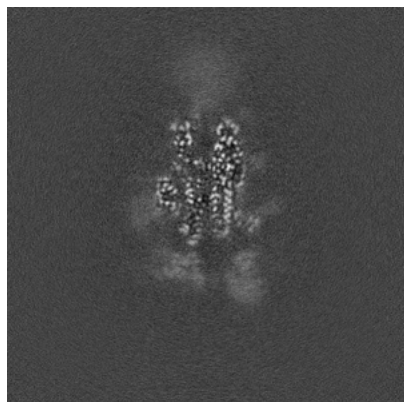


Y Index: 180

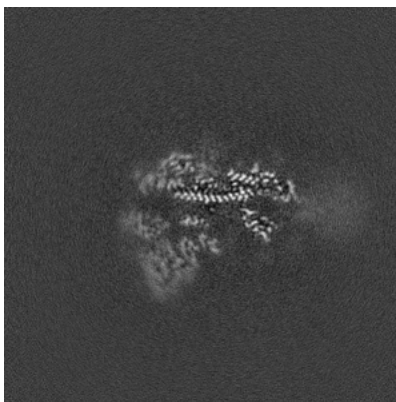


Z Index: 180

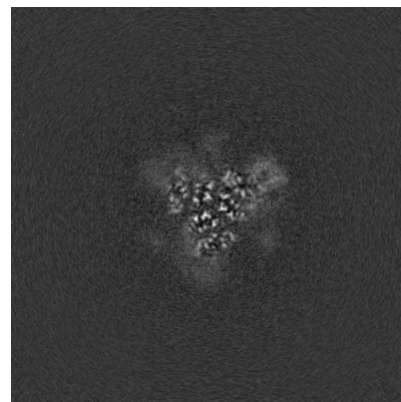
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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

