



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:28 PM UTC

PDB ID : 7CYC / pdb_00007cyc
EMDB ID : EMD-30496
Title : Cryo-EM structures of Alphacoronavirus spike glycoprotein
Authors : Song, X.; Shi, Y.; Ding, W.; Liu, Z.J.; Peng, G.
Deposited on : 2020-09-03
Resolution : 3.21 Å(reported)
Based on initial model : 5SZS

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:

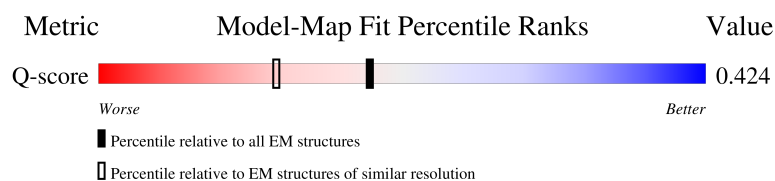
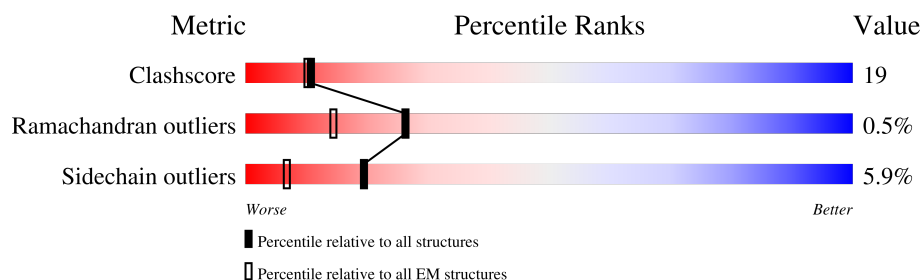
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	14613 (2.71 - 3.71)

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	1116	
1	B	1116	
1	C	1116	
2	D	7	

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Mol	Chain	Length	Quality of chain
2	H	7	
2	L	7	
3	E	3	
3	G	3	
3	I	3	
3	K	3	
3	M	3	
3	O	3	
4	F	2	
4	J	2	
4	N	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1201	-	-	X	-
5	NAG	B	1201	-	-	X	-
5	NAG	C	1201	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22521 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.

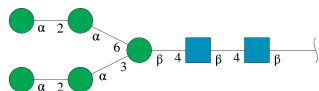
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		
1	B	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		
1	C	959	Total	C	N	O	S	0	0
			7094	4483	1225	1349	37		

There are 24 discrepancies between the modelled and reference sequences:

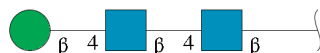
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	MET	ARG	variant	UNP P15423
A	681	ARG	THR	variant	UNP P15423
A	765	ALA	VAL	variant	UNP P15423
A	775	SER	ALA	variant	UNP P15423
A	871	ILE	THR	variant	UNP P15423
A	937	LEU	ILE	variant	UNP P15423
A	971	ARG	THR	variant	UNP P15423
A	1005	ILE	MET	variant	UNP P15423
B	642	MET	ARG	variant	UNP P15423
B	681	ARG	THR	variant	UNP P15423
B	765	ALA	VAL	variant	UNP P15423
B	775	SER	ALA	variant	UNP P15423
B	871	ILE	THR	variant	UNP P15423
B	937	LEU	ILE	variant	UNP P15423
B	971	ARG	THR	variant	UNP P15423
B	1005	ILE	MET	variant	UNP P15423
C	642	MET	ARG	variant	UNP P15423
C	681	ARG	THR	variant	UNP P15423
C	765	ALA	VAL	variant	UNP P15423
C	775	SER	ALA	variant	UNP P15423
C	871	ILE	THR	variant	UNP P15423
C	937	LEU	ILE	variant	UNP P15423
C	971	ARG	THR	variant	UNP P15423
C	1005	ILE	MET	variant	UNP P15423

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	7	Total	C	N	O	0	0
			83	46	2	35		
2	H	7	Total	C	N	O	0	0
			83	46	2	35		
2	L	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



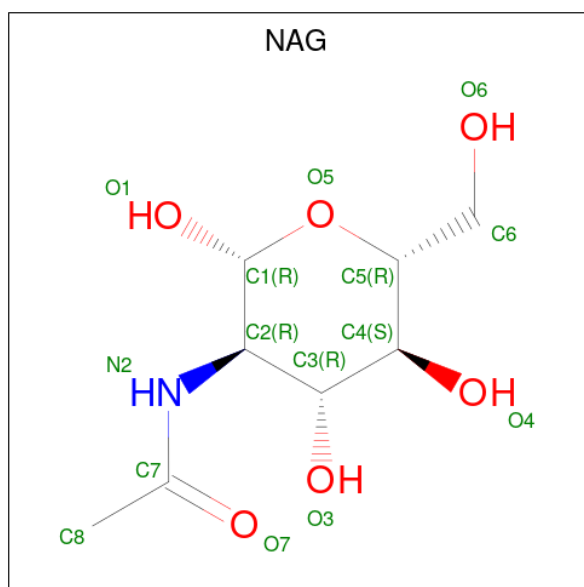
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		

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

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

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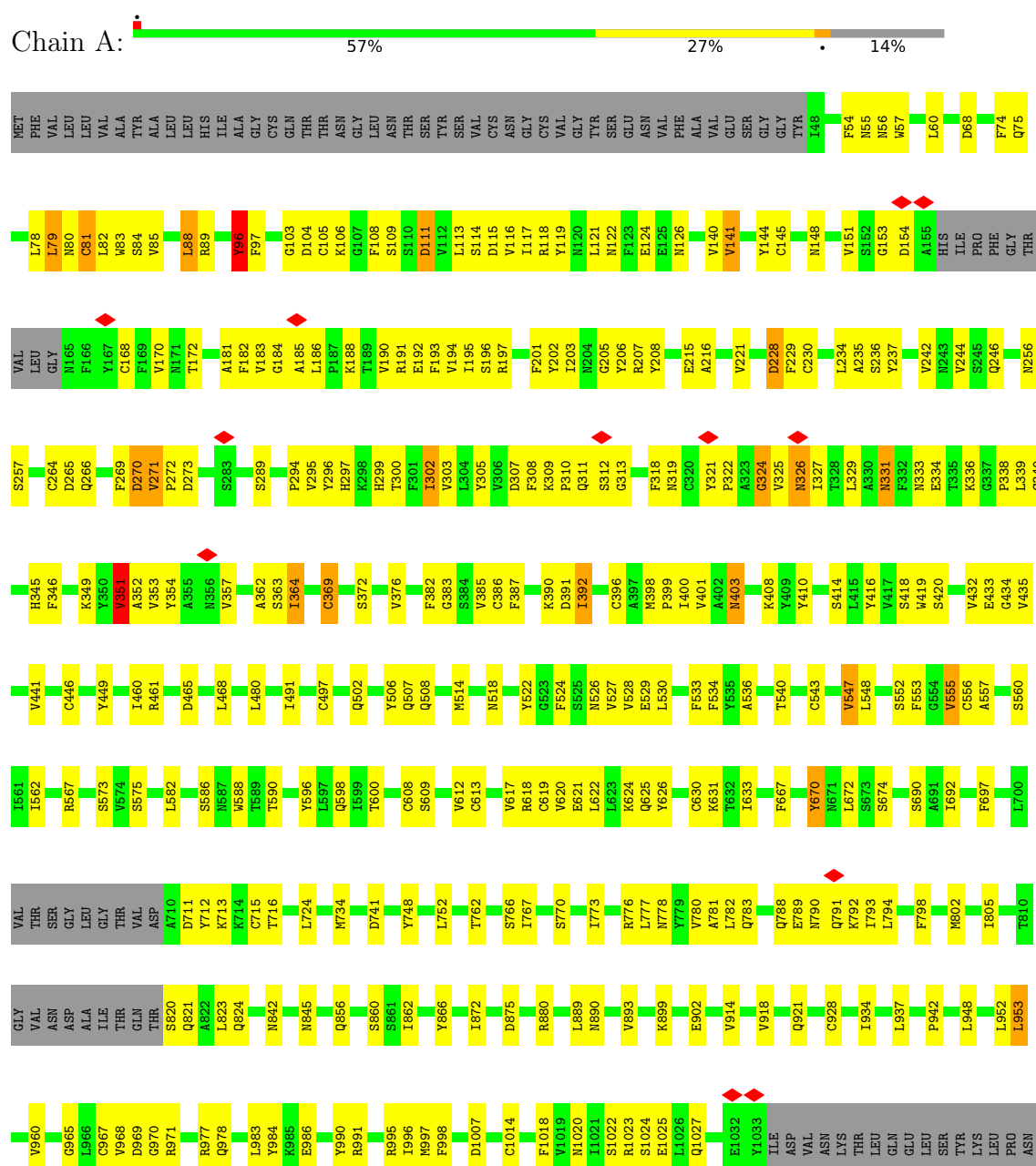
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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



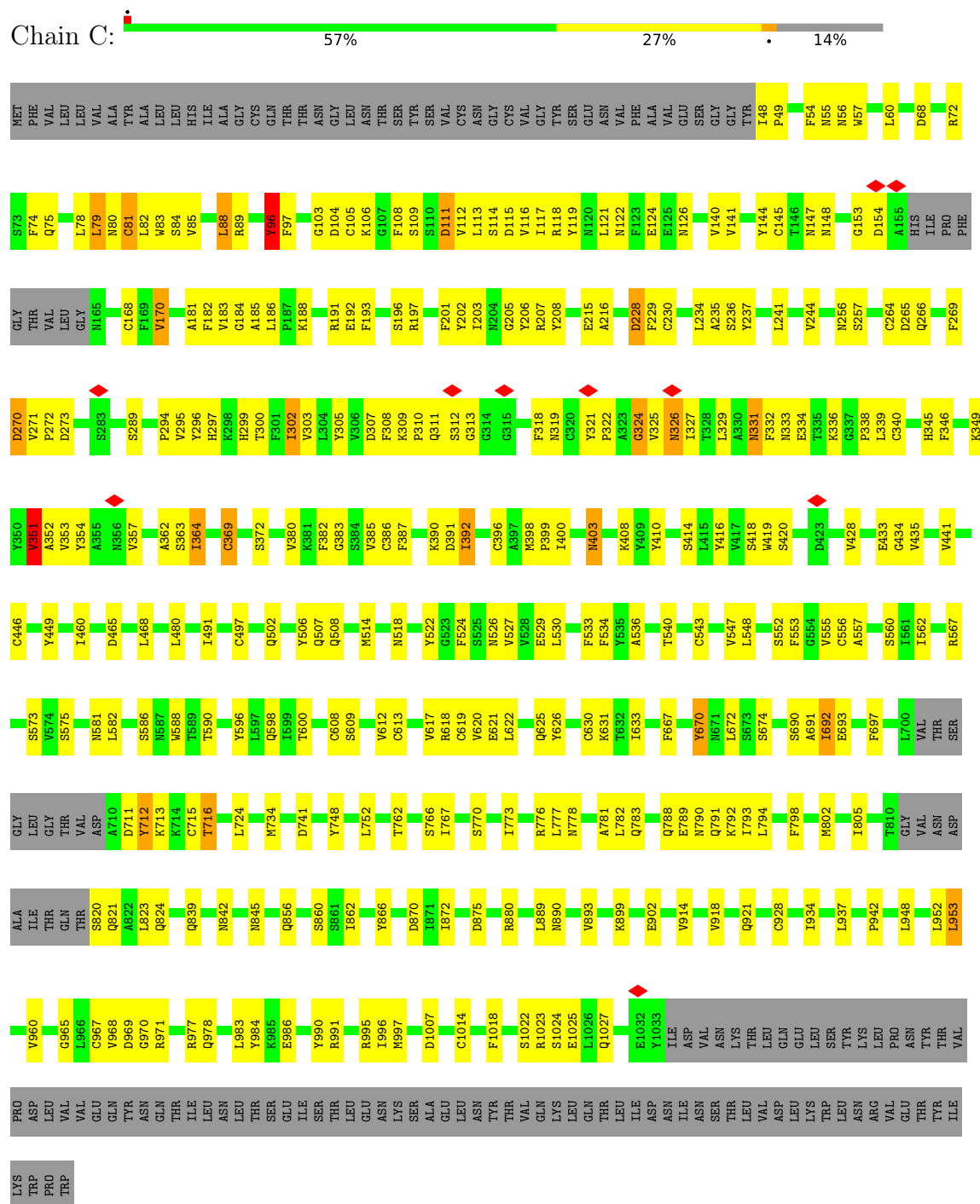
[illegible]

- Molecule 1: Spike glycoprotein



LYS	ASN	VAL	L700	I562	N441	L339	S257	PHE	GLY	SF73	MET
LEU	ARG	ASP	THR	R567	C446	C340	N260	GLY	THR	F74	
PRO	VAL	ALA	SER	L567	C446	H345	N260	VAL	VAL	Q75	
THR	THR	ILE	GLY	D572	N449	F346	R263	LEU	LEU	L78	
VAL	LYS	GLN	LEU	N573	I460	K349	D265	GLY	GLY	L79	
PRO	THR	THR	THR	N575	I460	K349	D265	N165	N165	N80	
ASP	SR20	VAL	VAL	L582	D465	V351	Q266	C168	C168	C81	
LEU	Q821	ASP	ASP	L582	I466	A352	F269	F169	F169	L82	
VAL	A822	VAL	A710	L582	I466	A352	D270	V170	V170	N83	
VAL	L823	VAL	D711	S586	F467	V353	N271	N171	N171	S84	
GLU	Q824	GLU	Y712	N587	I468	V354	P272	T172	T172	N85	
GLN	V968	GLN	K713	N588	I480	A355	D273	T172	T172		
TYR	D969	TYR	W714	T590	I491	V356		A181	A181	L88	
ASN	G970	ASN	T715	T590	I491	A362		F182	F182	R89	
GLN	R971	GLN	T716	Y596	C497	S363	S289	V183	V183	Y95	
THR		THR	L724	Y596	C497	S363		G184	G184	Y96	
ILE	Q856	ILE	D741	Q598	Q502	C369	L293	A185	A185	F97	
LEU	Q856	LEU	T600	Y599	Q502	C369	P294	G186	G186		
ASN	S860	ASN	L983	T600	Y506	V380	Y296	P187	P187	G103	
LEU	S861	LEU	Y748	T600	Q507	V380	K298	K188	K188	D104	
THR	I862	THR	L752	C608	Q508	K381	H299	T189	T189	C105	
LYS	I865	LYS	L752	S609	Q508	F382	H299	V190	V190	K106	
GLU	Y866	GLU	L752	S609	Q508	C383	T300	R191	R191	G107	
ILE	Y866	ILE	T762	V612	N514	S384	F301	E192	E192	F108	
SER	Y990	SER	T762	C613	N518	S385	I302	F193	F193	S109	
THR		THR	S766	V617	Y522	C386	Y305	V194	V194	S10	
LEU	I871	LEU	I767	R618	Q523	F387	V306	I195	I195	D111	
GLU	I871	GLU	S770	R618	Q523	K390	V306	S196	S196	V112	
ASN	I872	ASN	I773	C619	S525	D307	V306	R197	R197	V112	
LYS	D875	LYS	I773	S525	S525	D307	V306	L113	L113	S114	
SER	D879	SER	I773	E621	N526	F308	F308	D115	D115	S114	
ALA	R880	ALA	R776	N526	V527	K309	K309	V116	V116	D115	
LEU	I881	LEU	L776	L622	N528	P310	P310	I117	I117	D115	
ASN	I882	ASN	L777	L623	N528	Q311	Q311	M204	M204	R118	
THR	I889	THR	N778	R624	N528	A397	Q311	Y206	Y206	Y119	
VAL	N890	VAL	I780	Q625	L530	P399	G313	G205	G205	N120	
GLN	V893	GLN	L782	L631	T540	K408	V409	E215	E215	N120	
LYS	L897	LYS	Q783	L633	T540	V409	P322	A216	A216	E124	
THR	R898	THR	Q788	L633	T540	Y410	A323	Y221	Y221	E125	
LEU	K899	LEU	Q789	F667	T540	Y410	G324	V221	V221	V140	
ILE		ILE	N790		C543	S414	V325	D228	D228	V141	
ASP	E902	ASP	Q791	Y670	C543	S414	V325	F229	F229	Y144	
ASN	Y914	ASN	L672	N671	N547	Y416	N326	C230	C230	C145	
ASN	VAL	ASN	L793	L672	L548	V417	T327	L234	L234	T146	
SER	VAL	SER	L794	N673	S552	S418	T328	A235	A235	N147	
THR	ASN	THR	F798	N674	S553	V419	L329	S236	S236	N148	
LEU	Q921	LEU		N690	N554	S420	A330	Y237	Y237		
VAL		VAL	N802	A691	V555	V419	A330	V242	V242	G153	
LEU	C928	LEU	L692	A691	V555	V419	A330	N243	N243	D154	
GLN		GLN	1805	E693	A557	S420	N331	V244	V244	A155	
LYS	1934	LYS				D423	F332	HIS	HIS	D68	
LEU		LEU	N810	F697	S560	E433	T335	G337	G337	ILE	
THR		THR	GLY		N564	V435	K336				

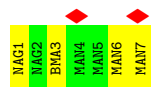
- Molecule 1: Spike glycoprotein



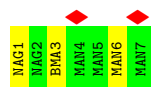
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 3: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 3: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 3: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 3: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose





- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36846	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.222	Depositor
Minimum map value	-10.273	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

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	0.42	0/7246	0.78	11/9752 (0.1%)
1	B	0.42	0/7246	0.78	11/9752 (0.1%)
1	C	0.42	0/7246	0.78	13/9752 (0.1%)
All	All	0.42	0/21738	0.78	35/29256 (0.1%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	716	THR	N-CA-C	-7.69	102.96	114.64
1	A	716	THR	N-CA-C	-7.66	103.00	114.64
1	B	716	THR	N-CA-C	-7.64	103.03	114.64
1	B	96	TYR	CB-CA-C	-7.62	100.56	111.76
1	C	96	TYR	CB-CA-C	-7.62	100.56	111.76
1	A	96	TYR	CB-CA-C	-7.60	100.59	111.76
1	A	872	ILE	N-CA-C	7.23	117.99	110.62
1	B	872	ILE	N-CA-C	7.20	117.97	110.62
1	C	872	ILE	N-CA-C	7.17	117.93	110.62
1	B	272	PRO	CB-CA-C	-6.98	102.45	111.46
1	C	272	PRO	CB-CA-C	-6.98	102.46	111.46
1	A	272	PRO	CB-CA-C	-6.95	102.50	111.46
1	C	272	PRO	CA-C-O	-6.35	114.10	121.34
1	A	272	PRO	CA-C-O	-6.33	114.13	121.34
1	B	272	PRO	CA-C-O	-6.33	114.13	121.34
1	C	712	TYR	CA-C-N	5.98	129.11	120.38
1	C	712	TYR	C-N-CA	5.98	129.11	120.38
1	A	326	ASN	CA-C-N	5.61	131.25	122.84
1	A	326	ASN	C-N-CA	5.61	131.25	122.84
1	C	326	ASN	CA-C-N	5.61	131.25	122.84
1	C	326	ASN	C-N-CA	5.61	131.25	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ASN	CA-C-N	5.58	131.21	122.84
1	B	326	ASN	C-N-CA	5.58	131.21	122.84
1	C	670	TYR	CB-CA-C	5.30	119.59	110.79
1	A	670	TYR	CB-CA-C	5.28	119.55	110.79
1	B	670	TYR	CB-CA-C	5.27	119.54	110.79
1	A	324	GLY	CA-C-N	5.10	131.15	121.97
1	A	324	GLY	C-N-CA	5.10	131.15	121.97
1	C	324	GLY	CA-C-N	5.09	131.13	121.97
1	C	324	GLY	C-N-CA	5.09	131.13	121.97
1	C	111	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	324	GLY	CA-C-N	5.08	131.11	121.97
1	B	324	GLY	C-N-CA	5.08	131.11	121.97
1	B	111	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	111	ASP	CA-CB-CG	5.04	117.64	112.60

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	7094	0	6274	283	0
1	B	7094	0	6273	291	0
1	C	7094	0	6273	270	0
2	D	83	0	70	0	0
2	H	83	0	70	0	0
2	L	83	0	70	0	0
3	E	39	0	34	0	0
3	G	39	0	34	2	0
3	I	39	0	34	0	0
3	K	39	0	34	2	0
3	M	39	0	34	0	0
3	O	39	0	34	2	0
4	F	28	0	25	0	0
4	J	28	0	25	0	0
4	N	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	224	0	208	15	0
5	B	224	0	208	14	0
5	C	224	0	208	15	0
All	All	22521	0	19933	788	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 19.

All (788) 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:B:230:CYS:SG	5:B:1202:NAG:H83	1.52	1.50
1:C:230:CYS:SG	5:C:1202:NAG:H83	1.52	1.49
1:A:230:CYS:SG	5:A:1202:NAG:H83	1.57	1.44
1:B:78:LEU:CD2	1:B:236:SER:HB2	1.65	1.27
1:A:78:LEU:CD2	1:A:236:SER:HB2	1.65	1.26
1:B:78:LEU:HD22	1:B:236:SER:CB	1.67	1.25
1:A:78:LEU:HD22	1:A:236:SER:CB	1.67	1.24
1:C:78:LEU:CD2	1:C:236:SER:HB2	1.65	1.24
1:C:78:LEU:HD22	1:C:236:SER:CB	1.67	1.23
1:B:79:LEU:HD11	1:B:108:PHE:CD1	1.80	1.16
1:A:79:LEU:HD11	1:A:108:PHE:CD1	1.81	1.15
1:C:79:LEU:HD11	1:C:108:PHE:CD1	1.81	1.14
1:B:122:ASN:ND2	1:B:230:CYS:SG	2.23	1.11
1:B:230:CYS:SG	5:B:1202:NAG:C8	2.38	1.11
1:C:230:CYS:SG	5:C:1202:NAG:C8	2.38	1.11
1:A:122:ASN:ND2	1:A:230:CYS:SG	2.23	1.10
1:C:122:ASN:ND2	1:C:230:CYS:SG	2.23	1.10
1:A:230:CYS:SG	5:A:1202:NAG:C8	2.41	1.08
1:B:79:LEU:HD23	1:B:79:LEU:H	1.19	1.06
1:C:68:ASP:HA	1:C:244:VAL:O	1.55	1.06
1:B:68:ASP:HA	1:B:244:VAL:O	1.55	1.05
1:A:68:ASP:HA	1:A:244:VAL:O	1.55	1.04
1:C:79:LEU:HD23	1:C:79:LEU:H	1.19	1.04
1:A:79:LEU:H	1:A:79:LEU:HD23	1.19	1.03
1:A:96:TYR:CD2	1:A:216:ALA:HB2	1.94	1.03
1:A:78:LEU:HD13	1:A:236:SER:O	1.58	1.02
1:C:78:LEU:HD13	1:C:236:SER:O	1.58	1.02
1:C:96:TYR:CD2	1:C:216:ALA:HB2	1.94	1.02
1:B:78:LEU:HD13	1:B:236:SER:O	1.58	1.01
1:B:96:TYR:CD2	1:B:216:ALA:HB2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HB2	1:A:230:CYS:SG	2.06	0.95
1:B:122:ASN:HB2	1:B:230:CYS:SG	2.06	0.95
1:C:122:ASN:HB2	1:C:230:CYS:SG	2.06	0.95
1:A:122:ASN:CB	1:A:230:CYS:SG	2.57	0.92
1:C:122:ASN:CB	1:C:230:CYS:SG	2.57	0.92
1:B:122:ASN:CB	1:B:230:CYS:SG	2.57	0.92
1:C:82:LEU:HB3	1:C:104:ASP:O	1.72	0.90
1:C:78:LEU:HD13	1:C:236:SER:C	1.96	0.90
1:A:713:LYS:HE2	1:B:534:PHE:CE1	2.07	0.89
1:B:78:LEU:HD13	1:B:236:SER:C	1.96	0.89
1:A:78:LEU:HD13	1:A:236:SER:C	1.96	0.89
1:B:82:LEU:HB3	1:B:104:ASP:O	1.72	0.88
1:A:82:LEU:HB3	1:A:104:ASP:O	1.72	0.88
1:A:713:LYS:HE2	1:B:534:PHE:HE1	1.38	0.87
1:C:80:ASN:O	1:C:109:SER:HB3	1.75	0.86
1:A:80:ASN:O	1:A:109:SER:HB3	1.76	0.86
1:B:80:ASN:O	1:B:109:SER:HB3	1.75	0.86
1:B:300:THR:OG1	1:B:346:PHE:CB	2.24	0.85
1:C:300:THR:OG1	1:C:346:PHE:CB	2.24	0.85
1:A:84:SER:HA	1:A:103:GLY:HA3	1.58	0.85
1:A:300:THR:OG1	1:A:346:PHE:CB	2.24	0.84
1:B:84:SER:HA	1:B:103:GLY:HA3	1.58	0.84
1:A:465:ASP:HB2	1:A:491:ILE:HD11	1.60	0.83
1:C:84:SER:HA	1:C:103:GLY:HA3	1.58	0.83
1:B:465:ASP:HB2	1:B:491:ILE:HD11	1.60	0.81
1:C:465:ASP:HB2	1:C:491:ILE:HD11	1.60	0.81
1:A:977:ARG:NH2	1:C:1007:ASP:OD1	2.14	0.81
1:A:96:TYR:CG	1:A:216:ALA:HB2	2.16	0.80
1:C:96:TYR:CG	1:C:216:ALA:HB2	2.16	0.80
1:B:96:TYR:CG	1:B:216:ALA:HB2	2.16	0.80
1:B:96:TYR:CE2	1:B:216:ALA:HB2	2.17	0.80
1:A:300:THR:OG1	1:A:346:PHE:HB3	1.82	0.80
1:A:96:TYR:CE2	1:A:216:ALA:HB2	2.17	0.79
1:A:575:SER:OG	1:A:995:ARG:HD2	1.83	0.79
1:C:575:SER:OG	1:C:995:ARG:HD2	1.83	0.79
1:C:96:TYR:CE2	1:C:216:ALA:HB2	2.17	0.79
1:C:300:THR:OG1	1:C:346:PHE:HB3	1.82	0.78
1:B:897:LEU:HD13	1:C:839:GLN:HE22	1.47	0.78
1:B:575:SER:OG	1:B:995:ARG:HD2	1.83	0.77
1:B:300:THR:OG1	1:B:346:PHE:HB3	1.82	0.77
1:A:340:CYS:HB2	1:A:386:CYS:SG	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:PHE:CE1	1:C:713:LYS:HE2	2.22	0.75
1:C:340:CYS:HB2	1:C:386:CYS:SG	2.26	0.75
1:B:340:CYS:HB2	1:B:386:CYS:SG	2.26	0.74
1:A:182:PHE:HB2	1:B:296:TYR:HB2	1.70	0.74
1:A:96:TYR:CD2	5:A:1201:NAG:H83	2.22	0.74
1:C:79:LEU:H	1:C:79:LEU:CD2	1.97	0.74
1:C:79:LEU:HD23	1:C:79:LEU:N	2.01	0.74
1:C:96:TYR:CD2	5:C:1201:NAG:H83	2.23	0.73
1:B:96:TYR:CD2	5:B:1201:NAG:H83	2.23	0.72
1:B:56:ASN:OD1	1:B:191:ARG:NH2	2.22	0.72
1:A:56:ASN:OD1	1:A:191:ARG:NH2	2.22	0.72
1:C:56:ASN:OD1	1:C:191:ARG:NH2	2.22	0.72
1:C:983:LEU:HD11	1:C:990:TYR:HB3	1.72	0.72
1:B:79:LEU:H	1:B:79:LEU:CD2	1.97	0.72
1:A:631:LYS:HE2	1:B:266:GLN:HA	1.72	0.71
1:A:1007:ASP:OD1	1:B:977:ARG:NH2	2.23	0.71
1:B:983:LEU:HD11	1:B:990:TYR:HB3	1.72	0.71
1:A:78:LEU:HB2	1:A:236:SER:H	1.56	0.70
1:A:185:ALA:HB2	1:B:294:PRO:HB2	1.74	0.70
1:A:79:LEU:H	1:A:79:LEU:CD2	1.97	0.70
1:A:983:LEU:HD11	1:A:990:TYR:HB3	1.72	0.70
1:A:79:LEU:HD23	1:A:79:LEU:N	2.01	0.70
1:B:79:LEU:HD23	1:B:79:LEU:N	2.01	0.70
1:C:788:GLN:O	1:C:792:LYS:NZ	2.24	0.70
1:B:1023:ARG:O	1:B:1027:GLN:NE2	2.25	0.70
1:B:78:LEU:HB2	1:B:236:SER:H	1.56	0.70
1:A:319:ASN:HB2	1:A:410:TYR:HB2	1.73	0.70
1:A:1023:ARG:O	1:A:1027:GLN:NE2	2.25	0.70
1:C:1023:ARG:O	1:C:1027:GLN:NE2	2.24	0.70
1:B:598:GLN:NE2	1:B:600:THR:O	2.25	0.70
1:A:788:GLN:O	1:A:792:LYS:NZ	2.24	0.69
1:B:788:GLN:O	1:B:792:LYS:NZ	2.24	0.69
1:C:78:LEU:HB2	1:C:236:SER:H	1.56	0.69
1:C:776:ARG:HB3	1:C:921:GLN:OE1	1.92	0.69
1:A:534:PHE:HE1	1:C:713:LYS:HE2	1.56	0.69
1:C:598:GLN:NE2	1:C:600:THR:O	2.25	0.69
1:A:228:ASP:N	1:A:228:ASP:OD1	2.25	0.69
1:C:80:ASN:C	1:C:109:SER:HB3	2.17	0.69
1:A:598:GLN:NE2	1:A:600:THR:O	2.25	0.69
1:A:953:LEU:HD21	3:G:1:NAG:H3	1.75	0.69
1:C:228:ASP:OD1	1:C:228:ASP:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ASN:HB2	1:C:410:TYR:HB2	1.73	0.69
1:A:80:ASN:C	1:A:109:SER:HB3	2.17	0.69
1:B:122:ASN:CG	1:B:230:CYS:SG	2.76	0.69
1:A:182:PHE:HB2	1:B:296:TYR:HD2	1.58	0.68
1:A:776:ARG:HB3	1:A:921:GLN:OE1	1.93	0.68
1:B:319:ASN:HB2	1:B:410:TYR:HB2	1.74	0.68
1:B:776:ARG:HB3	1:B:921:GLN:OE1	1.93	0.68
1:C:122:ASN:CG	1:C:230:CYS:SG	2.76	0.68
1:A:122:ASN:CG	1:A:230:CYS:SG	2.76	0.68
1:B:80:ASN:C	1:B:109:SER:HB3	2.17	0.68
1:A:184:GLY:HA3	1:B:295:VAL:HA	1.76	0.68
1:A:266:GLN:HA	1:C:631:LYS:HE2	1.76	0.67
1:A:300:THR:OG1	1:A:346:PHE:HB2	1.93	0.67
1:C:300:THR:OG1	1:C:346:PHE:HB2	1.94	0.67
1:C:588:TRP:CH2	1:C:997:MET:HG2	2.30	0.67
1:B:228:ASP:OD1	1:B:228:ASP:N	2.26	0.67
1:B:588:TRP:CH2	1:B:997:MET:HG2	2.30	0.67
1:A:296:TYR:HD2	1:C:182:PHE:HB2	1.58	0.66
1:A:588:TRP:CH2	1:A:997:MET:HG2	2.30	0.66
1:B:85:VAL:HG12	1:B:88:LEU:HB3	1.78	0.66
1:B:300:THR:OG1	1:B:346:PHE:HB2	1.93	0.66
1:A:777:LEU:HD22	1:A:783:GLN:HB2	1.78	0.66
1:C:119:TYR:HB2	1:C:193:PHE:HB3	1.77	0.66
1:C:124:GLU:OE2	1:C:126:ASN:ND2	2.28	0.66
1:B:119:TYR:HB2	1:B:193:PHE:HB3	1.77	0.66
1:B:124:GLU:OE2	1:B:126:ASN:ND2	2.28	0.66
1:C:777:LEU:HD22	1:C:783:GLN:HB2	1.78	0.66
1:A:96:TYR:CD1	5:A:1201:NAG:H82	2.31	0.65
1:A:119:TYR:HB2	1:A:193:PHE:HB3	1.77	0.65
1:A:124:GLU:OE2	1:A:126:ASN:ND2	2.28	0.65
1:C:85:VAL:HG12	1:C:88:LEU:HB3	1.78	0.65
1:B:622:LEU:HD21	1:B:875:ASP:HB3	1.78	0.65
1:B:777:LEU:HD22	1:B:783:GLN:HB2	1.78	0.65
1:C:622:LEU:HD21	1:C:875:ASP:HB3	1.78	0.64
1:A:622:LEU:HD21	1:A:875:ASP:HB3	1.78	0.64
1:B:1007:ASP:OD1	1:C:977:ARG:NH2	2.30	0.64
1:A:85:VAL:HG12	1:A:88:LEU:HB3	1.78	0.64
1:A:118:ARG:NH2	1:A:192:GLU:OE2	2.30	0.64
1:C:556:CYS:SG	1:C:557:ALA:N	2.71	0.64
1:B:556:CYS:SG	1:B:557:ALA:N	2.71	0.63
1:B:56:ASN:HA	1:B:191:ARG:HH12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:CYS:SG	1:A:557:ALA:N	2.71	0.63
1:A:74:PHE:O	1:A:75:GLN:NE2	2.31	0.63
1:A:182:PHE:CB	1:B:296:TYR:HB2	2.28	0.63
1:B:74:PHE:O	1:B:75:GLN:NE2	2.31	0.63
1:C:80:ASN:OD1	1:C:235:ALA:HA	1.99	0.63
1:C:115:ASP:OD2	1:C:237:TYR:N	2.32	0.63
1:A:56:ASN:HA	1:A:191:ARG:HH12	1.64	0.63
1:B:115:ASP:OD2	1:B:237:TYR:N	2.32	0.63
1:B:713:LYS:HE2	1:C:534:PHE:CE1	2.34	0.63
1:B:96:TYR:CD1	5:B:1201:NAG:H82	2.34	0.62
1:C:74:PHE:O	1:C:75:GLN:NE2	2.31	0.62
1:A:78:LEU:CD1	1:A:236:SER:O	2.43	0.62
1:B:118:ARG:NH2	1:B:192:GLU:OE2	2.30	0.62
1:A:80:ASN:OD1	1:A:235:ALA:HA	1.99	0.62
1:C:609:SER:O	1:C:613:CYS:HB2	2.00	0.62
1:B:80:ASN:OD1	1:B:235:ALA:HA	1.99	0.62
1:A:115:ASP:OD2	1:A:237:TYR:N	2.32	0.62
1:A:96:TYR:CG	5:A:1201:NAG:C8	2.83	0.61
1:C:88:LEU:HD11	1:C:229:PHE:HB2	1.82	0.61
1:A:631:LYS:CE	1:B:266:GLN:HA	2.31	0.61
1:C:339:LEU:HG	1:C:387:PHE:O	2.00	0.61
1:A:88:LEU:HD11	1:A:229:PHE:HB2	1.82	0.61
1:A:339:LEU:HG	1:A:387:PHE:O	2.00	0.61
1:A:609:SER:O	1:A:613:CYS:HB2	2.00	0.61
1:B:96:TYR:CG	5:B:1201:NAG:C8	2.83	0.61
1:B:339:LEU:HG	1:B:387:PHE:O	2.00	0.61
1:B:609:SER:O	1:B:613:CYS:HB2	2.00	0.61
1:C:56:ASN:HA	1:C:191:ARG:HH12	1.64	0.61
1:C:96:TYR:CG	5:C:1201:NAG:C8	2.83	0.61
1:C:96:TYR:CD1	5:C:1201:NAG:H82	2.34	0.61
1:C:118:ARG:NH2	1:C:192:GLU:OE2	2.30	0.61
1:B:631:LYS:HE2	1:C:266:GLN:HA	1.83	0.61
1:A:182:PHE:HB2	1:B:296:TYR:CD2	2.35	0.60
1:B:713:LYS:HE2	1:C:534:PHE:HE1	1.65	0.60
1:B:96:TYR:CD2	5:B:1201:NAG:C8	2.85	0.60
1:A:821:GLN:O	1:A:824:GLN:HG2	2.02	0.60
1:B:78:LEU:CD1	1:B:236:SER:O	2.43	0.60
1:A:294:PRO:HB2	1:C:185:ALA:HB2	1.84	0.60
1:C:862:ILE:HD12	1:C:862:ILE:H	1.66	0.60
1:A:862:ILE:HD12	1:A:862:ILE:H	1.66	0.60
1:B:624:LYS:HG3	1:C:72:ARG:NH2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD11	1:B:229:PHE:HB2	1.82	0.59
1:B:821:GLN:O	1:B:824:GLN:HG2	2.02	0.59
1:C:96:TYR:CD2	5:C:1201:NAG:C8	2.85	0.59
1:A:96:TYR:CD2	5:A:1201:NAG:C8	2.85	0.59
1:A:326:ASN:HB3	5:A:1205:NAG:O5	2.02	0.59
1:B:862:ILE:HD12	1:B:862:ILE:H	1.66	0.59
1:C:529:GLU:HG3	1:C:534:PHE:CE1	2.38	0.59
1:C:821:GLN:O	1:C:824:GLN:HG2	2.02	0.59
1:A:398:MET:O	1:A:414:SER:O	2.21	0.59
1:C:967:CYS:SG	1:C:1018:PHE:HB2	2.42	0.59
1:A:311:GLN:OE1	1:A:311:GLN:N	2.30	0.59
1:A:206:TYR:HE1	1:A:208:TYR:CZ	2.21	0.59
1:A:307:ASP:HA	1:A:354:TYR:HB3	1.85	0.59
1:A:529:GLU:HG3	1:A:534:PHE:CE1	2.38	0.59
1:B:529:GLU:HG3	1:B:534:PHE:CE1	2.37	0.59
1:B:967:CYS:SG	1:B:1018:PHE:HB2	2.42	0.59
1:C:398:MET:O	1:C:414:SER:O	2.21	0.59
1:A:567:ARG:NH2	3:G:1:NAG:O6	2.36	0.58
1:B:115:ASP:OD1	1:B:116:VAL:N	2.37	0.58
1:B:311:GLN:OE1	1:B:311:GLN:N	2.30	0.58
1:A:88:LEU:HD21	1:A:229:PHE:HB2	1.85	0.58
1:B:88:LEU:HD21	1:B:229:PHE:HB2	1.85	0.58
1:B:307:ASP:HA	1:B:354:TYR:HB3	1.85	0.58
1:B:398:MET:O	1:B:414:SER:O	2.21	0.58
1:B:206:TYR:HE1	1:B:208:TYR:CZ	2.21	0.58
1:C:115:ASP:OD1	1:C:116:VAL:N	2.37	0.58
1:A:507:GLN:C	1:A:508:GLN:OE1	2.47	0.58
1:A:967:CYS:SG	1:A:1018:PHE:HB2	2.43	0.58
1:C:88:LEU:HD21	1:C:229:PHE:HB2	1.86	0.58
1:B:184:GLY:HA3	1:C:295:VAL:HA	1.85	0.58
1:B:507:GLN:C	1:B:508:GLN:OE1	2.47	0.58
1:A:168:CYS:SG	1:A:186:LEU:HD22	2.44	0.58
1:A:631:LYS:HZ1	1:B:266:GLN:HA	1.69	0.58
1:B:83:TRP:CD1	1:B:85:VAL:H	2.22	0.58
1:C:507:GLN:C	1:C:508:GLN:OE1	2.47	0.58
1:A:54:PHE:HB2	1:A:57:TRP:HB2	1.86	0.57
1:A:115:ASP:OD1	1:A:116:VAL:N	2.37	0.57
1:B:81:CYS:H	1:B:234:LEU:HD21	1.69	0.57
1:C:168:CYS:SG	1:C:186:LEU:HD22	2.44	0.57
1:C:206:TYR:HE1	1:C:208:TYR:CZ	2.21	0.57
1:C:300:THR:HG1	1:C:346:PHE:CB	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TRP:CD1	1:A:85:VAL:H	2.22	0.57
1:B:168:CYS:SG	1:B:186:LEU:HD22	2.44	0.57
1:B:54:PHE:HB2	1:B:57:TRP:HB2	1.86	0.57
1:A:96:TYR:CG	5:A:1201:NAG:H83	2.40	0.57
1:A:391:ASP:HA	1:A:416:TYR:CG	2.39	0.57
1:B:300:THR:HG1	1:B:346:PHE:HB3	1.68	0.57
1:B:914:VAL:O	1:B:918:VAL:CB	2.53	0.57
1:C:300:THR:HG1	1:C:346:PHE:HB3	1.69	0.57
1:C:307:ASP:HA	1:C:354:TYR:HB3	1.85	0.57
1:B:391:ASP:HA	1:B:416:TYR:CG	2.39	0.57
1:A:300:THR:HG1	1:A:346:PHE:HB3	1.68	0.57
1:C:391:ASP:HA	1:C:416:TYR:CG	2.39	0.57
1:C:83:TRP:CD1	1:C:85:VAL:H	2.22	0.57
1:A:81:CYS:H	1:A:234:LEU:HD21	1.69	0.56
1:C:54:PHE:HB2	1:C:57:TRP:HB2	1.86	0.56
1:C:914:VAL:O	1:C:918:VAL:CB	2.53	0.56
1:B:114:SER:HB2	1:B:234:LEU:HD12	1.87	0.56
1:A:914:VAL:O	1:A:918:VAL:CB	2.53	0.56
1:C:82:LEU:H	1:C:105:CYS:HA	1.71	0.56
1:A:391:ASP:N	1:A:391:ASP:OD1	2.39	0.56
1:C:114:SER:HB2	1:C:234:LEU:HD12	1.87	0.56
1:A:82:LEU:H	1:A:105:CYS:HA	1.71	0.56
1:C:81:CYS:H	1:C:234:LEU:HD21	1.69	0.56
1:C:78:LEU:CD1	1:C:236:SER:O	2.43	0.56
1:C:114:SER:OG	1:C:235:ALA:N	2.39	0.56
1:C:953:LEU:HD21	3:O:1:NAG:H3	1.88	0.56
1:B:953:LEU:HD21	3:K:1:NAG:H3	1.88	0.55
1:A:270:ASP:OD1	1:A:270:ASP:N	2.40	0.55
1:A:608:CYS:O	1:A:612:VAL:HG22	2.06	0.55