6.3 Largest variance slices [i](#)

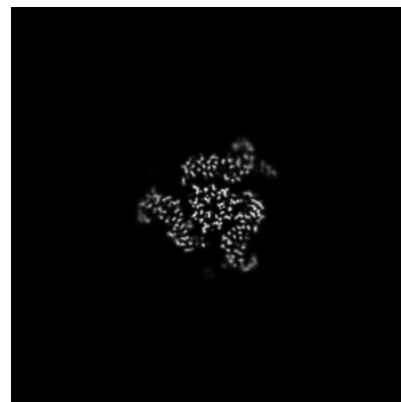
6.3.1 Primary map



X Index: 175

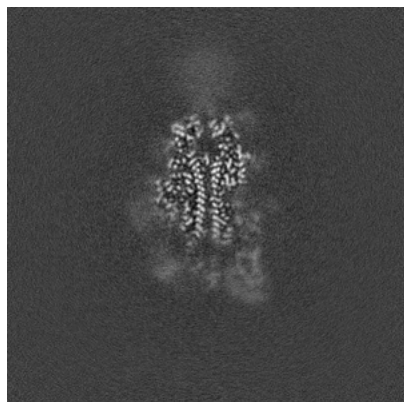


Y Index: 173

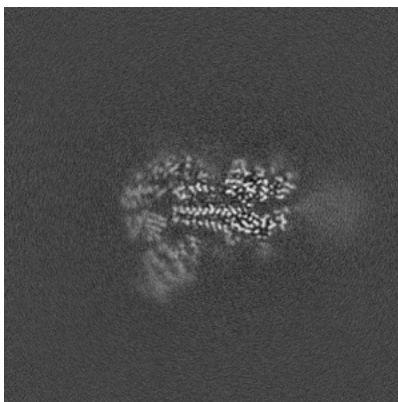


Z Index: 165

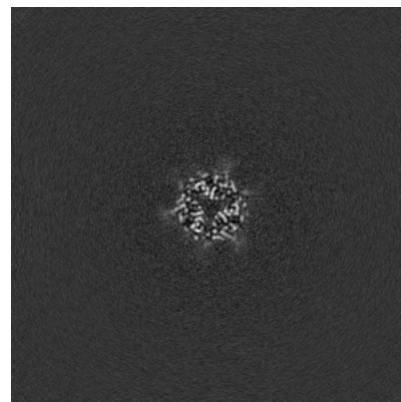
6.3.2 Raw map



X Index: 175



Y Index: 173

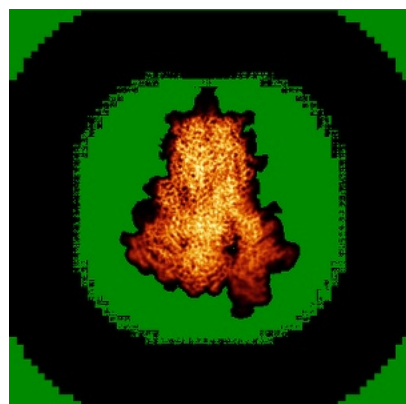


Z Index: 234

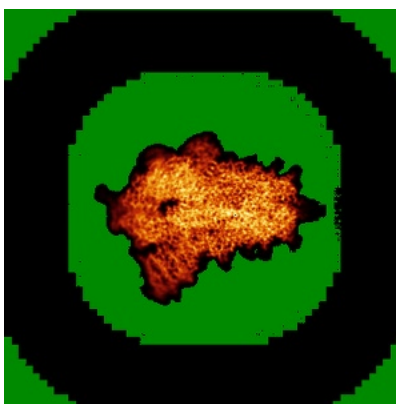
The images above show the largest variance slices of the map in three orthogonal directions.

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

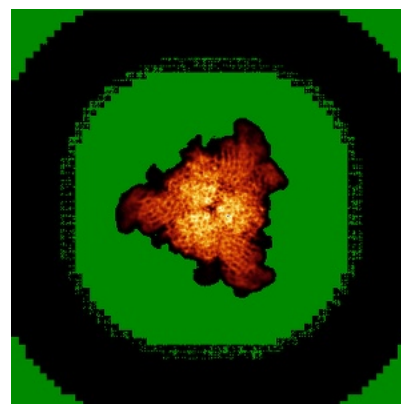
6.4.1 Primary map



X

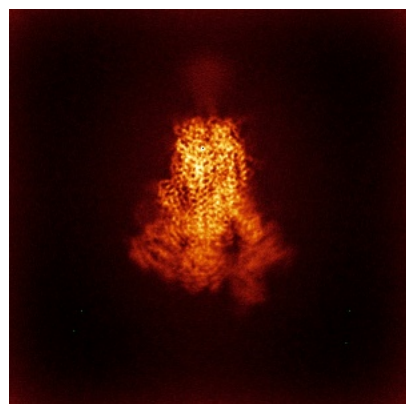


Y

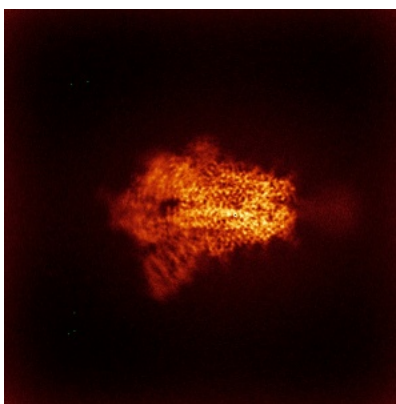


Z

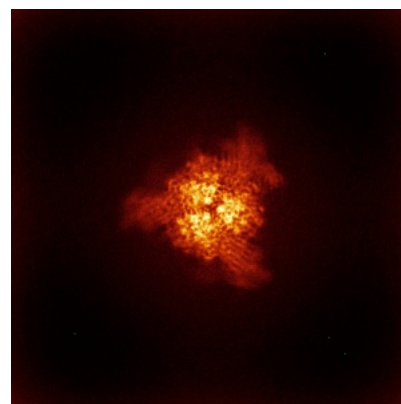
6.4.2 Raw map



X



Y



Z

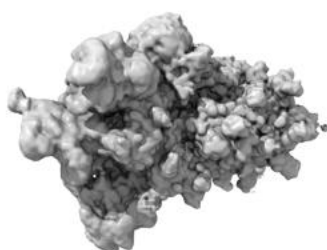
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

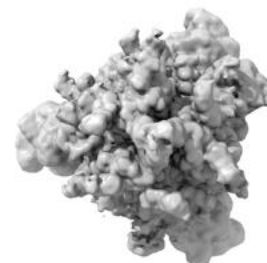
6.5.1 Primary map



X



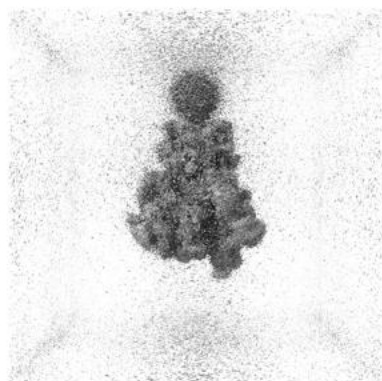
Y



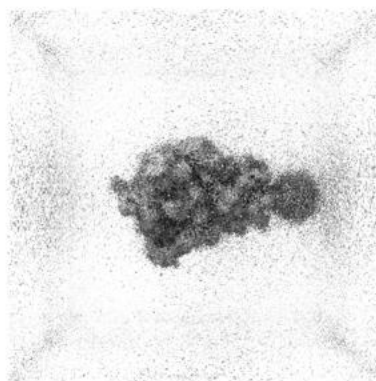
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

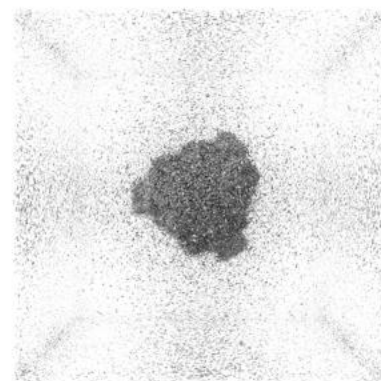
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

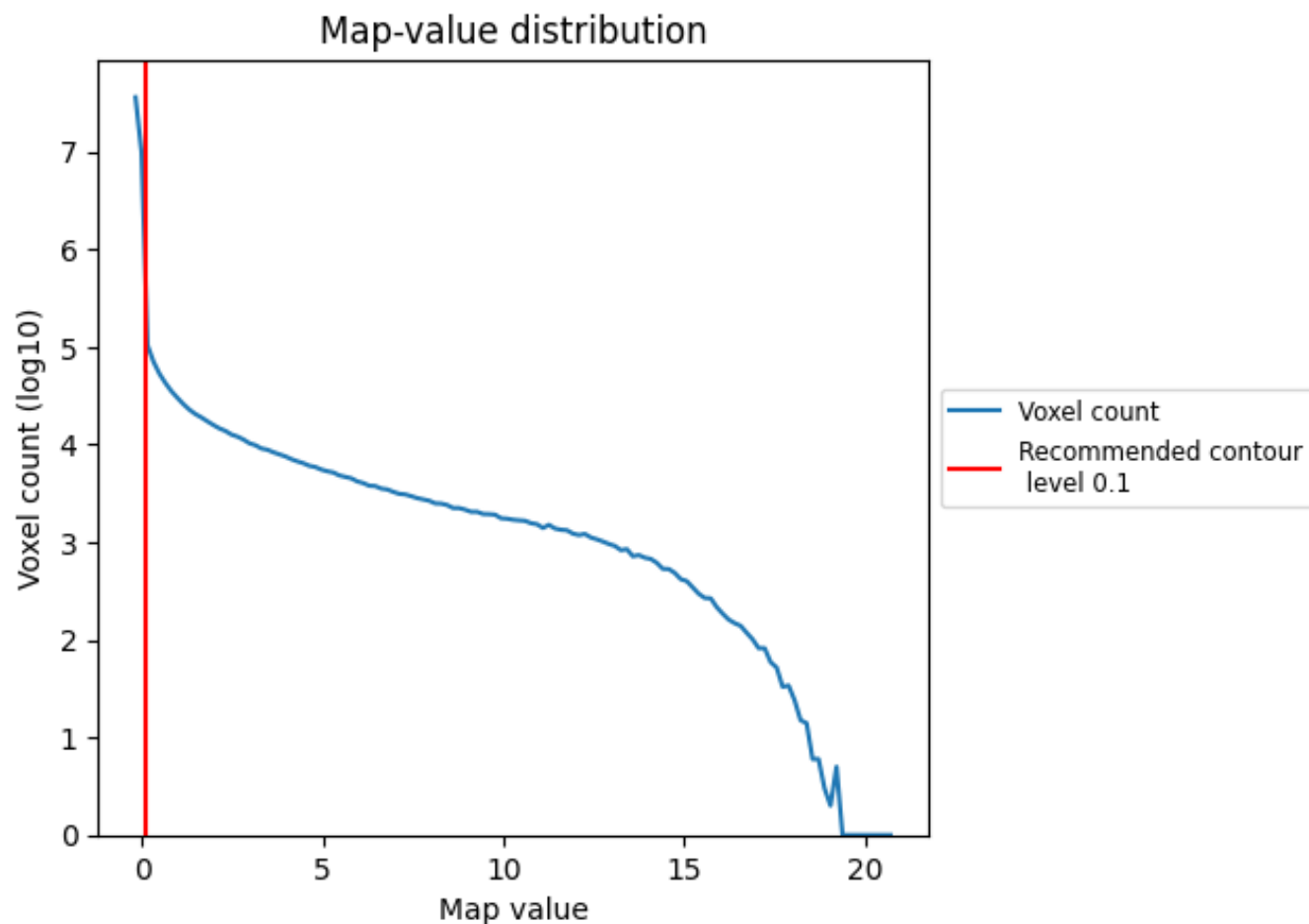
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