1:C:79:LEU:HD11	1:C:108:PHE:CG	2.40	0.55
1:C:608:CYS:O	1:C:612:VAL:HG12	2.06	0.55
1:B:82:LEU:H	1:B:105:CYS:HA	1.70	0.55
1:A:114:SER:HB2	1:A:234:LEU:HD12	1.87	0.55
1:A:185:ALA:HB2	1:B:294:PRO:CB	2.36	0.55
1:B:608:CYS:O	1:B:612:VAL:HG22	2.06	0.55
1:B:712:TYR:O	1:B:715:CYS:N	2.29	0.55
1:C:311:GLN:OE1	1:C:311:GLN:N	2.30	0.55
1:B:114:SER:OG	1:B:235:ALA:N	2.39	0.55
1:A:114:SER:OG	1:A:235:ALA:N	2.39	0.54
1:C:468:LEU:HD23	1:C:468:LEU:H	1.72	0.54
1:A:502:GLN:HB3	1:A:514:MET:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD22	5:A:1202:NAG:H83	1.73	0.54
1:A:821:GLN:H	1:A:821:GLN:CD	2.15	0.54
1:B:369:CYS:N	1:B:396:CYS:SG	2.81	0.54
1:A:369:CYS:N	1:A:396:CYS:SG	2.81	0.54
1:B:567:ARG:NH2	3:K:1:NAG:O6	2.41	0.54
1:C:552:SER:HG	1:C:553:PHE:HD2	1.54	0.54
1:C:821:GLN:CD	1:C:821:GLN:H	2.15	0.54
1:C:369:CYS:N	1:C:396:CYS:SG	2.81	0.54
1:C:502:GLN:HB3	1:C:514:MET:HB2	1.90	0.54
1:B:978:GLN:N	1:B:978:GLN:OE1	2.41	0.54
1:B:170:VAL:O	1:B:181:ALA:HB3	2.08	0.54
1:B:502:GLN:HB3	1:B:514:MET:HB2	1.90	0.54
1:B:326:ASN:HB3	5:B:1205:NAG:O5	2.08	0.54
1:C:96:TYR:CG	5:C:1201:NAG:H83	2.43	0.54
1:C:170:VAL:O	1:C:181:ALA:HB3	2.08	0.54
1:A:296:TYR:CD2	1:C:182:PHE:HB2	2.41	0.53
1:B:468:LEU:HD23	1:B:468:LEU:H	1.72	0.53
1:B:613:CYS:HA	1:B:619:CYS:SG	2.48	0.53
1:C:978:GLN:OE1	1:C:978:GLN:N	2.41	0.53
1:A:115:ASP:CG	1:A:236:SER:HA	2.33	0.53
1:B:391:ASP:OD1	1:B:391:ASP:N	2.39	0.53
1:C:115:ASP:CG	1:C:236:SER:HA	2.33	0.53
1:C:270:ASP:N	1:C:270:ASP:OD1	2.40	0.53
1:C:567:ARG:NH2	3:O:1:NAG:O6	2.40	0.53
1:C:613:CYS:HA	1:C:619:CYS:SG	2.48	0.53
1:A:468:LEU:HD23	1:A:468:LEU:H	1.72	0.53
1:B:588:TRP:HH2	1:B:997:MET:HG2	1.74	0.53
1:B:821:GLN:CD	1:B:821:GLN:H	2.15	0.53
1:C:712:TYR:O	1:C:715:CYS:N	2.29	0.53
1:A:170:VAL:O	1:A:181:ALA:HB3	2.08	0.53
1:A:978:GLN:N	1:A:978:GLN:OE1	2.41	0.53
1:B:354:TYR:OH	1:B:362:ALA:N	2.42	0.53
1:C:303:VAL:O	1:C:329:LEU:HB2	2.08	0.53
1:C:354:TYR:OH	1:C:362:ALA:N	2.42	0.53
1:C:633:ILE:HD13	1:C:889:LEU:HD23	1.91	0.53
1:A:303:VAL:O	1:A:329:LEU:HB2	2.08	0.53
1:B:96:TYR:CG	5:B:1201:NAG:H83	2.43	0.53
1:B:256:ASN:OD1	1:B:257:SER:N	2.42	0.53
1:C:391:ASP:OD1	1:C:391:ASP:N	2.39	0.53
1:B:115:ASP:CG	1:B:236:SER:HA	2.33	0.53
1:C:256:ASN:OD1	1:C:257:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:CYS:HB3	1:B:109:SER:OG	2.09	0.53
1:B:633:ILE:HD13	1:B:889:LEU:HD23	1.91	0.53
1:C:105:CYS:HB3	1:C:109:SER:OG	2.09	0.53
1:C:326:ASN:HB3	5:C:1205:NAG:O5	2.08	0.53
1:A:208:TYR:CD1	1:B:293:LEU:HD11	2.43	0.52
1:A:842:ASN:HA	1:A:845:ASN:HB2	1.91	0.52
1:A:613:CYS:HA	1:A:619:CYS:SG	2.48	0.52
1:B:590:THR:CG2	1:B:794:LEU:HB2	2.39	0.52
1:A:354:TYR:OH	1:A:362:ALA:N	2.42	0.52
1:A:588:TRP:HH2	1:A:997:MET:HG2	1.73	0.52
1:B:300:THR:HG1	1:B:346:PHE:CB	2.22	0.52
1:B:303:VAL:O	1:B:329:LEU:HB2	2.09	0.52
1:B:332:PHE:HA	1:B:336:LYS:HZ2	1.74	0.52
1:B:552:SER:HG	1:B:553:PHE:HD2	1.57	0.52
1:C:322:PRO:C	1:C:324:GLY:H	2.18	0.52
1:C:78:LEU:HD22	1:C:236:SER:HB2	0.73	0.52
1:C:124:GLU:OE1	1:C:124:GLU:N	2.36	0.52
1:C:311:GLN:OE1	1:C:322:PRO:HB2	2.09	0.52
1:A:68:ASP:CA	1:A:244:VAL:O	2.44	0.52
1:A:88:LEU:HD23	1:A:88:LEU:H	1.75	0.52
1:B:270:ASP:OD1	1:B:270:ASP:N	2.40	0.52
1:B:322:PRO:C	1:B:324:GLY:H	2.18	0.52
1:B:529:GLU:HG3	1:B:534:PHE:HE1	1.75	0.52
1:A:327:ILE:O	1:A:327:ILE:HG13	2.10	0.52
1:B:78:LEU:HD22	1:B:236:SER:HB2	0.73	0.52
1:A:144:TYR:OH	1:A:154:ASP:O	2.27	0.52
1:B:182:PHE:HB2	1:C:296:TYR:HD2	1.75	0.52
1:B:311:GLN:OE1	1:B:322:PRO:HB2	2.09	0.52
1:A:122:ASN:H	1:A:229:PHE:HD1	1.57	0.51
1:A:79:LEU:HD11	1:A:108:PHE:CG	2.40	0.51
1:A:590:THR:CG2	1:A:794:LEU:HB2	2.39	0.51
1:B:122:ASN:H	1:B:229:PHE:HD1	1.57	0.51
1:B:762:THR:N	1:C:582:LEU:HA	2.25	0.51
1:C:773:ILE:HD11	1:C:791:GLN:HG2	1.92	0.51
1:C:842:ASN:HA	1:C:845:ASN:HB2	1.91	0.51
1:A:105:CYS:HB3	1:A:109:SER:OG	2.09	0.51
1:A:311:GLN:OE1	1:A:322:PRO:HB2	2.09	0.51
1:B:820:SER:OG	1:B:823:LEU:HD23	2.11	0.51
1:B:842:ASN:HA	1:B:845:ASN:HB2	1.91	0.51
1:A:529:GLU:HG3	1:A:534:PHE:HE1	1.75	0.51
1:A:633:ILE:HD13	1:A:889:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD23	1:B:88:LEU:H	1.75	0.51
1:C:590:THR:CG2	1:C:794:LEU:HB2	2.39	0.51
1:B:790:ASN:HA	1:B:793:ILE:HG12	1.93	0.51
1:C:88:LEU:H	1:C:88:LEU:HD23	1.75	0.51
1:C:122:ASN:HD22	5:C:1202:NAG:H83	1.76	0.51
1:C:529:GLU:HG3	1:C:534:PHE:HE1	1.75	0.51
1:A:300:THR:HG1	1:A:346:PHE:CB	2.21	0.51
1:A:790:ASN:HA	1:A:793:ILE:HG12	1.93	0.51
1:A:97:PHE:O	1:A:113:LEU:HD12	2.11	0.51
1:B:870:ASP:OD1	1:C:372:SER:CB	2.59	0.51
1:A:266:GLN:HA	1:C:631:LYS:CE	2.40	0.51
1:C:122:ASN:H	1:C:229:PHE:HD1	1.57	0.51
1:A:256:ASN:OD1	1:A:257:SER:N	2.42	0.50
1:A:295:VAL:HA	1:C:184:GLY:HA3	1.92	0.50
1:B:97:PHE:O	1:B:113:LEU:HD12	2.11	0.50
1:A:530:LEU:HD23	1:A:533:PHE:CE1	2.46	0.50
1:A:631:LYS:NZ	1:B:266:GLN:HA	2.25	0.50
1:A:773:ILE:HD11	1:A:791:GLN:HG2	1.92	0.50
1:A:820:SER:OG	1:A:823:LEU:HD23	2.11	0.50
1:B:79:LEU:HD11	1:B:108:PHE:CG	2.40	0.50
1:B:530:LEU:HD23	1:B:533:PHE:CE1	2.46	0.50
1:A:322:PRO:C	1:A:324:GLY:H	2.18	0.50
1:B:773:ILE:HD11	1:B:791:GLN:HG2	1.92	0.50
1:A:296:TYR:HB2	1:C:182:PHE:HB2	1.94	0.50
1:A:308:PHE:HE2	1:A:318:PHE:CE2	2.30	0.50
1:B:327:ILE:O	1:B:327:ILE:HG13	2.10	0.50
1:C:820:SER:OG	1:C:823:LEU:HD23	2.11	0.50
1:A:762:THR:N	1:B:582:LEU:HA	2.27	0.50
1:C:327:ILE:HG13	1:C:327:ILE:O	2.10	0.50
1:B:122:ASN:HD22	5:B:1202:NAG:H83	1.76	0.50
1:B:124:GLU:H	1:B:124:GLU:CD	2.18	0.50
1:B:188:LYS:HD2	1:B:188:LYS:C	2.37	0.50
1:C:97:PHE:O	1:C:113:LEU:HD12	2.11	0.50
1:A:624:LYS:HG3	1:B:72:ARG:NH2	2.26	0.50
1:C:530:LEU:HD23	1:C:533:PHE:CE1	2.46	0.50
1:A:383:GLY:N	1:A:420:SER:O	2.33	0.50
1:B:522:TYR:HB2	1:B:524:PHE:HD2	1.77	0.50
1:A:372:SER:CB	1:C:870:ASP:OD1	2.60	0.49
1:B:308:PHE:HE2	1:B:318:PHE:CE2	2.30	0.49
1:B:78:LEU:HD11	1:B:237:TYR:O	2.12	0.49
1:B:793:ILE:HG13	1:B:794:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PHE:HA	1:C:336:LYS:HZ2	1.77	0.49
1:C:188:LYS:HD2	1:C:188:LYS:C	2.37	0.49
1:A:188:LYS:C	1:A:188:LYS:HD2	2.37	0.49
1:C:308:PHE:HE2	1:C:318:PHE:CE2	2.29	0.49
1:A:124:GLU:H	1:A:124:GLU:CD	2.18	0.49
1:A:185:ALA:HB2	1:B:294:PRO:HD2	1.95	0.49
1:A:522:TYR:HB2	1:A:524:PHE:HD2	1.77	0.49
1:B:345:HIS:HB3	1:B:433:GLU:OE1	2.12	0.49
1:C:790:ASN:HA	1:C:793:ILE:HG12	1.93	0.49
1:C:124:GLU:H	1:C:124:GLU:CD	2.18	0.49
1:C:308:PHE:HD1	1:C:324:GLY:HA2	1.78	0.49
1:A:345:HIS:HB3	1:A:433:GLU:OE1	2.12	0.49
1:C:345:HIS:HB3	1:C:433:GLU:OE1	2.12	0.49
1:B:308:PHE:HD1	1:B:324:GLY:HA2	1.78	0.49
1:C:78:LEU:HD11	1:C:237:TYR:O	2.12	0.49
1:A:78:LEU:HD11	1:A:237:TYR:O	2.12	0.48
1:A:246:GLN:HB3	1:B:467:PHE:HE1	1.78	0.48
1:C:588:TRP:HH2	1:C:997:MET:HG2	1.74	0.48
1:A:446:CYS:SG	1:A:497:CYS:HB2	2.53	0.48
1:A:145:CYS:HA	1:A:168:CYS:HA	1.96	0.48
1:A:308:PHE:HD1	1:A:324:GLY:HA2	1.78	0.48
1:B:85:VAL:HG12	1:B:85:VAL:O	2.13	0.48
1:C:144:TYR:OH	1:C:154:ASP:O	2.27	0.48
1:A:766:SER:OG	1:A:767:ILE:N	2.47	0.48
1:A:971:ARG:O	1:A:1014:CYS:HB2	2.14	0.48
1:B:446:CYS:SG	1:B:497:CYS:HB2	2.53	0.48
1:C:85:VAL:HG12	1:C:85:VAL:O	2.13	0.48
1:C:446:CYS:SG	1:C:497:CYS:HB2	2.53	0.48
1:C:522:TYR:HB2	1:C:524:PHE:HD2	1.77	0.48
1:C:793:ILE:HG13	1:C:794:LEU:N	2.28	0.48
1:A:712:TYR:O	1:A:715:CYS:N	2.29	0.48
1:A:793:ILE:HG13	1:A:794:LEU:N	2.28	0.48
1:B:631:LYS:HZ1	1:C:266:GLN:HA	1.78	0.48
1:B:766:SER:OG	1:B:767:ILE:N	2.47	0.48
1:A:856:GLN:HB3	1:A:880:ARG:HD3	1.96	0.48
1:B:201:PHE:O	1:B:207:ARG:HG2	2.14	0.48
1:B:202:TYR:CE2	1:B:207:ARG:HB2	2.49	0.48
1:B:390:LYS:O	1:B:416:TYR:HB2	2.14	0.48
1:C:322:PRO:C	1:C:324:GLY:N	2.72	0.48
1:C:96:TYR:CG	5:C:1201:NAG:H82	2.48	0.48
1:C:201:PHE:O	1:C:207:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:SER:OG	1:C:767:ILE:N	2.47	0.48
1:C:965:GLY:C	1:C:1018:PHE:HB3	2.39	0.48
1:A:85:VAL:HG12	1:A:85:VAL:O	2.13	0.48
1:A:96:TYR:CD1	5:A:1201:NAG:C8	2.97	0.48
1:A:202:TYR:CE2	1:A:207:ARG:HB2	2.49	0.48
1:A:302:ILE:HG12	1:A:302:ILE:O	2.14	0.48
1:B:145:CYS:HA	1:B:168:CYS:HA	1.96	0.48
1:B:856:GLN:HB3	1:B:880:ARG:HD3	1.96	0.48
1:A:78:LEU:HD22	1:A:236:SER:HB2	0.73	0.48
1:A:201:PHE:O	1:A:207:ARG:HG2	2.14	0.48
1:B:144:TYR:OH	1:B:154:ASP:O	2.27	0.47
1:B:68:ASP:CA	1:B:244:VAL:O	2.44	0.47
1:B:741:ASP:OD1	1:B:741:ASP:N	2.43	0.47
1:C:202:TYR:CE2	1:C:207:ARG:HB2	2.49	0.47
1:A:96:TYR:CG	5:A:1201:NAG:H82	2.49	0.47
1:A:390:LYS:O	1:A:416:TYR:HB2	2.14	0.47
1:B:971:ARG:O	1:B:1014:CYS:HB2	2.14	0.47
1:C:390:LYS:O	1:C:416:TYR:HB2	2.13	0.47
1:C:741:ASP:N	1:C:741:ASP:OD1	2.43	0.47
1:A:965:GLY:C	1:A:1018:PHE:HB3	2.39	0.47
1:C:971:ARG:O	1:C:1014:CYS:HB2	2.14	0.47
1:B:965:GLY:C	1:B:1018:PHE:HB3	2.39	0.47
1:C:115:ASP:HA	1:C:197:ARG:HH12	1.80	0.47
1:C:68:ASP:CA	1:C:244:VAL:O	2.44	0.47
1:C:302:ILE:O	1:C:302:ILE:HG12	2.14	0.47
1:C:331:ASN:HB3	1:C:339:LEU:HD22	1.96	0.47
1:C:618:ARG:HB2	1:C:866:TYR:CE2	2.49	0.47
1:A:518:ASN:HD22	5:A:1206:NAG:C7	2.28	0.47
1:A:618:ARG:HB2	1:A:866:TYR:CE2	2.49	0.47
1:B:322:PRO:C	1:B:324:GLY:N	2.72	0.47
1:B:618:ARG:HB2	1:B:866:TYR:CE2	2.49	0.47
1:C:145:CYS:HA	1:C:168:CYS:HA	1.96	0.47
1:B:115:ASP:HA	1:B:197:ARG:HH12	1.80	0.47
1:B:302:ILE:O	1:B:302:ILE:HG12	2.14	0.47
1:B:383:GLY:N	1:B:420:SER:O	2.33	0.47
1:C:540:THR:O	1:C:560:SER:OG	2.33	0.47
1:C:969:ASP:HB3	1:C:1022:SER:HA	1.97	0.47
1:A:1020:ASN:HB3	5:A:1216:NAG:N2	2.29	0.47
1:B:230:CYS:CB	5:B:1202:NAG:H83	2.42	0.47
1:C:575:SER:OG	1:C:995:ARG:CD	2.59	0.47
1:A:331:ASN:HB3	1:A:339:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:HG	1:A:553:PHE:HD2	1.59	0.46
1:C:934:ILE:HD11	1:C:952:LEU:HD11	1.97	0.46
1:B:331:ASN:HB3	1:B:339:LEU:HD22	1.96	0.46
1:B:969:ASP:HB3	1:B:1022:SER:HA	1.97	0.46
1:C:297:HIS:HB2	1:C:434:GLY:N	2.30	0.46
1:C:617:VAL:O	1:C:621:GLU:HG2	2.16	0.46
1:C:856:GLN:HB3	1:C:880:ARG:HD3	1.96	0.46
1:A:297:HIS:HB2	1:A:434:GLY:N	2.31	0.46
1:C:333:ASN:OD1	1:C:334:GLU:N	2.49	0.46
1:A:322:PRO:C	1:A:324:GLY:N	2.72	0.46
1:B:297:HIS:HB2	1:B:434:GLY:N	2.30	0.46
1:B:984:TYR:CE2	1:B:986:GLU:HB2	2.51	0.46
1:A:115:ASP:HA	1:A:197:ARG:HH12	1.80	0.46
1:B:983:LEU:HD12	1:B:984:TYR:H	1.81	0.46
1:C:385:VAL:O	1:C:418:SER:O	2.34	0.46
1:A:461:ARG:NH1	1:C:716:THR:O	2.48	0.46
1:A:543:CYS:HA	1:A:562:ILE:HD11	1.98	0.46
1:B:631:LYS:CE	1:C:266:GLN:HA	2.45	0.46
1:C:991:ARG:HD3	1:C:991:ARG:HA	1.67	0.46
1:A:385:VAL:O	1:A:418:SER:O	2.34	0.46
1:B:96:TYR:CG	1:B:216:ALA:CB	2.95	0.46
1:A:333:ASN:OD1	1:A:334:GLU:N	2.49	0.46
1:B:124:GLU:OE1	1:B:124:GLU:N	2.36	0.46
1:C:983:LEU:HD12	1:C:984:TYR:H	1.80	0.46
1:A:969:ASP:HB3	1:A:1022:SER:HA	1.96	0.46
1:A:984:TYR:CE2	1:A:986:GLU:HB2	2.51	0.46
1:B:338:PRO:HG3	1:B:392:ILE:HD11	1.98	0.46
1:B:543:CYS:HA	1:B:562:ILE:HD11	1.97	0.46
1:B:617:VAL:O	1:B:621:GLU:HG2	2.16	0.46
1:A:789:GLU:O	1:A:793:ILE:HG12	2.16	0.46
1:B:96:TYR:CG	5:B:1201:NAG:H82	2.48	0.46
1:A:305:TYR:CE1	1:A:351:VAL:HG11	2.51	0.45
1:A:934:ILE:HD11	1:A:952:LEU:HD11	1.97	0.45
1:A:983:LEU:HD12	1:A:984:TYR:H	1.81	0.45
1:A:991:ARG:HA	1:A:991:ARG:HD3	1.67	0.45
1:B:106:LYS:HG2	1:B:106:LYS:O	2.16	0.45
1:A:540:THR:O	1:A:560:SER:OG	2.33	0.45
1:A:617:VAL:O	1:A:621:GLU:HG2	2.16	0.45
1:A:289:SER:OG	1:A:441:VAL:HA	2.16	0.45
1:B:305:TYR:CE1	1:B:351:VAL:HG21	2.51	0.45
1:B:333:ASN:OD1	1:B:334:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:ILE:H	1:B:692:ILE:HG12	1.52	0.45
1:B:789:GLU:O	1:B:793:ILE:HG12	2.16	0.45
1:B:995:ARG:CZ	1:B:996:ILE:HD11	2.47	0.45
1:C:106:LYS:O	1:C:106:LYS:HG2	2.16	0.45
1:C:789:GLU:O	1:C:793:ILE:HG12	2.16	0.45
1:C:984:TYR:CE2	1:C:986:GLU:HB2	2.51	0.45
1:A:55:ASN:OD1	1:A:56:ASN:N	2.50	0.45