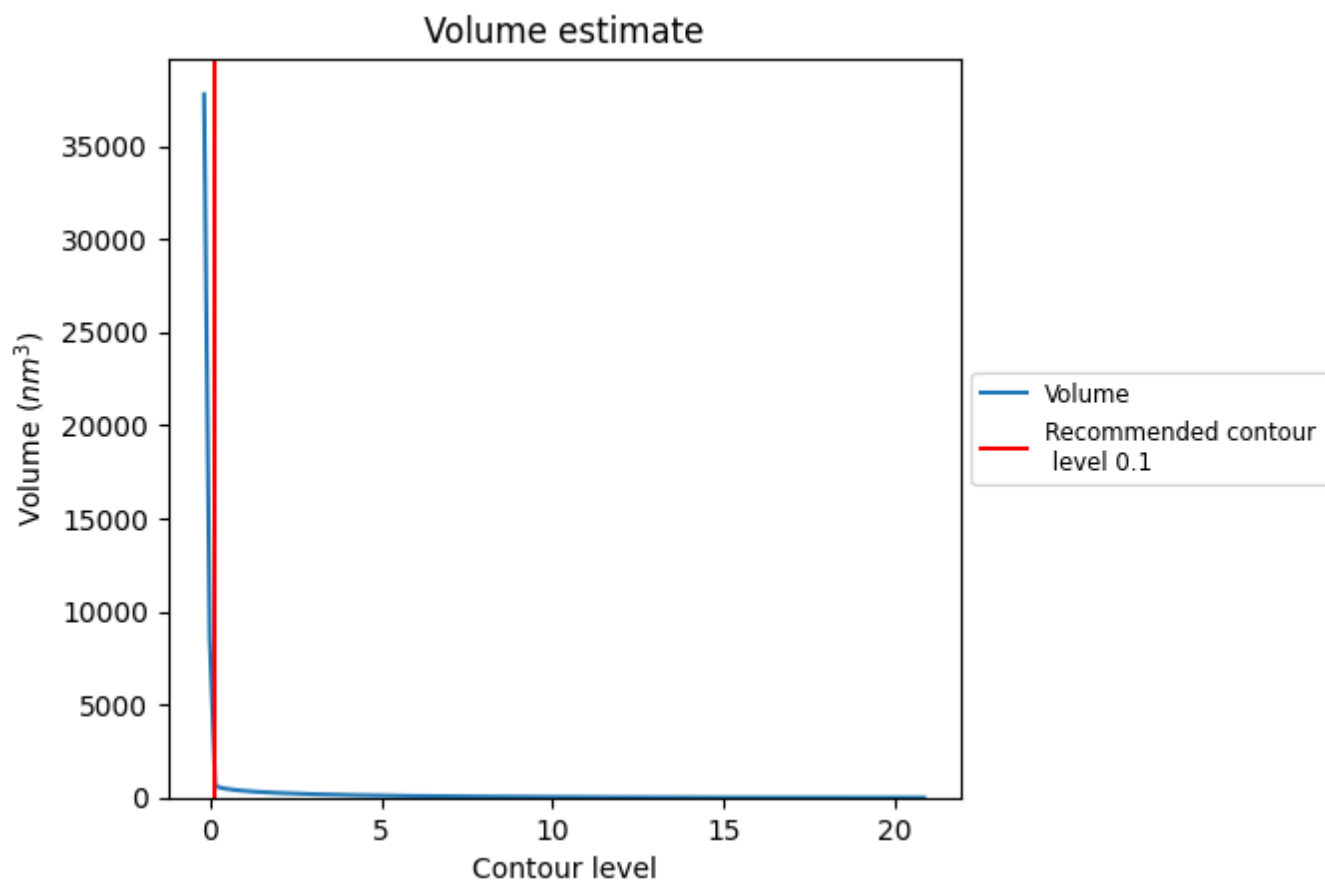
This section contains the results of statistical analysis of the map.