1:A:124:GLU:OE1	1:A:124:GLU:N	2.36	0.45
1:B:385:VAL:O	1:B:418:SER:O	2.34	0.45
1:C:88:LEU:O	1:C:89:ARG:HD3	2.17	0.45
1:C:305:TYR:CE1	1:C:351:VAL:HG11	2.51	0.45
1:C:338:PRO:HG3	1:C:392:ILE:HD11	1.98	0.45
1:A:741:ASP:N	1:A:741:ASP:OD1	2.43	0.45
1:B:575:SER:OG	1:B:995:ARG:CD	2.59	0.45
1:B:937:LEU:HB2	1:B:948:LEU:HB2	1.99	0.45
1:C:526:ASN:OD1	1:C:527:VAL:N	2.50	0.45
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.79	0.45
1:B:88:LEU:O	1:B:89:ARG:HD3	2.17	0.45
1:C:289:SER:OG	1:C:441:VAL:HA	2.16	0.45
1:A:185:ALA:HB2	1:B:294:PRO:CD	2.47	0.45
1:A:338:PRO:HG3	1:A:392:ILE:HD11	1.98	0.45
1:A:995:ARG:CZ	1:A:996:ILE:HD11	2.47	0.45
1:B:55:ASN:OD1	1:B:56:ASN:N	2.50	0.45
1:B:526:ASN:OD1	1:B:527:VAL:N	2.50	0.45
1:B:624:LYS:HZ2	1:C:72:ARG:CZ	2.30	0.45
1:B:934:ILE:HD11	1:B:952:LEU:HD11	1.97	0.45
1:C:78:LEU:HB2	1:C:236:SER:N	2.28	0.45
1:A:670:TYR:HD2	1:A:798:PHE:CD2	2.35	0.45
1:B:148:ASN:HB3	1:B:153:GLY:HA2	1.99	0.45
1:B:336:LYS:HD2	1:B:336:LYS:HA	1.78	0.45
1:A:106:LYS:O	1:A:106:LYS:HG2	2.16	0.45
1:A:460:ILE:HD12	1:A:460:ILE:N	2.32	0.45
1:B:460:ILE:N	1:B:460:ILE:HD12	2.32	0.45
1:B:582:LEU:O	1:B:960:VAL:N	2.50	0.45
1:C:78:LEU:HB3	1:C:80:ASN:ND2	2.32	0.45
1:C:543:CYS:HA	1:C:562:ILE:HD11	1.98	0.45
1:C:582:LEU:O	1:C:960:VAL:N	2.50	0.45
1:A:351:VAL:HG12	1:A:352:ALA:H	1.82	0.45
1:B:289:SER:OG	1:B:441:VAL:HA	2.16	0.45
1:A:273:ASP:HB3	1:A:506:TYR:HA	1.99	0.44
1:A:364:ILE:HD12	1:A:364:ILE:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:CYS:SG	5:B:1202:NAG:C7	3.03	0.44
1:B:273:ASP:HB3	1:B:506:TYR:HA	1.99	0.44
1:B:351:VAL:HG22	1:B:352:ALA:H	1.82	0.44
1:B:540:THR:O	1:B:560:SER:OG	2.33	0.44
1:A:410:TYR:CE1	1:B:338:PRO:HD2	2.52	0.44
1:A:762:THR:H	1:B:582:LEU:HA	1.83	0.44
1:A:899:LYS:O	1:A:902:GLU:HG3	2.17	0.44
1:A:995:ARG:C	1:A:996:ILE:HD13	2.43	0.44
1:A:526:ASN:OD1	1:A:527:VAL:N	2.50	0.44
1:B:890:ASN:HA	1:B:893:VAL:HG12	2.00	0.44
1:C:692:ILE:H	1:C:692:ILE:HG12	1.52	0.44
1:C:995:ARG:CZ	1:C:996:ILE:HD11	2.47	0.44
1:A:78:LEU:HB3	1:A:80:ASN:ND2	2.32	0.44
1:A:88:LEU:O	1:A:89:ARG:HD3	2.17	0.44
1:B:78:LEU:HB3	1:B:80:ASN:ND2	2.32	0.44
1:C:148:ASN:HB3	1:C:153:GLY:HA2	1.99	0.44
1:C:273:ASP:HB3	1:C:506:TYR:HA	1.99	0.44
1:C:995:ARG:C	1:C:996:ILE:HD13	2.43	0.44
1:A:321:TYR:HB2	1:A:410:TYR:CE2	2.53	0.44
1:C:321:TYR:HB2	1:C:410:TYR:CE2	2.53	0.44
1:C:383:GLY:N	1:C:420:SER:O	2.33	0.44
1:C:460:ILE:HD12	1:C:460:ILE:N	2.32	0.44
1:A:148:ASN:HB3	1:A:153:GLY:HA2	1.99	0.44
1:C:670:TYR:HD2	1:C:798:PHE:CD2	2.35	0.44
1:C:674:SER:O	1:C:690:SER:HB3	2.18	0.44
1:A:185:ALA:CB	1:B:294:PRO:HB2	2.45	0.44
1:A:969:ASP:OD1	1:A:970:GLY:N	2.50	0.44
1:A:575:SER:OG	1:A:995:ARG:CD	2.59	0.44
1:A:937:LEU:HB2	1:A:948:LEU:HB2	1.99	0.44
1:B:78:LEU:HB2	1:B:236:SER:N	2.28	0.44
1:C:55:ASN:OD1	1:C:56:ASN:N	2.50	0.44
1:A:890:ASN:HA	1:A:893:VAL:HG12	2.00	0.44
1:B:547:VAL:HG11	1:B:557:ALA:HA	2.00	0.44
1:C:899:LYS:O	1:C:902:GLU:HG3	2.17	0.44
5:C:1201:NAG:O7	5:C:1201:NAG:O3	2.34	0.44
1:B:321:TYR:HB2	1:B:410:TYR:CE2	2.53	0.43
1:B:899:LYS:O	1:B:902:GLU:HG3	2.17	0.43
1:B:995:ARG:C	1:B:996:ILE:HD13	2.43	0.43
1:B:264:CYS:SG	1:B:265:ASP:N	2.91	0.43
1:B:382:PHE:HE1	1:B:419:TRP:CG	2.36	0.43
1:C:349:LYS:HE3	1:C:349:LYS:HB2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.92	0.43
1:B:670:TYR:HD2	1:B:798:PHE:CD2	2.35	0.43
1:C:969:ASP:OD1	1:C:970:GLY:N	2.50	0.43
1:A:582:LEU:O	1:A:960:VAL:N	2.50	0.43
1:B:96:TYR:CD2	1:B:215:GLU:HG2	2.54	0.43
1:B:691:ALA:C	1:B:693:GLU:N	2.75	0.43
1:B:802:MET:HA	1:B:805:ILE:HG12	2.01	0.43
1:C:382:PHE:HE1	1:C:419:TRP:CG	2.36	0.43
1:C:697:PHE:HE1	1:C:942:PRO:HG3	1.84	0.43
1:C:890:ASN:HA	1:C:893:VAL:HG12	2.00	0.43
1:C:937:LEU:HB2	1:C:948:LEU:HB2	1.99	0.43
1:A:96:TYR:CD2	1:A:215:GLU:HG2	2.54	0.43
1:A:264:CYS:SG	1:A:265:ASP:N	2.91	0.43
1:A:310:PRO:CB	1:A:322:PRO:HG2	2.48	0.43
1:A:382:PHE:HE1	1:A:419:TRP:CG	2.36	0.43
1:B:185:ALA:N	1:C:294:PRO:O	2.42	0.43
1:B:234:LEU:HD23	1:B:234:LEU:H	1.83	0.43
1:B:596:TYR:CD1	1:B:596:TYR:C	2.97	0.43
1:B:697:PHE:HE1	1:B:942:PRO:HG3	1.84	0.43
1:C:802:MET:HA	1:C:805:ILE:HG12	2.01	0.43
1:A:96:TYR:CG	1:A:216:ALA:CB	2.95	0.43
1:A:674:SER:O	1:A:690:SER:HB3	2.18	0.43
1:B:310:PRO:CB	1:B:322:PRO:HG2	2.48	0.43
1:B:969:ASP:OD1	1:B:970:GLY:N	2.50	0.43
1:C:96:TYR:CD2	1:C:215:GLU:HG2	2.54	0.43
1:C:206:TYR:HE1	1:C:208:TYR:CE2	2.37	0.43
1:C:310:PRO:CB	1:C:322:PRO:HG2	2.48	0.43
1:C:351:VAL:HG12	1:C:352:ALA:H	1.82	0.43
1:A:697:PHE:HE1	1:A:942:PRO:HG3	1.84	0.43
1:B:116:VAL:HG22	1:B:196:SER:CB	2.49	0.43
1:C:121:LEU:HD12	1:C:229:PHE:CE1	2.54	0.43
1:C:264:CYS:SG	1:C:265:ASP:N	2.91	0.43
1:C:596:TYR:CD1	1:C:596:TYR:C	2.97	0.43
1:A:182:PHE:CD1	1:B:296:TYR:N	2.87	0.43
1:A:208:TYR:CE1	1:B:293:LEU:HD11	2.54	0.43
1:A:289:SER:O	1:A:449:TYR:HA	2.19	0.43
1:A:547:VAL:HG11	1:A:557:ALA:HA	2.00	0.43
1:C:116:VAL:HG12	1:C:196:SER:CB	2.49	0.43
1:C:299:HIS:HD2	1:C:433:GLU:HB2	1.84	0.43
1:C:734:MET:HE3	1:C:734:MET:HB2	1.86	0.43
1:A:299:HIS:HD2	1:A:433:GLU:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:TYR:CD1	1:A:596:TYR:C	2.97	0.43
1:B:299:HIS:HD2	1:B:433:GLU:HB2	1.84	0.43
1:C:289:SER:O	1:C:449:TYR:HA	2.19	0.43
1:A:116:VAL:HG22	1:A:196:SER:CB	2.49	0.42
1:A:782:LEU:O	1:A:783:GLN:C	2.61	0.42
1:A:802:MET:HA	1:A:805:ILE:HG12	2.01	0.42
1:B:121:LEU:HD12	1:B:229:PHE:CE1	2.54	0.42
1:B:674:SER:O	1:B:690:SER:HB3	2.18	0.42
1:C:299:HIS:HA	1:C:433:GLU:OE1	2.19	0.42
1:C:547:VAL:HG21	1:C:557:ALA:HA	2.00	0.42
1:A:234:LEU:H	1:A:234:LEU:HD23	1.83	0.42
1:B:526:ASN:O	1:B:536:ALA:HA	2.20	0.42
1:A:625:GLN:HG3	1:A:626:TYR:CD1	2.54	0.42
1:A:734:MET:HE3	1:A:734:MET:HB2	1.86	0.42
1:B:289:SER:O	1:B:449:TYR:HA	2.19	0.42
1:B:782:LEU:O	1:B:783:GLN:C	2.61	0.42
1:C:782:LEU:O	1:C:783:GLN:C	2.61	0.42
1:A:78:LEU:HB2	1:A:236:SER:N	2.28	0.42
1:A:121:LEU:HD12	1:A:229:PHE:CE1	2.54	0.42
1:A:230:CYS:SG	5:A:1202:NAG:C7	3.05	0.42
1:B:206:TYR:HE1	1:B:208:TYR:CE2	2.37	0.42
1:B:762:THR:CB	1:C:581:ASN:HB3	2.48	0.42
1:B:967:CYS:HB3	1:B:1014:CYS:SG	2.60	0.42
1:B:1024:SER:OG	1:B:1025:GLU:N	2.53	0.42
1:C:230:CYS:CB	5:C:1202:NAG:H83	2.43	0.42
1:A:206:TYR:HE1	1:A:208:TYR:CE2	2.37	0.42
1:A:372:SER:HB2	1:C:870:ASP:OD1	2.18	0.42
1:A:1024:SER:OG	1:A:1025:GLU:N	2.53	0.42
1:B:299:HIS:HA	1:B:433:GLU:OE1	2.19	0.42
1:C:1024:SER:OG	1:C:1025:GLU:N	2.53	0.42
1:A:299:HIS:HA	1:A:433:GLU:OE1	2.19	0.42
1:A:526:ASN:O	1:A:536:ALA:HA	2.20	0.42
1:B:96:TYR:CZ	1:B:216:ALA:HB2	2.54	0.42
1:B:297:HIS:HB3	1:B:433:GLU:HB3	2.02	0.42
1:C:297:HIS:HB3	1:C:433:GLU:HB3	2.02	0.42
1:C:297:HIS:HB3	1:C:433:GLU:HG2	2.01	0.42
1:A:582:LEU:HA	1:C:762:THR:N	2.35	0.42
1:B:96:TYR:O	1:B:97:PHE:C	2.62	0.42
1:C:234:LEU:H	1:C:234:LEU:HD23	1.83	0.42
1:C:297:HIS:CD2	1:C:345:HIS:CE1	3.08	0.42
1:A:195:ILE:HD12	1:A:195:ILE:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:OD1	1:A:309:LYS:HB2	2.20	0.42
1:B:60:LEU:HD23	1:B:205:GLY:HA2	2.01	0.42
1:B:865:ILE:HD13	1:B:865:ILE:HA	1.92	0.42
1:C:60:LEU:HD23	1:C:205:GLY:HA2	2.01	0.42
1:C:364:ILE:HD12	1:C:364:ILE:HA	1.73	0.42
1:C:625:GLN:HG3	1:C:626:TYR:CD1	2.54	0.42
1:C:748:TYR:CE2	1:C:752:LEU:HD11	2.55	0.42
1:A:297:HIS:CD2	1:A:345:HIS:CE1	3.08	0.42
1:A:967:CYS:HB3	1:A:1014:CYS:SG	2.60	0.42
1:B:297:HIS:HB3	1:B:433:GLU:HG2	2.01	0.42
1:B:518:ASN:HB2	1:B:534:PHE:CE2	2.55	0.42
1:C:967:CYS:HB3	1:C:1014:CYS:SG	2.60	0.42
1:A:312:SER:OG	1:A:313:GLY:N	2.53	0.42
1:B:85:VAL:CG1	1:B:88:LEU:HB3	2.48	0.42
1:B:195:ILE:HD12	1:B:195:ILE:HA	1.93	0.42
1:C:518:ASN:HB2	1:C:534:PHE:CE2	2.55	0.42
1:A:297:HIS:HB3	1:A:433:GLU:HB3	2.02	0.41
1:B:96:TYR:CD1	1:B:216:ALA:HB2	2.55	0.41
1:B:297:HIS:NE2	1:B:345:HIS:HE1	2.18	0.41
1:B:307:ASP:OD1	1:B:309:LYS:HB2	2.20	0.41
1:B:349:LYS:HE3	1:B:349:LYS:HB2	1.74	0.41
1:B:625:GLN:HG3	1:B:626:TYR:CD1	2.54	0.41
1:C:295:VAL:O	1:C:297:HIS:HD2	2.03	0.41
1:A:299:HIS:CD2	1:A:433:GLU:HB2	2.56	0.41
1:B:81:CYS:HB2	1:B:234:LEU:CD2	2.51	0.41
1:C:297:HIS:NE2	1:C:345:HIS:HE1	2.18	0.41
1:A:96:TYR:O	1:A:97:PHE:C	2.62	0.41
1:A:295:VAL:O	1:A:297:HIS:HD2	2.03	0.41
1:A:480:LEU:H	1:A:480:LEU:HD23	1.85	0.41
1:B:96:TYR:CD1	5:B:1201:NAG:C8	3.01	0.41
1:B:141:VAL:HA	1:B:172:THR:HA	2.02	0.41
1:B:480:LEU:H	1:B:480:LEU:HD23	1.85	0.41
1:B:748:TYR:CE2	1:B:752:LEU:HD11	2.55	0.41
1:C:57:TRP:CZ3	1:C:118:ARG:NE	2.88	0.41
1:C:269:PHE:CD1	1:C:269:PHE:N	2.88	0.41
1:A:297:HIS:HB3	1:A:433:GLU:HG2	2.01	0.41
1:A:748:TYR:CE2	1:A:752:LEU:HD11	2.55	0.41
1:A:778:ASN:HA	1:A:781:ALA:O	2.21	0.41
5:A:1201:NAG:O7	5:A:1201:NAG:O3	2.34	0.41
1:C:480:LEU:HD23	1:C:480:LEU:H	1.85	0.41
1:C:613:CYS:SG	1:C:620:VAL:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD23	1:A:205:GLY:HA2	2.01	0.41
1:A:297:HIS:NE2	1:A:345:HIS:HE1	2.18	0.41
1:C:526:ASN:O	1:C:536:ALA:HA	2.19	0.41
1:C:778:ASN:HA	1:C:781:ALA:O	2.21	0.41
1:B:57:TRP:CZ3	1:B:118:ARG:NE	2.88	0.41
1:B:295:VAL:O	1:B:297:HIS:HD2	2.03	0.41
1:B:572:ASP:OD1	1:B:572:ASP:N	2.53	0.41
1:C:48:ILE:HA	1:C:49:PRO:HD3	1.92	0.41
1:C:312:SER:OG	1:C:313:GLY:N	2.53	0.41
1:A:141:VAL:HA	1:A:172:THR:HA	2.02	0.41
1:A:518:ASN:HB2	1:A:534:PHE:CE2	2.55	0.41
1:B:147:ASN:HB3	1:B:154:ASP:OD2	2.21	0.41
1:B:879:ASP:O	1:B:882:ILE:HG12	2.21	0.41
1:C:299:HIS:CD2	1:C:433:GLU:HB2	2.56	0.41
1:C:691:ALA:C	1:C:693:GLU:N	2.75	0.41
1:C:711:ASP:OD1	1:C:711:ASP:O	2.39	0.41
1:A:613:CYS:SG	1:A:620:VAL:HA	2.60	0.41
1:B:269:PHE:CD1	1:B:269:PHE:N	2.88	0.41
1:B:403:ASN:HA	1:B:408:LYS:O	2.20	0.41
1:C:96:TYR:CD1	5:C:1201:NAG:C8	3.01	0.41
1:A:81:CYS:HB2	1:A:234:LEU:CD2	2.50	0.41
1:A:96:TYR:CD1	1:A:216:ALA:HB2	2.55	0.41
1:A:208:TYR:HD1	1:B:293:LEU:HD11	1.85	0.41
1:A:403:ASN:HA	1:A:408:LYS:O	2.20	0.41
1:A:998:PHE:O	1:A:998:PHE:CD2	2.74	0.41
1:B:230:CYS:CB	5:B:1202:NAG:C8	2.99	0.41
1:B:297:HIS:CD2	1:B:345:HIS:CE1	3.08	0.41
1:B:711:ASP:O	1:B:711:ASP:OD1	2.39	0.41
1:C:81:CYS:HB2	1:C:234:LEU:CD2	2.50	0.41
1:C:96:TYR:CG	1:C:216:ALA:CB	2.95	0.41
1:C:96:TYR:O	1:C:97:PHE:C	2.62	0.41
1:C:147:ASN:HB3	1:C:154:ASP:OD2	2.21	0.41
1:C:230:CYS:SG	5:C:1202:NAG:C7	3.03	0.41
1:C:403:ASN:HA	1:C:408:LYS:O	2.20	0.41
1:C:548:LEU:HB3	1:C:555:VAL:CG2	2.51	0.41
1:B:81:CYS:HB2	1:B:234:LEU:HD21	2.03	0.41
1:C:72:ARG:HA	1:C:241:LEU:HA	2.03	0.41
1:C:85:VAL:CG1	1:C:88:LEU:HB3	2.48	0.41
1:A:185:ALA:N	1:B:294:PRO:O	2.36	0.40
1:A:269:PHE:CD1	1:A:269:PHE:N	2.88	0.40
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:SER:OG	1:A:1023:ARG:N	2.54	0.40
1:B:548:LEU:HB3	1:B:555:VAL:CG2	2.51	0.40
1:A:711:ASP:O	1:A:711:ASP:OD1	2.39	0.40
1:B:312:SER:OG	1:B:313:GLY:N	2.53	0.40
1:B:613:CYS:SG	1:B:620:VAL:HA	2.60	0.40
1:C:81:CYS:HB2	1:C:234:LEU:HD21	2.03	0.40
1:C:307:ASP:OD1	1:C:309:LYS:HB2	2.20	0.40
1:C:1022:SER:OG	1:C:1023:ARG:N	2.54	0.40
1:A:271:VAL:H	1:A:271:VAL:HG12	1.62	0.40
1:A:548:LEU:HB3	1:A:555:VAL:CG1	2.51	0.40
1:B:260:ASN:OD1	1:B:263:ARG:NH1	2.53	0.40
1:B:299:HIS:CD2	1:B:433:GLU:HB2	2.56	0.40
1:B:778:ASN:HA	1:B:781:ALA:O	2.21	0.40
1:C:230:CYS:CB	5:C:1202:NAG:C8	2.99	0.40
1:A:81:CYS:HB2	1:A:234:LEU:HD21	2.03	0.40
1:A:96:TYR:CZ	1:A:216:ALA:HB2	2.54	0.40
1:A:182:PHE:HE2	1:B:298:LYS:HD2	1.86	0.40
1:B:998:PHE:O	1:B:998:PHE:CD2	2.74	0.40
1:A:410:TYR:HE1	1:B:338:PRO:HD2	1.85	0.40
1:B:862:ILE:HD12	1:B:862:ILE:N	2.36	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	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	24	58
1	B	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	24	58
1	C	951/1116 (85%)	893 (94%)	53 (6%)	5 (0%)	24	58
All	All	2853/3348 (85%)	2679 (94%)	159 (6%)	15 (0%)	26	58