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.

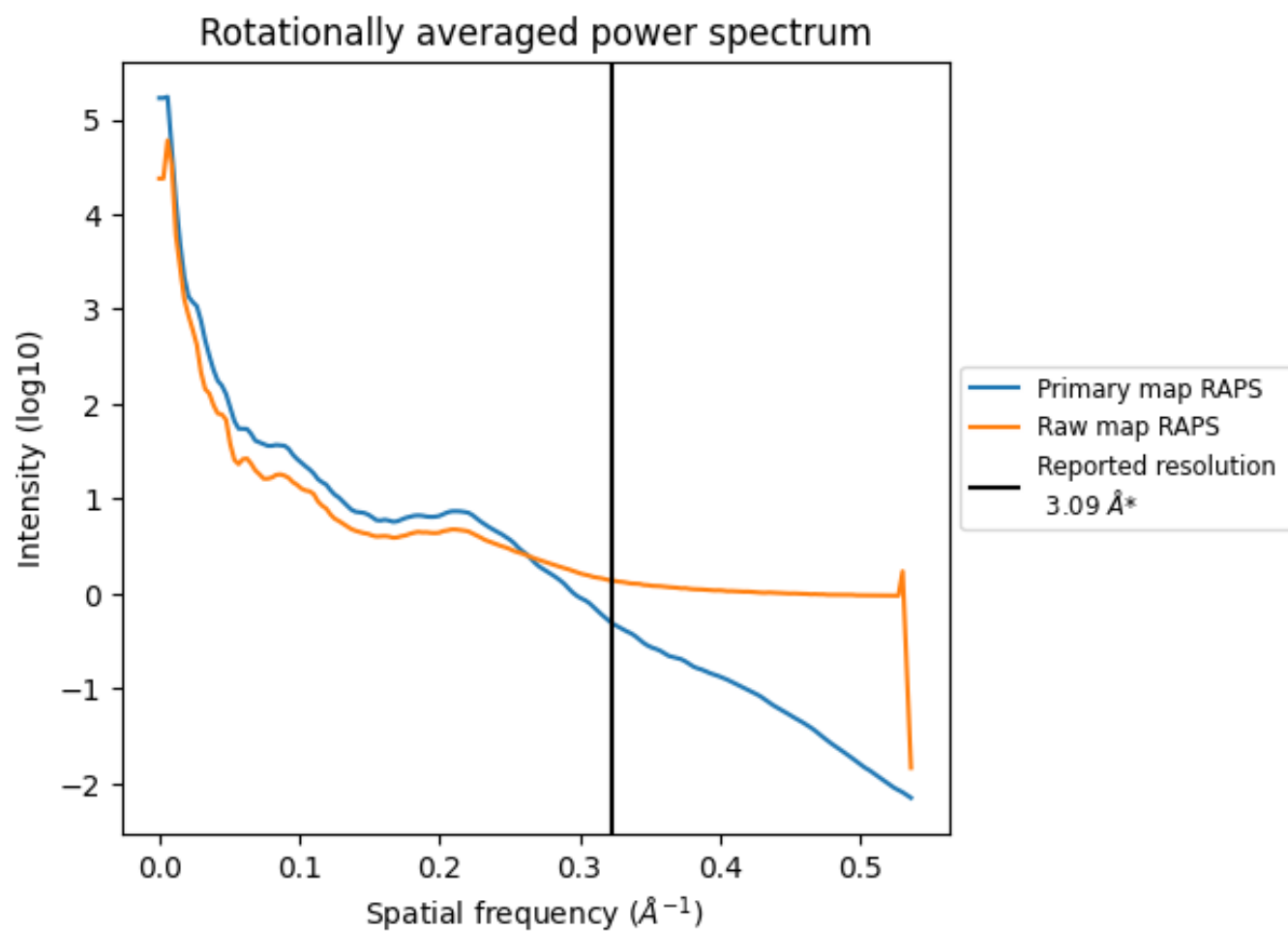
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2794 nm^3 ; this corresponds to an approximate mass of 2524 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 [i](#)