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	VAL
1	A	331	ASN
1	A	351	VAL
1	B	325	VAL
1	B	331	ASN
1	B	351	VAL
1	C	325	VAL
1	C	331	ASN
1	C	351	VAL
1	A	399	PRO
1	B	399	PRO
1	B	667	PHE
1	C	399	PRO
1	A	667	PHE
1	C	667	PHE

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	731/969 (75%)	684 (94%)	47 (6%)	16	46
1	B	721/969 (74%)	679 (94%)	42 (6%)	18	49
1	C	723/969 (75%)	684 (95%)	39 (5%)	20	51
All	All	2175/2907 (75%)	2047 (94%)	128 (6%)	19	48

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	81	CYS
1	A	88	LEU
1	A	96	TYR
1	A	111	ASP
1	A	117	ILE

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Mol	Chain	Res	Type
1	A	140	VAL
1	A	141	VAL
1	A	151	VAL
1	A	183	VAL
1	A	190	VAL
1	A	194	VAL
1	A	203	ILE
1	A	221	VAL
1	A	228	ASP
1	A	242	VAL
1	A	270	ASP
1	A	271	VAL
1	A	302	ILE
1	A	351	VAL
1	A	353	VAL
1	A	357	VAL
1	A	363	SER
1	A	364	ILE
1	A	369	CYS
1	A	376	VAL
1	A	392	ILE
1	A	400	ILE
1	A	401	VAL
1	A	403	ASN
1	A	432	VAL
1	A	435	VAL
1	A	528	VAL
1	A	547	VAL
1	A	555	VAL
1	A	573	SER
1	A	586	SER
1	A	630	CYS
1	A	672	LEU
1	A	692	ILE
1	A	724	LEU
1	A	770	SER
1	A	780	VAL
1	A	860	SER
1	A	928	CYS
1	A	953	LEU
1	A	968	VAL
1	B	79	LEU

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Mol	Chain	Res	Type
1	B	81	CYS
1	B	88	LEU
1	B	95	VAL
1	B	96	TYR
1	B	111	ASP
1	B	112	VAL
1	B	117	ILE
1	B	140	VAL
1	B	170	VAL
1	B	183	VAL
1	B	190	VAL
1	B	194	VAL
1	B	203	ILE
1	B	221	VAL
1	B	228	ASP
1	B	242	VAL
1	B	270	ASP
1	B	302	ILE
1	B	353	VAL
1	B	363	SER
1	B	364	ILE
1	B	369	CYS
1	B	380	VAL
1	B	392	ILE
1	B	400	ILE
1	B	403	ASN
1	B	435	VAL
1	B	441	VAL
1	B	547	VAL
1	B	573	SER
1	B	586	SER
1	B	630	CYS
1	B	672	LEU
1	B	692	ILE
1	B	724	LEU
1	B	770	SER
1	B	780	VAL
1	B	860	SER
1	B	928	CYS
1	B	953	LEU
1	B	968	VAL
1	C	79	LEU

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Mol	Chain	Res	Type
1	C	81	CYS
1	C	88	LEU
1	C	96	TYR
1	C	111	ASP
1	C	112	VAL
1	C	117	ILE
1	C	140	VAL
1	C	141	VAL
1	C	170	VAL
1	C	183	VAL
1	C	203	ILE
1	C	228	ASP
1	C	270	ASP
1	C	271	VAL
1	C	302	ILE
1	C	351	VAL
1	C	353	VAL
1	C	357	VAL
1	C	363	SER
1	C	364	ILE
1	C	369	CYS
1	C	380	VAL
1	C	392	ILE
1	C	400	ILE
1	C	403	ASN
1	C	428	VAL
1	C	435	VAL
1	C	573	SER
1	C	586	SER
1	C	630	CYS
1	C	672	LEU
1	C	692	ILE
1	C	724	LEU
1	C	770	SER
1	C	860	SER
1	C	928	CYS
1	C	953	LEU
1	C	968	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	266	GLN
1	A	299	HIS
1	A	345	HIS
1	A	403	ASN
1	A	774	GLN
1	A	791	GLN
1	A	850	GLN
1	A	856	GLN
1	A	890	ASN
1	A	921	GLN
1	A	933	HIS
1	A	949	HIS
1	B	75	GLN
1	B	299	HIS
1	B	345	HIS
1	B	403	ASN
1	B	774	GLN
1	B	791	GLN
1	B	850	GLN
1	B	856	GLN
1	B	890	ASN
1	B	921	GLN
1	B	933	HIS
1	B	949	HIS
1	C	75	GLN
1	C	299	HIS
1	C	345	HIS
1	C	403	ASN
1	C	469	ASN
1	C	774	GLN
1	C	791	GLN
1	C	839	GLN
1	C	850	GLN
1	C	856	GLN
1	C	890	ASN
1	C	921	GLN
1	C	933	HIS
1	C	949	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

45 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	2,1	14,14,15	0.40	0	17,19,21	1.12	2 (11%)
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.75	0
2	BMA	D	3	2	11,11,12	0.35	0	15,15,17	1.48	3 (20%)
2	MAN	D	4	2	11,11,12	0.19	0	15,15,17	0.74	0
2	MAN	D	5	2	11,11,12	0.20	0	15,15,17	0.60	0
2	MAN	D	6	2	11,11,12	0.18	0	15,15,17	0.99	1 (6%)
2	MAN	D	7	2	11,11,12	0.22	0	15,15,17	0.91	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.64	0	17,19,21	0.78	0
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	0.40	0
3	BMA	E	3	3	11,11,12	0.49	0	15,15,17	0.93	1 (6%)
4	NAG	F	1	1,4	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.60	0
3	NAG	G	1	1,3	14,14,15	0.67	0	17,19,21	0.71	1 (5%)
3	NAG	G	2	3	14,14,15	0.49	0	17,19,21	0.40	0
3	BMA	G	3	3	11,11,12	0.51	0	15,15,17	0.94	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.41	0	17,19,21	1.11	2 (11%)
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.77	0
2	BMA	H	3	2	11,11,12	0.35	0	15,15,17	1.49	3 (20%)
2	MAN	H	4	2	11,11,12	0.19	0	15,15,17	0.73	0
2	MAN	H	5	2	11,11,12	0.18	0	15,15,17	0.61	0
2	MAN	H	6	2	11,11,12	0.19	0	15,15,17	1.00	1 (6%)
2	MAN	H	7	2	11,11,12	0.22	0	15,15,17	0.92	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.63	0	17,19,21	0.78	0
3	NAG	I	2	3	14,14,15	0.59	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	I	3	3	11,11,12	0.50	0	15,15,17	0.93	1 (6%)
4	NAG	J	1	1,4	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	J	2	4	14,14,15	0.22	0	17,19,21	0.61	0
3	NAG	K	1	1,3	14,14,15	0.67	0	17,19,21	0.71	1 (5%)
3	NAG	K	2	3	14,14,15	0.51	0	17,19,21	0.41	0
3	BMA	K	3	3	11,11,12	0.50	0	15,15,17	0.94	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.39	0	17,19,21	1.12	2 (11%)
2	NAG	L	2	2	14,14,15	0.31	0	17,19,21	0.75	0
2	BMA	L	3	2	11,11,12	0.35	0	15,15,17	1.48	3 (20%)
2	MAN	L	4	2	11,11,12	0.20	0	15,15,17	0.73	0
2	MAN	L	5	2	11,11,12	0.20	0	15,15,17	0.61	0
2	MAN	L	6	2	11,11,12	0.17	0	15,15,17	1.00	1 (6%)
2	MAN	L	7	2	11,11,12	0.21	0	15,15,17	0.90	0
3	NAG	M	1	1,3	14,14,15	0.64	0	17,19,21	0.77	0
3	NAG	M	2	3	14,14,15	0.59	0	17,19,21	0.40	0
3	BMA	M	3	3	11,11,12	0.50	0	15,15,17	0.93	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	N	2	4	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	O	1	1,3	14,14,15	0.67	0	17,19,21	0.70	1 (5%)
3	NAG	O	2	3	14,14,15	0.50	0	17,19,21	0.40	0
3	BMA	O	3	3	11,11,12	0.50	0	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	1/1/1/1
2	MAN	D	6	2	-	0/2/19/22	1/1/1/1
2	MAN	D	7	2	-	0/2/19/22	1/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	MAN	H	5	2	-	1/2/19/22	1/1/1/1
2	MAN	H	6	2	-	0/2/19/22	1/1/1/1
2	MAN	H	7	2	-	0/2/19/22	1/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1
2	MAN	L	5	2	-	1/2/19/22	1/1/1/1
2	MAN	L	6	2	-	0/2/19/22	1/1/1/1
2	MAN	L	7	2	-	0/2/19/22	1/1/1/1
3	NAG	M	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	BMA	C3-C4-C5	3.66	116.88	110.23
2	L	3	BMA	C3-C4-C5	3.64	116.83	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C3-C4-C5	3.63	116.82	110.23
2	L	1	NAG	O5-C1-C2	-3.41	106.01	111.29
2	D	1	NAG	O5-C1-C2	-3.37	106.07	111.29
2	H	1	NAG	O5-C1-C2	-3.37	106.08	111.29
2	D	6	MAN	C2-C3-C4	-2.70	106.11	110.86
2	L	6	MAN	C2-C3-C4	-2.69	106.14	110.86
2	H	6	MAN	C2-C3-C4	-2.67	106.17	110.86
2	L	3	BMA	C6-C5-C4	-2.50	106.87	113.02
2	D	3	BMA	C6-C5-C4	-2.50	106.89	113.02
2	H	3	BMA	C6-C5-C4	-2.48	106.93	113.02
3	O	3	BMA	C1-O5-C5	2.26	115.22	112.19
3	K	3	BMA	C1-O5-C5	2.26	115.21	112.19
3	G	3	BMA	C1-O5-C5	2.25	115.20	112.19
3	M	3	BMA	C1-O5-C5	2.25	115.20	112.19
3	I	3	BMA	C1-O5-C5	2.23	115.17	112.19
3	E	3	BMA	C1-O5-C5	2.20	115.14	112.19
2	D	1	NAG	C2-N2-C7	-2.13	120.04	122.90
2	L	1	NAG	C2-N2-C7	-2.13	120.05	122.90
2	H	1	NAG	C2-N2-C7	-2.10	120.08	122.90
2	H	3	BMA	O3-C3-C4	-2.10	105.44	110.38
2	D	3	BMA	O3-C3-C4	-2.09	105.45	110.38
2	L	3	BMA	O3-C3-C4	-2.08	105.48	110.38
3	K	1	NAG	C4-C3-C2	-2.06	108.00	111.02
2	H	7	MAN	C1-C2-C3	-2.04	106.67	109.64
2	D	7	MAN	C1-C2-C3	-2.04	106.67	109.64
3	G	1	NAG	C4-C3-C2	-2.04	108.03	111.02
3	O	1	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	D	5	MAN	O5-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
2	L	5	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6

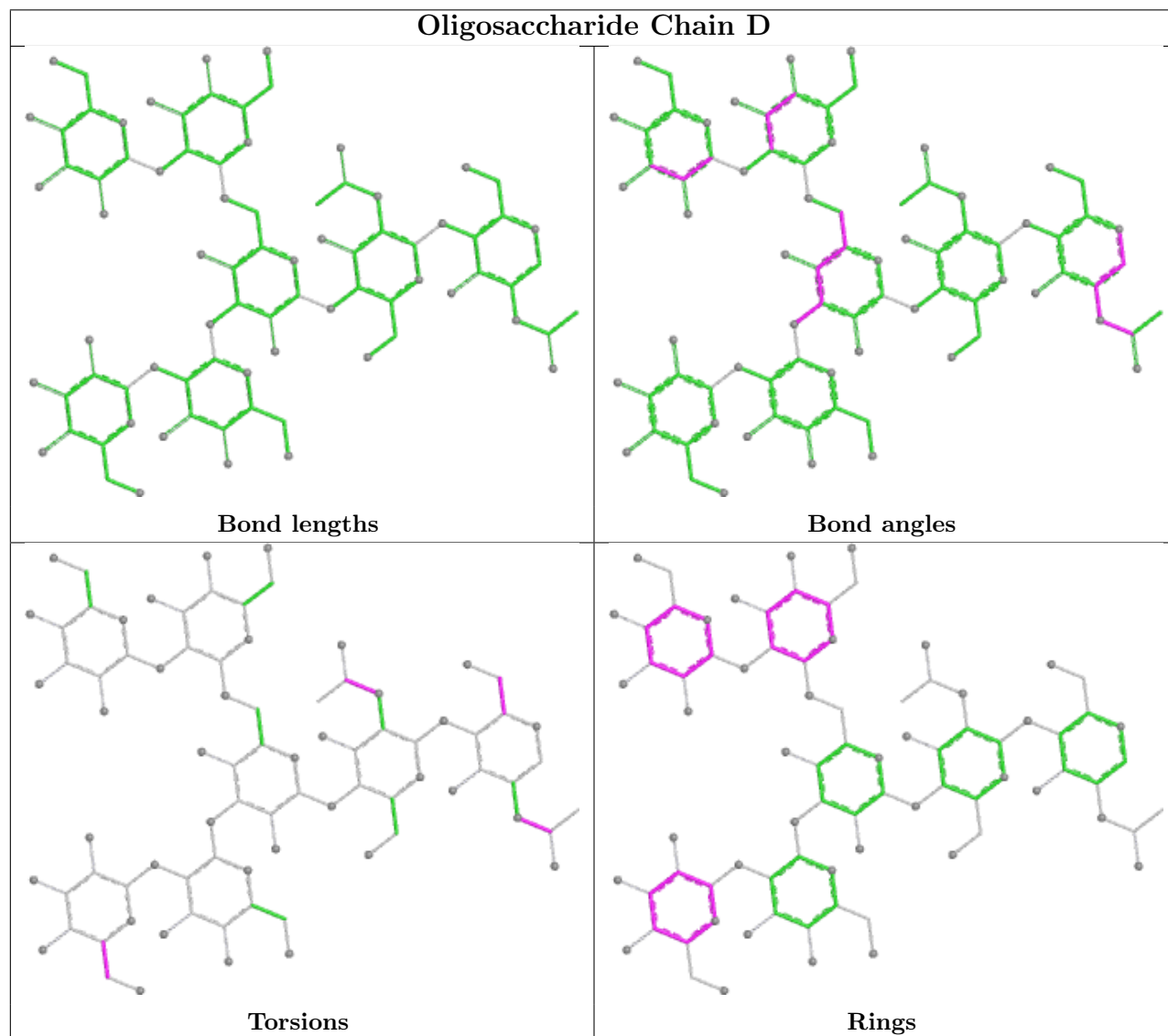
All (9) ring outliers are listed below:

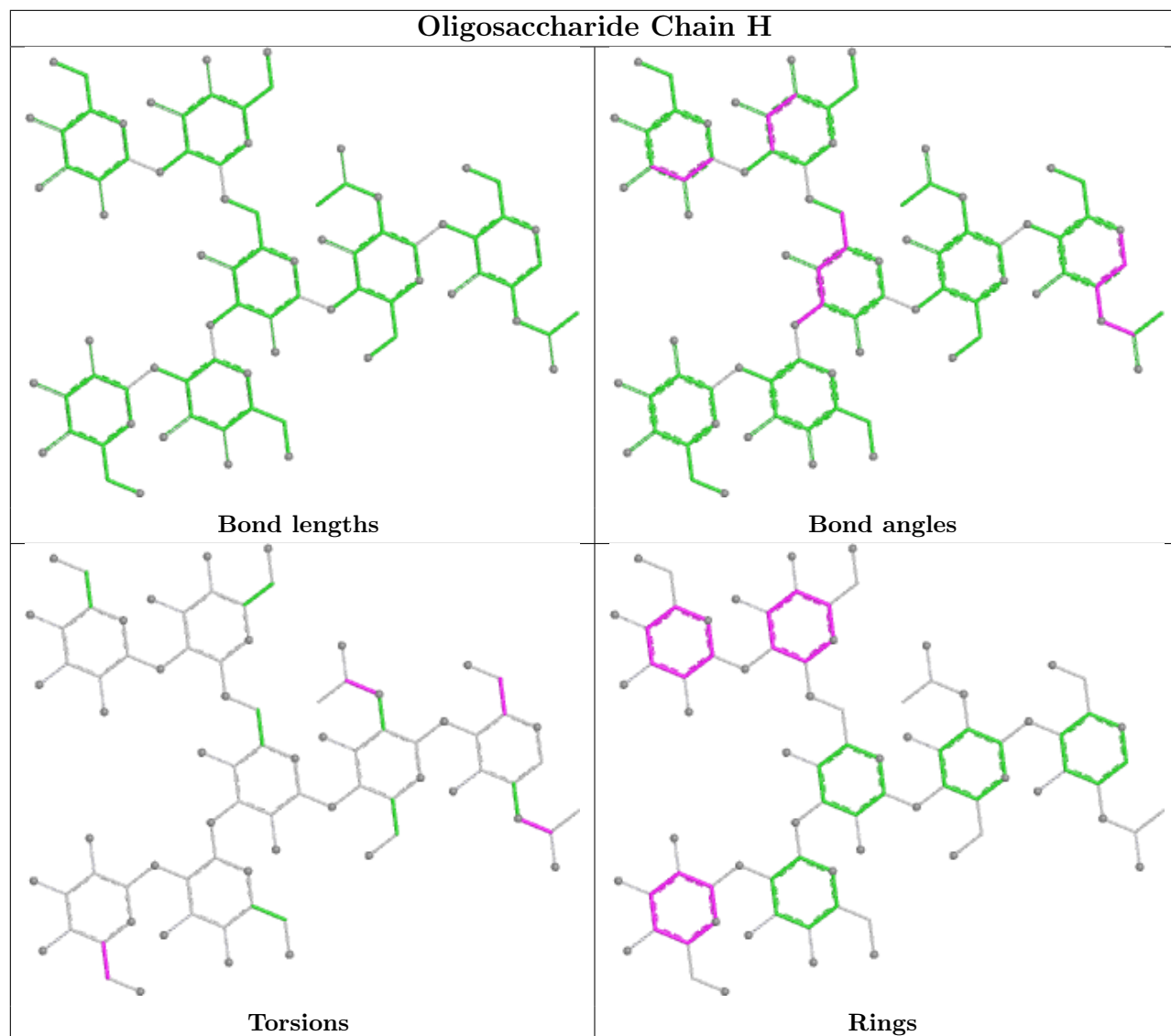
Mol	Chain	Res	Type	Atoms
2	D	7	MAN	C1-C2-C3-C4-C5-O5
2	H	7	MAN	C1-C2-C3-C4-C5-O5
2	L	7	MAN	C1-C2-C3-C4-C5-O5
2	H	5	MAN	C1-C2-C3-C4-C5-O5
2	L	5	MAN	C1-C2-C3-C4-C5-O5
2	D	5	MAN	C1-C2-C3-C4-C5-O5
2	H	6	MAN	C1-C2-C3-C4-C5-O5
2	D	6	MAN	C1-C2-C3-C4-C5-O5
2	L	6	MAN	C1-C2-C3-C4-C5-O5

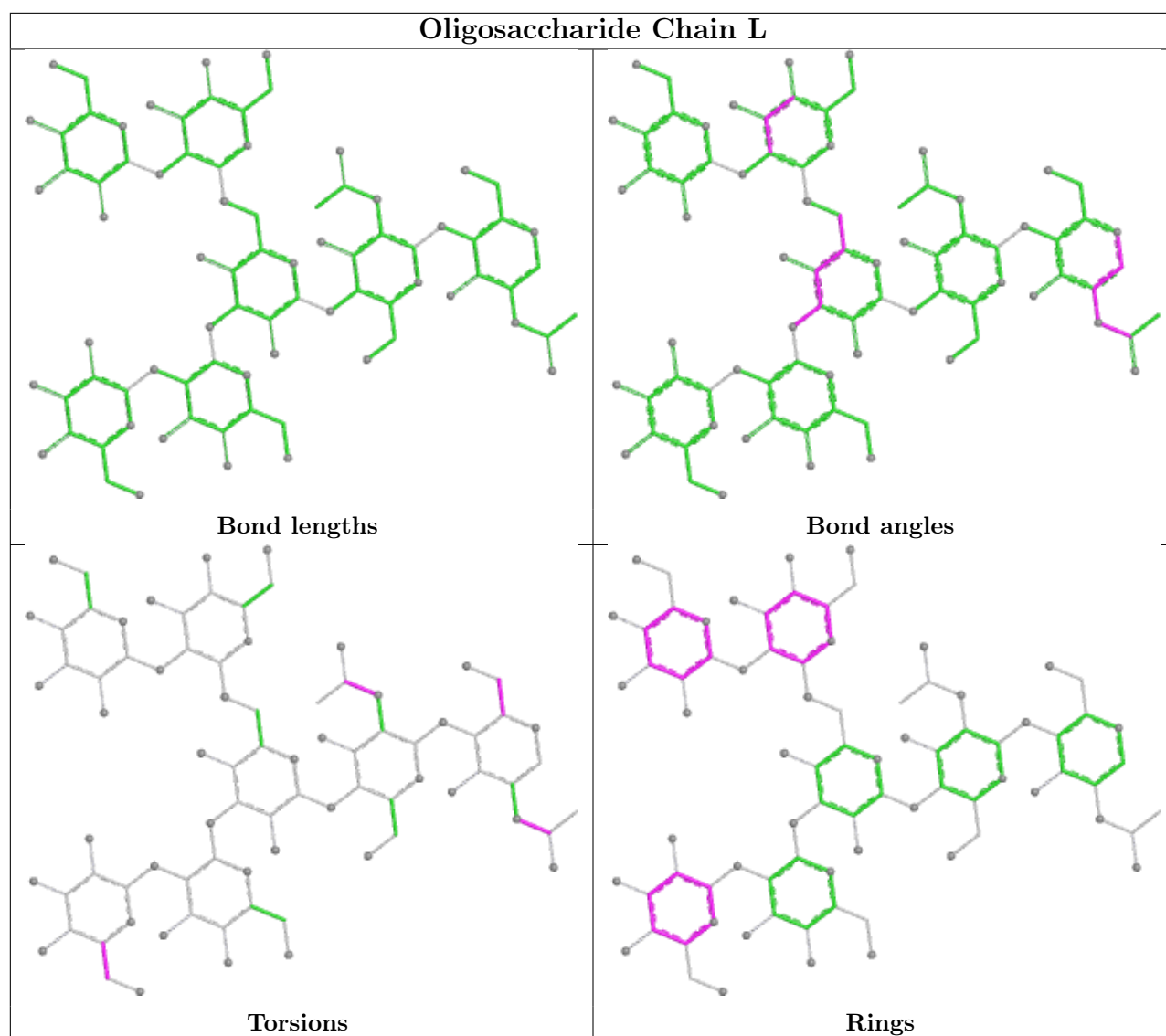
3 monomers are involved in 6 short contacts:

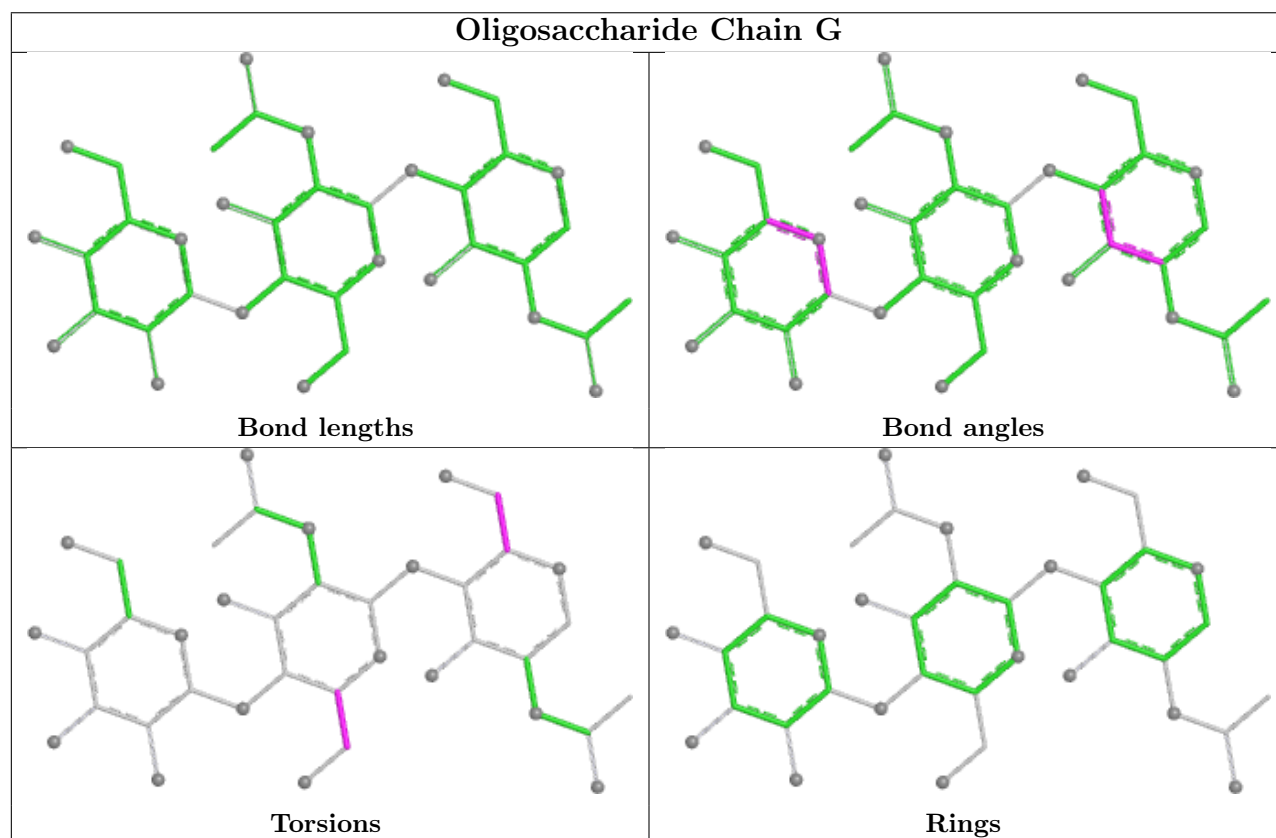
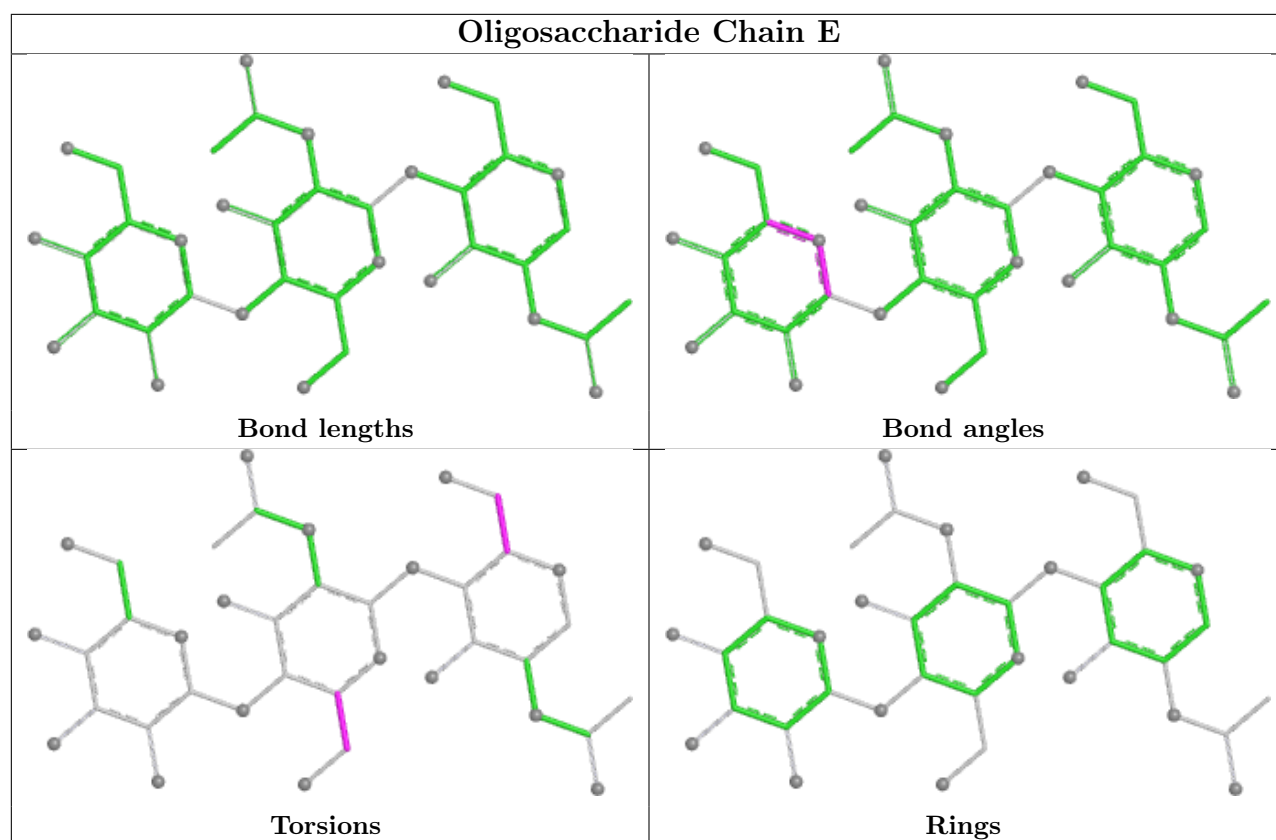
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	2	0
3	O	1	NAG	2	0
3	G	1	NAG	2	0