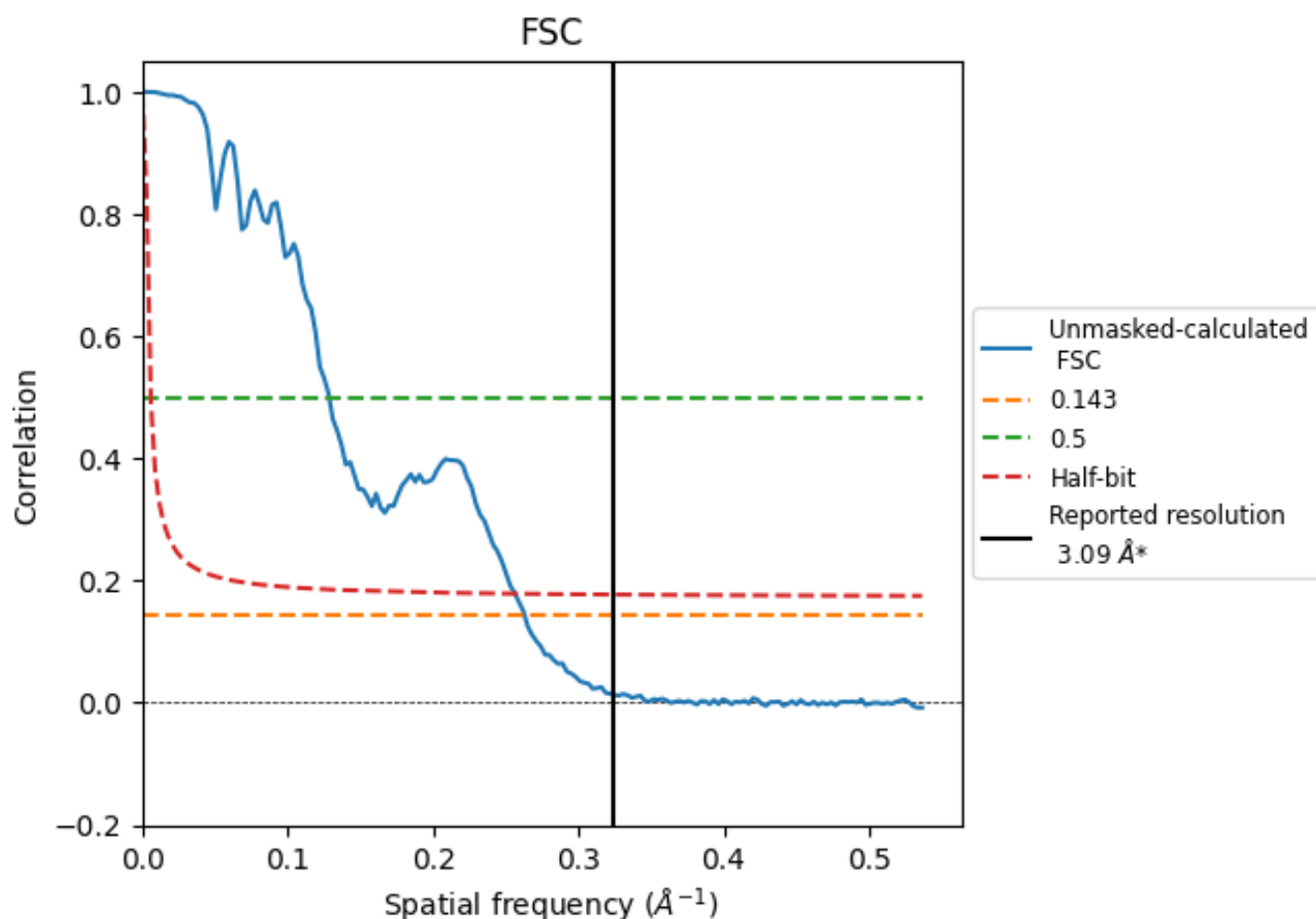


*Reported resolution corresponds to spatial frequency of $0.324 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

8.2 Resolution estimates [i](#)

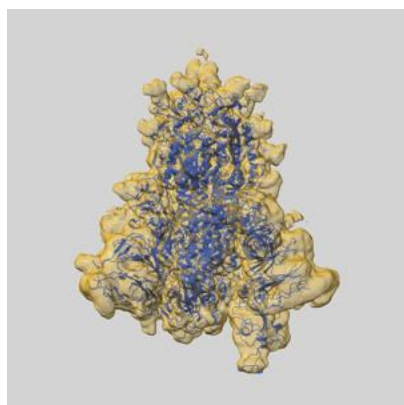
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	7.78	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.09 by more than 10 %