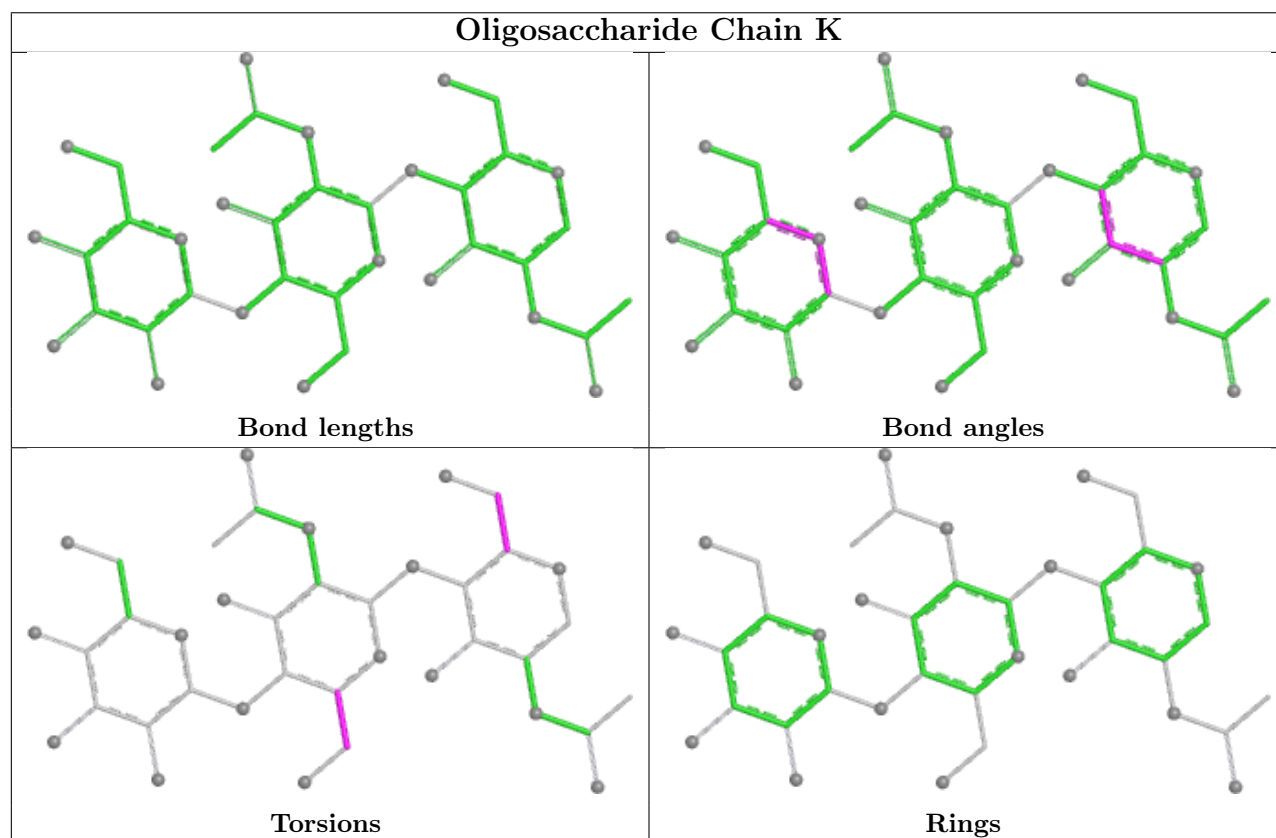
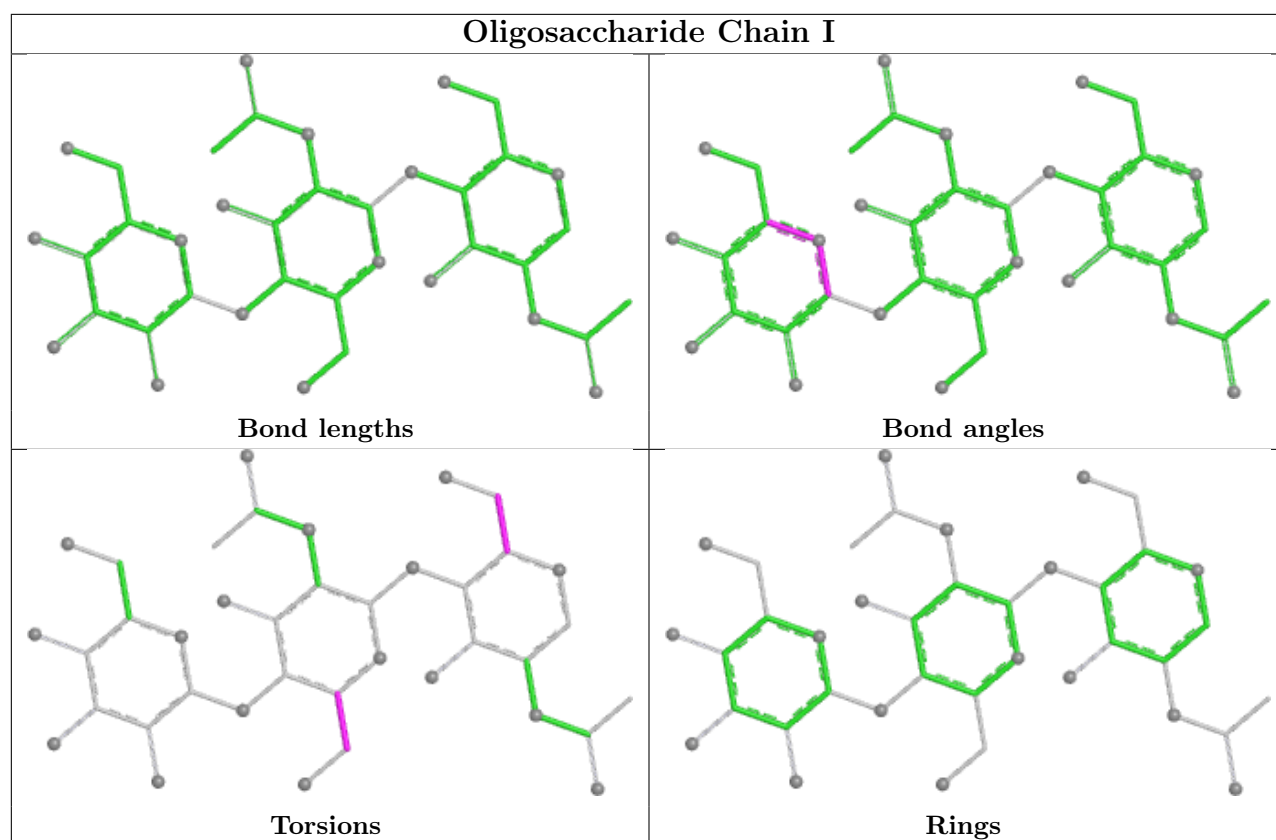
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

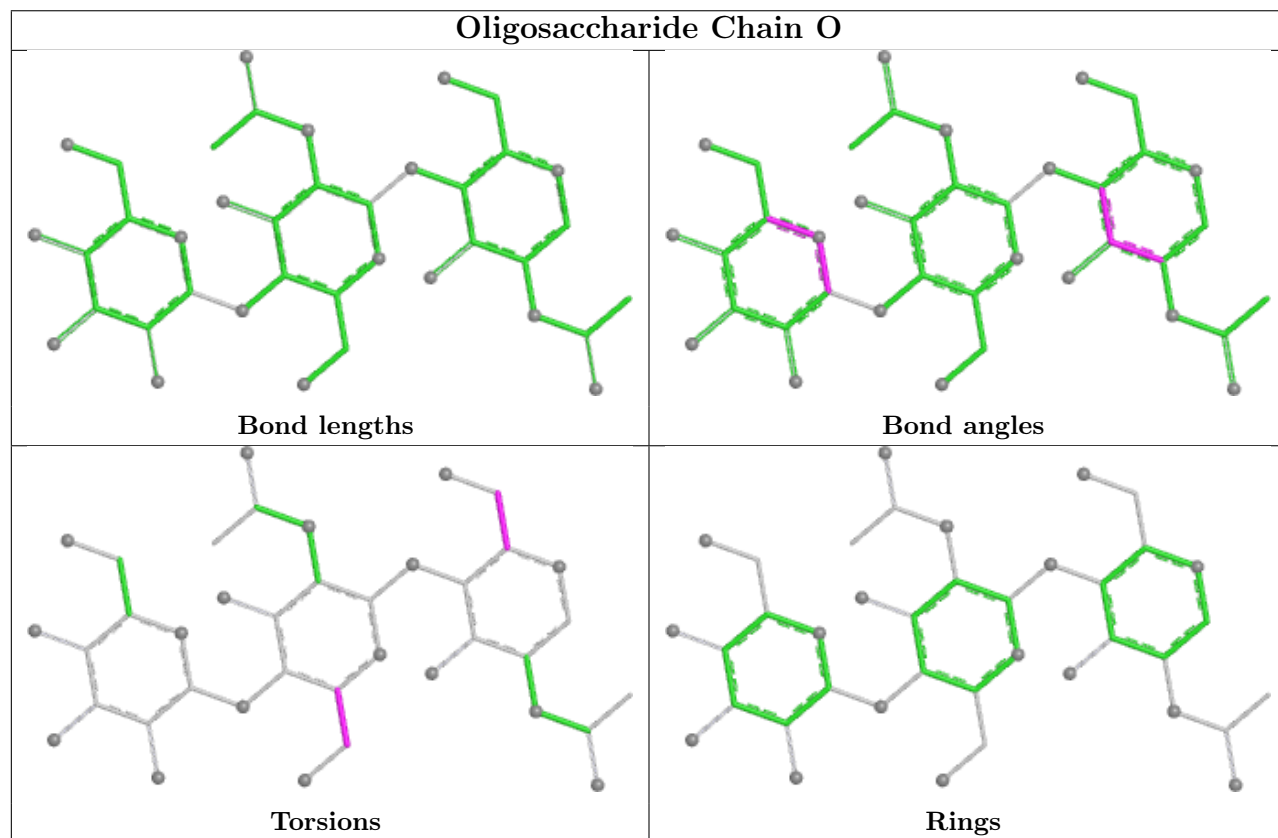
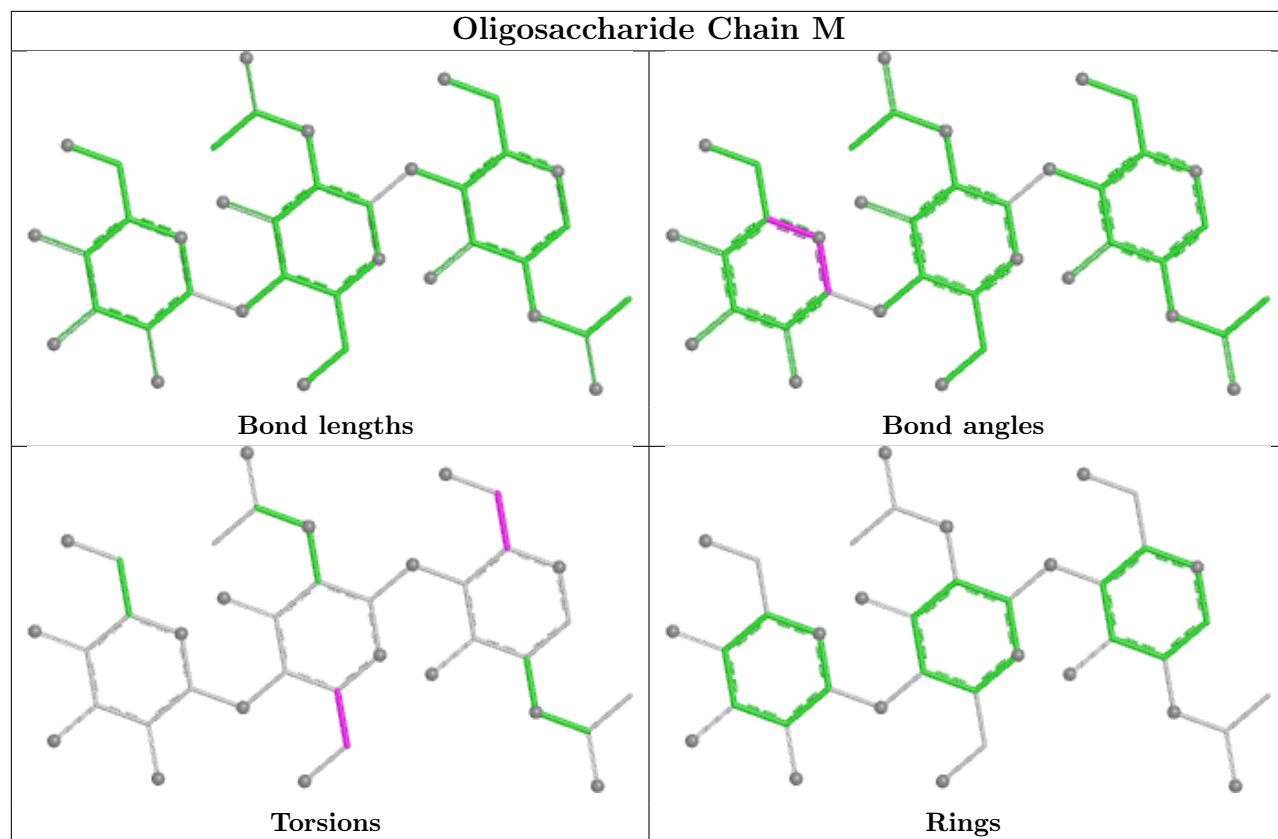