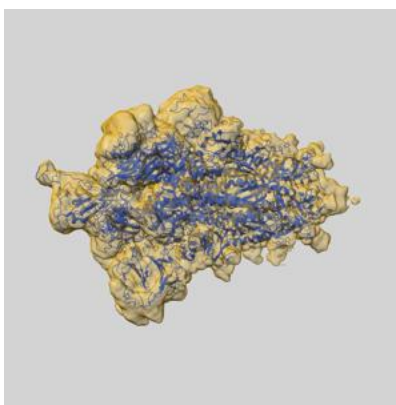
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63757 and PDB model 9MAO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

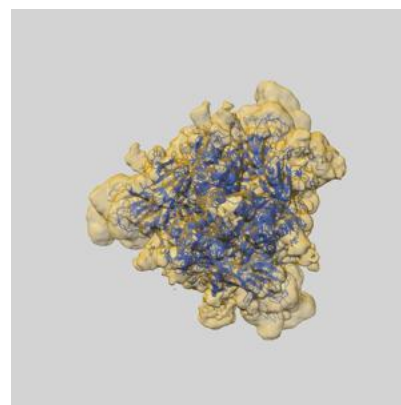
9.1 Map-model overlay [i](#)



X



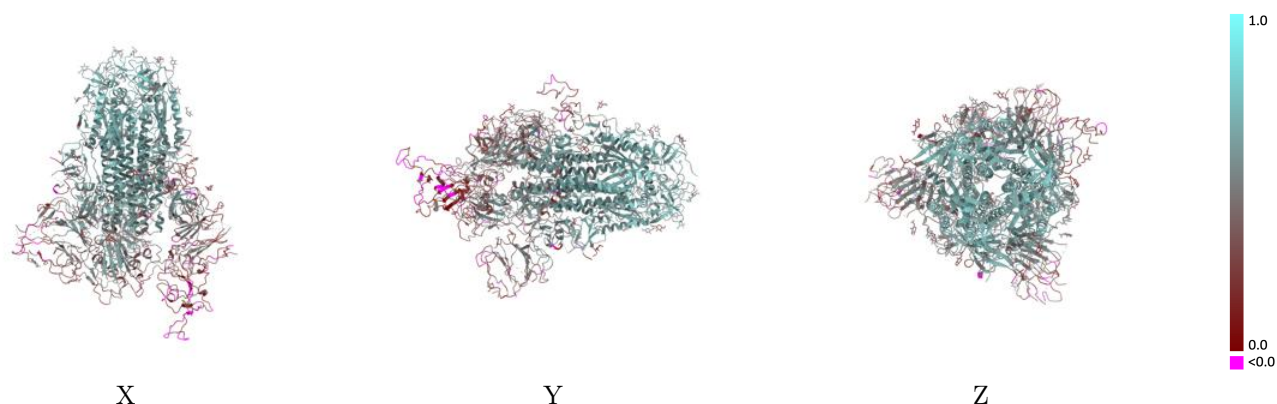
Y



Z

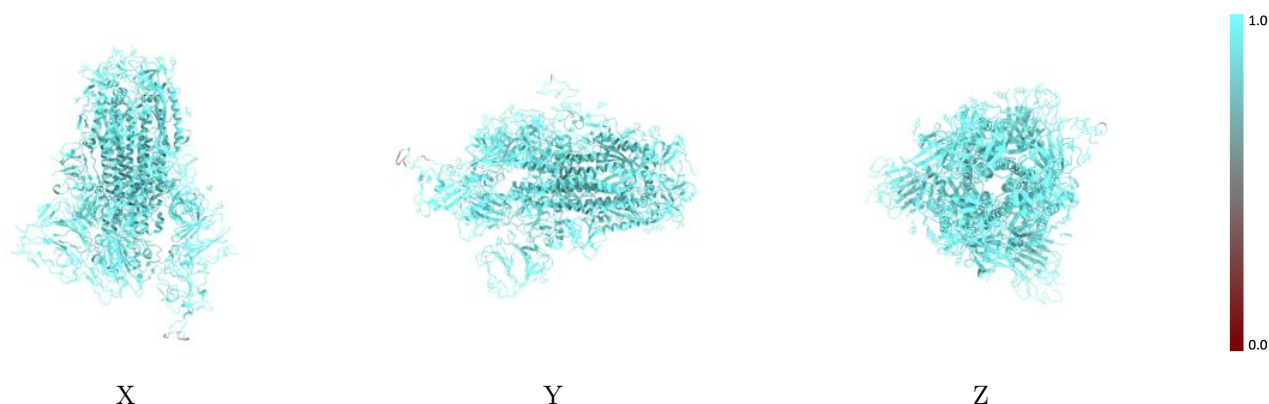
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



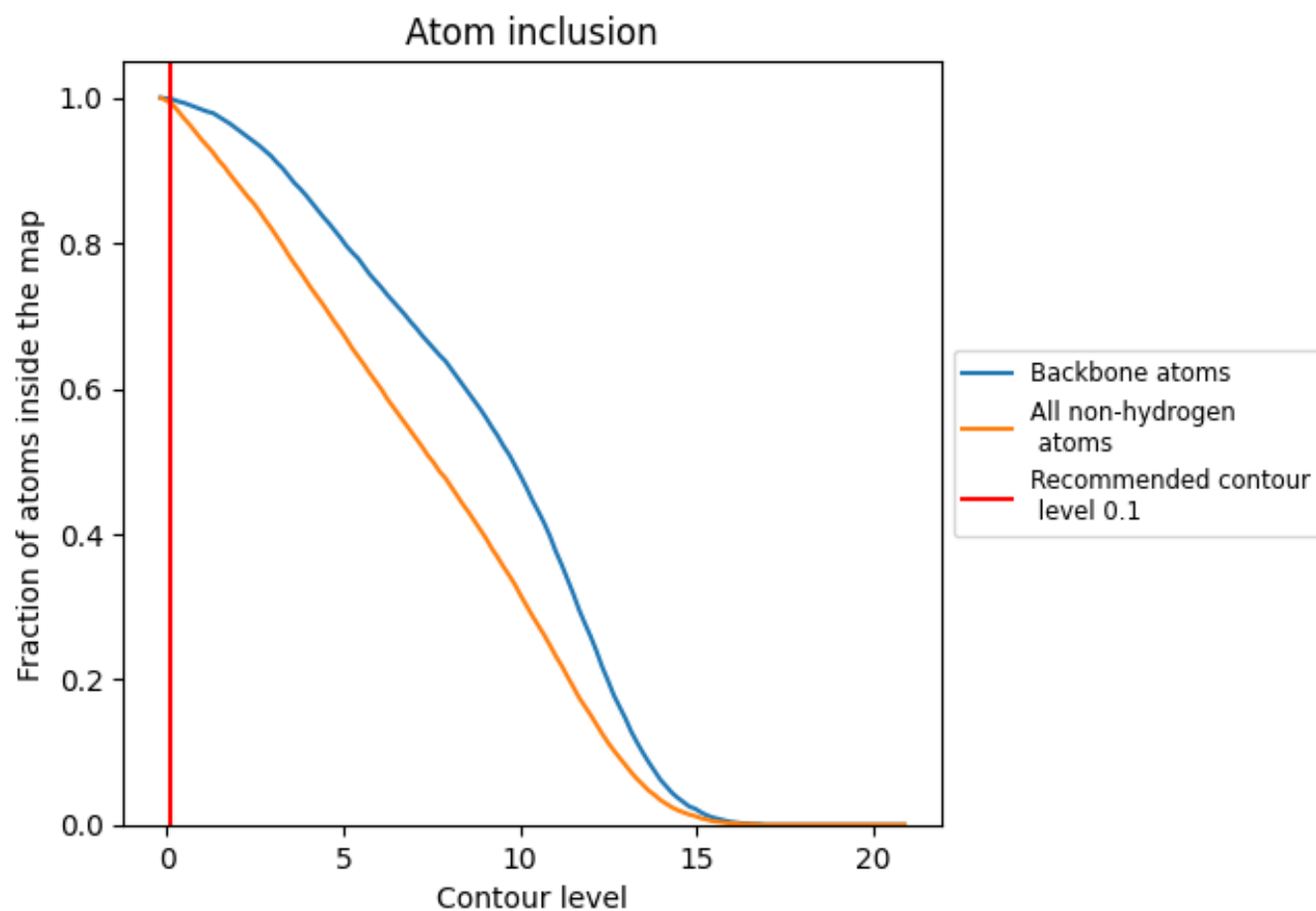
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.4740
A	0.9970	0.4890
B	0.9960	0.4890
C	0.9870	0.4490
D	0.9730	0.2010