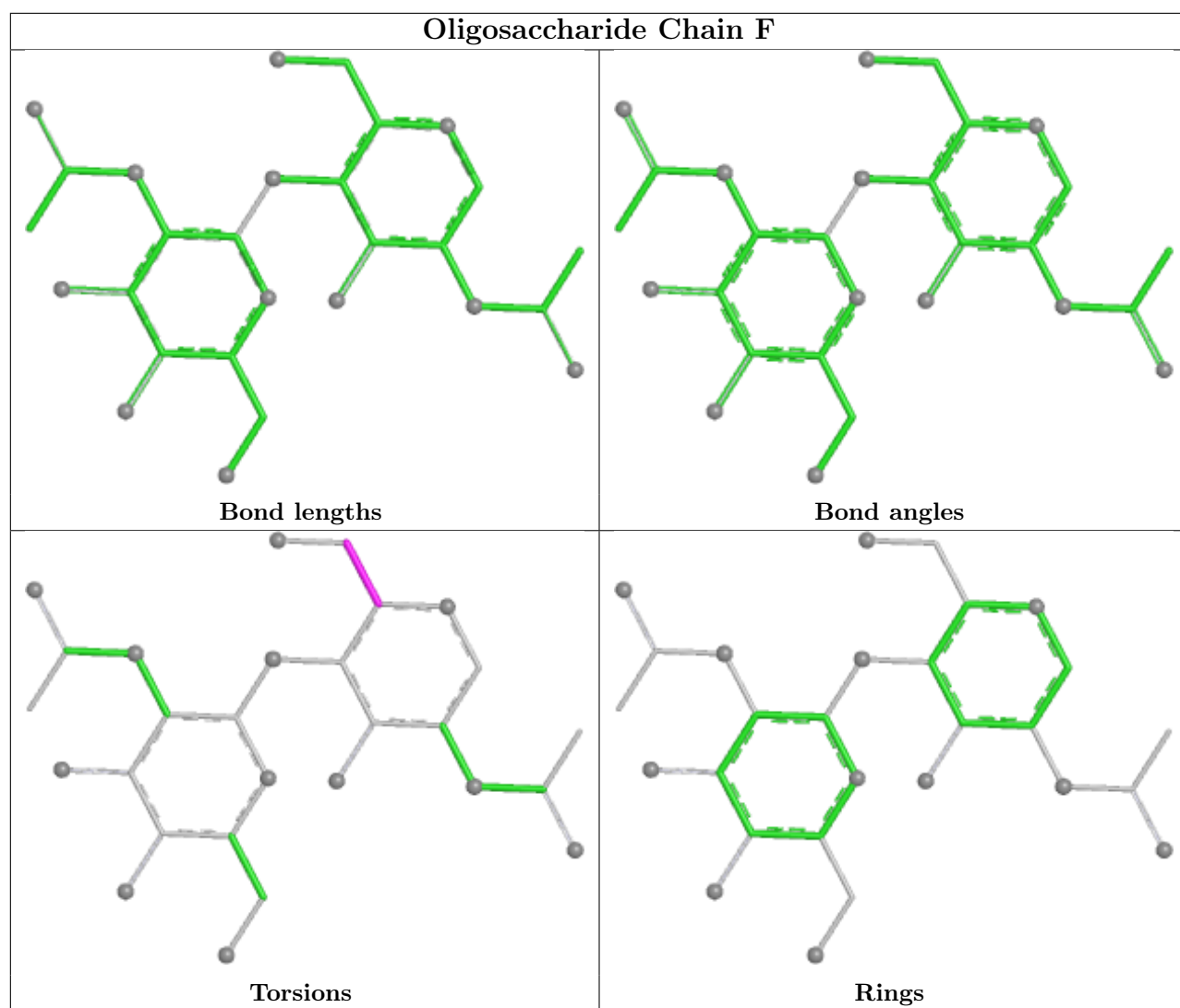


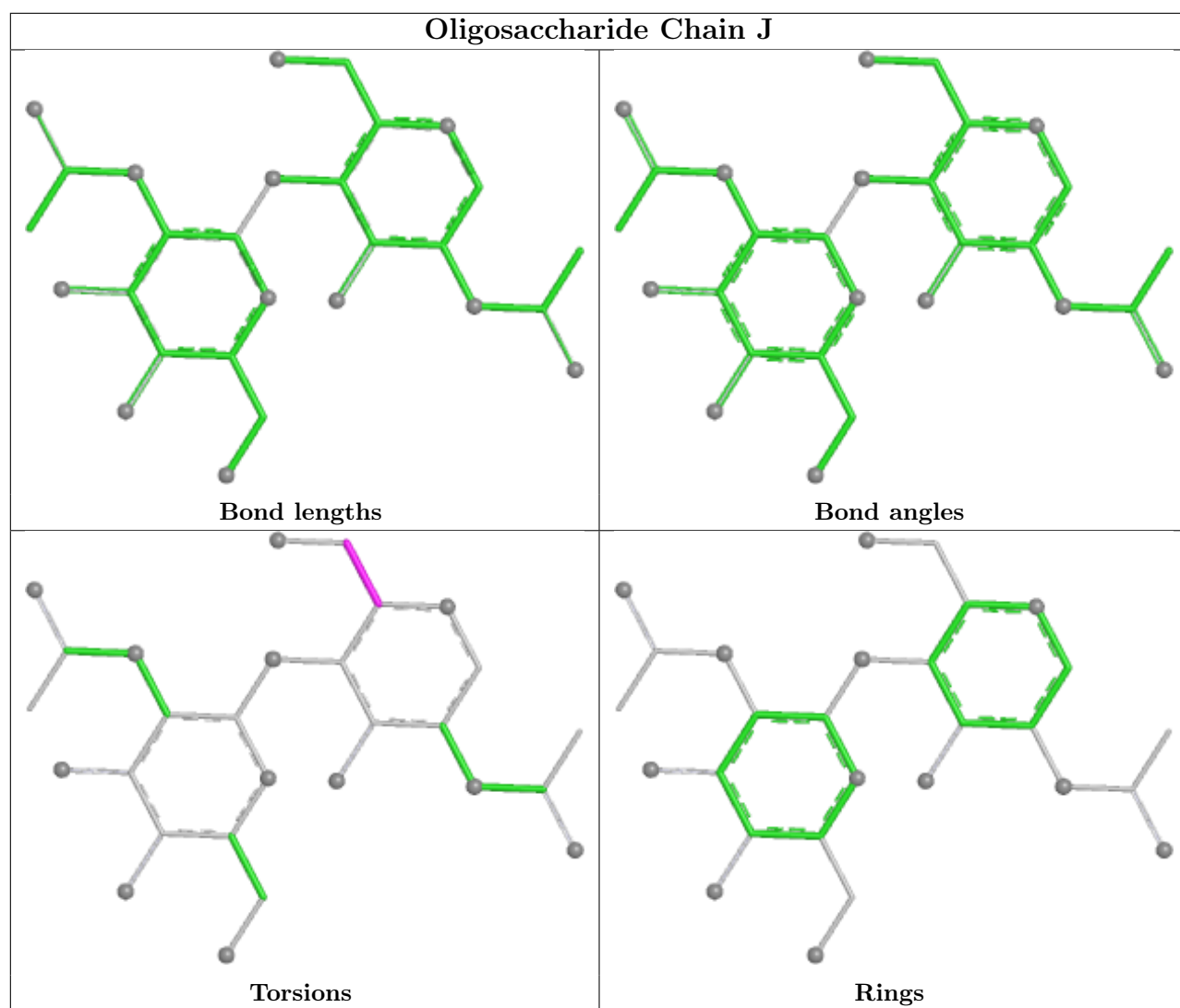


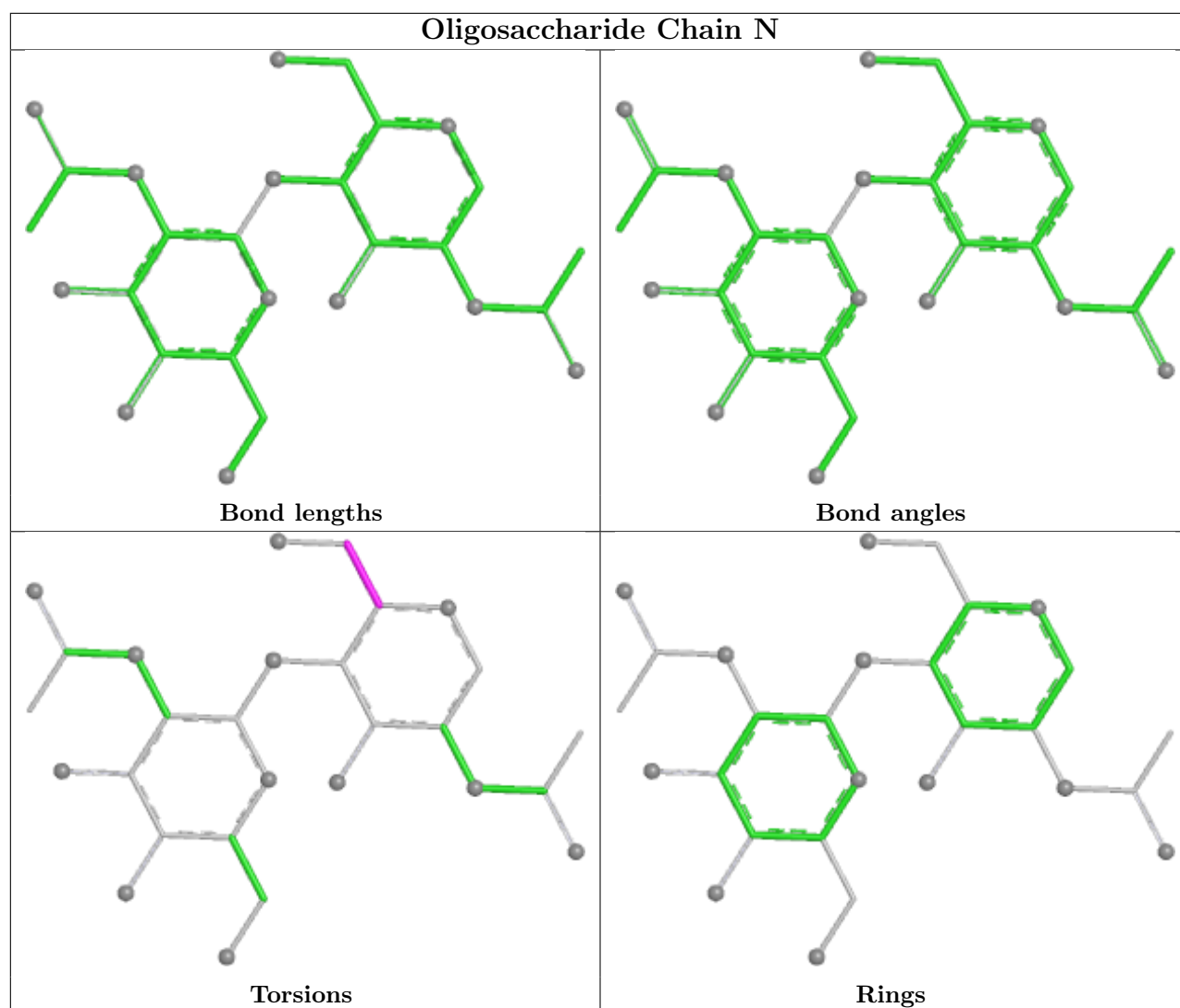












5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1210	1	14,14,15	0.33	0	17,19,21	0.49	0
5	NAG	A	1213	1	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
5	NAG	B	1208	1	14,14,15	0.13	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1216	1	14,14,15	0.50	0	17,19,21	0.41	0
5	NAG	A	1206	1	14,14,15	0.21	0	17,19,21	0.38	0
5	NAG	C	1205	1	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
5	NAG	A	1204	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	C	1206	1	14,14,15	0.18	0	17,19,21	0.37	0
5	NAG	C	1201	1	14,14,15	0.53	0	17,19,21	0.47	0
5	NAG	A	1215	1	14,14,15	0.39	0	17,19,21	0.34	0
5	NAG	A	1212	1	14,14,15	0.27	0	17,19,21	0.38	0
5	NAG	A	1201	1	14,14,15	0.53	0	17,19,21	0.48	0
5	NAG	A	1208	1	14,14,15	0.13	0	17,19,21	0.61	0
5	NAG	B	1202	1	14,14,15	0.62	0	17,19,21	0.48	0
5	NAG	B	1209	1	14,14,15	0.76	1 (7%)	17,19,21	0.45	0
5	NAG	B	1201	1	14,14,15	0.53	0	17,19,21	0.48	0
5	NAG	C	1203	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	A	1203	1	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	C	1202	1	14,14,15	0.60	0	17,19,21	0.47	0
5	NAG	C	1209	1	14,14,15	0.77	1 (7%)	17,19,21	0.45	0
5	NAG	A	1205	1	14,14,15	0.35	0	17,19,21	0.80	1 (5%)
5	NAG	A	1209	1	14,14,15	0.77	1 (7%)	17,19,21	0.44	0
5	NAG	B	1203	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	B	1211	1	14,14,15	1.28	1 (7%)	17,19,21	1.69	2 (11%)
5	NAG	C	1210	1	14,14,15	0.33	0	17,19,21	0.48	0
5	NAG	C	1213	1	14,14,15	0.21	0	17,19,21	0.75	1 (5%)
5	NAG	B	1207	1	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
5	NAG	B	1212	1	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	A	1211	1	14,14,15	1.31	1 (7%)	17,19,21	1.69	2 (11%)
5	NAG	B	1214	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
5	NAG	C	1208	1	14,14,15	0.13	0	17,19,21	0.63	0
5	NAG	B	1205	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
5	NAG	A	1202	1	14,14,15	0.60	0	17,19,21	0.47	0
5	NAG	B	1210	1	14,14,15	0.33	0	17,19,21	0.47	0
5	NAG	A	1216	1	14,14,15	0.50	0	17,19,21	0.41	0
5	NAG	B	1206	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	C	1211	1	14,14,15	1.31	1 (7%)	17,19,21	1.71	2 (11%)
5	NAG	C	1212	1	14,14,15	0.28	0	17,19,21	0.37	0
5	NAG	C	1215	1	14,14,15	0.38	0	17,19,21	0.34	0
5	NAG	C	1214	1	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
5	NAG	C	1207	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
5	NAG	A	1207	1	14,14,15	0.28	0	17,19,21	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1213	1	14,14,15	0.22	0	17,19,21	0.75	1 (5%)
5	NAG	B	1204	1	14,14,15	0.22	0	17,19,21	0.38	0
5	NAG	A	1214	1	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
5	NAG	B	1215	1	14,14,15	0.38	0	17,19,21	0.34	0
5	NAG	C	1204	1	14,14,15	0.22	0	17,19,21	0.38	0
5	NAG	C	1216	1	14,14,15	0.52	0	17,19,21	0.41	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
5	NAG	A	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1213	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1208	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1216	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1206	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1205	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1206	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1201	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1201	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1208	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1201	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1205	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1203	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1211	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1213	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1211	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1214	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1208	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1205	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1202	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1210	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1216	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1206	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1211	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1212	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1214	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1213	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1214	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1215	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1216	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1211	NAG	C1-C2	4.51	1.58	1.52
5	A	1211	NAG	C1-C2	4.50	1.58	1.52
5	B	1211	NAG	C1-C2	4.37	1.58	1.52
5	C	1209	NAG	O5-C1	-2.53	1.39	1.43
5	A	1209	NAG	O5-C1	-2.50	1.39	1.43
5	B	1209	NAG	O5-C1	-2.44	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1211	NAG	C1-O5-C5	5.71	119.84	112.19
5	A	1211	NAG	C1-O5-C5	5.67	119.78	112.19
5	B	1211	NAG	C1-O5-C5	5.66	119.78	112.19
5	C	1211	NAG	C4-C3-C2	3.59	116.28	111.02
5	A	1211	NAG	C4-C3-C2	3.56	116.24	111.02
5	B	1211	NAG	C4-C3-C2	3.55	116.23	111.02
5	A	1207	NAG	C1-O5-C5	3.08	116.32	112.19
5	B	1207	NAG	C1-O5-C5	3.08	116.31	112.19
5	C	1207	NAG	C1-O5-C5	3.05	116.27	112.19
5	C	1213	NAG	C1-O5-C5	2.59	115.66	112.19
5	B	1213	NAG	C1-O5-C5	2.58	115.64	112.19
5	A	1213	NAG	C1-O5-C5	2.57	115.62	112.19
5	B	1205	NAG	C1-O5-C5	2.19	115.12	112.19
5	A	1205	NAG	C1-O5-C5	2.16	115.08	112.19
5	C	1205	NAG	C1-O5-C5	2.14	115.05	112.19
5	A	1214	NAG	C1-O5-C5	2.08	114.98	112.19
5	C	1214	NAG	C1-O5-C5	2.05	114.94	112.19
5	B	1214	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1214	NAG	C4-C5-C6-O6
5	A	1214	NAG	C4-C5-C6-O6
5	B	1214	NAG	C4-C5-C6-O6
5	A	1208	NAG	O5-C5-C6-O6
5	A	1209	NAG	O5-C5-C6-O6
5	B	1208	NAG	O5-C5-C6-O6
5	B	1209	NAG	O5-C5-C6-O6
5	C	1208	NAG	O5-C5-C6-O6
5	C	1209	NAG	O5-C5-C6-O6
5	A	1211	NAG	O5-C5-C6-O6
5	B	1211	NAG	O5-C5-C6-O6
5	C	1211	NAG	O5-C5-C6-O6
5	A	1212	NAG	C4-C5-C6-O6
5	B	1212	NAG	C4-C5-C6-O6
5	C	1212	NAG	C4-C5-C6-O6
5	A	1205	NAG	O5-C5-C6-O6
5	A	1206	NAG	O5-C5-C6-O6
5	A	1212	NAG	O5-C5-C6-O6
5	B	1205	NAG	O5-C5-C6-O6
5	B	1206	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1212	NAG	O5-C5-C6-O6
5	C	1206	NAG	O5-C5-C6-O6
5	C	1212	NAG	O5-C5-C6-O6
5	C	1205	NAG	O5-C5-C6-O6
5	A	1214	NAG	O5-C5-C6-O6
5	B	1214	NAG	O5-C5-C6-O6
5	C	1214	NAG	O5-C5-C6-O6
5	A	1205	NAG	C4-C5-C6-O6
5	A	1209	NAG	C4-C5-C6-O6
5	B	1205	NAG	C4-C5-C6-O6
5	B	1209	NAG	C4-C5-C6-O6
5	C	1205	NAG	C4-C5-C6-O6
5	C	1209	NAG	C4-C5-C6-O6
5	A	1208	NAG	C4-C5-C6-O6
5	B	1208	NAG	C4-C5-C6-O6
5	C	1208	NAG	C4-C5-C6-O6
5	A	1211	NAG	C4-C5-C6-O6
5	B	1211	NAG	C4-C5-C6-O6
5	C	1211	NAG	C4-C5-C6-O6
5	A	1202	NAG	C8-C7-N2-C2
5	A	1202	NAG	O7-C7-N2-C2
5	A	1203	NAG	C8-C7-N2-C2
5	A	1203	NAG	O7-C7-N2-C2
5	A	1215	NAG	C8-C7-N2-C2
5	A	1215	NAG	O7-C7-N2-C2
5	A	1216	NAG	C8-C7-N2-C2
5	A	1216	NAG	O7-C7-N2-C2
5	B	1202	NAG	C8-C7-N2-C2
5	B	1202	NAG	O7-C7-N2-C2
5	B	1203	NAG	C8-C7-N2-C2
5	B	1203	NAG	O7-C7-N2-C2
5	B	1215	NAG	C8-C7-N2-C2
5	B	1215	NAG	O7-C7-N2-C2
5	B	1216	NAG	C8-C7-N2-C2
5	B	1216	NAG	O7-C7-N2-C2
5	C	1202	NAG	C8-C7-N2-C2
5	C	1202	NAG	O7-C7-N2-C2
5	C	1203	NAG	C8-C7-N2-C2
5	C	1203	NAG	O7-C7-N2-C2
5	C	1215	NAG	C8-C7-N2-C2
5	C	1215	NAG	O7-C7-N2-C2
5	C	1216	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	C	1216	NAG	O7-C7-N2-C2
5	A	1202	NAG	O5-C5-C6-O6
5	B	1202	NAG	O5-C5-C6-O6
5	C	1202	NAG	O5-C5-C6-O6
5	B	1206	NAG	C4-C5-C6-O6
5	C	1206	NAG	C4-C5-C6-O6
5	A	1206	NAG	C4-C5-C6-O6
5	A	1215	NAG	O5-C5-C6-O6
5	B	1215	NAG	O5-C5-C6-O6
5	C	1215	NAG	O5-C5-C6-O6
5	A	1208	NAG	C1-C2-N2-C7
5	B	1208	NAG	C1-C2-N2-C7
5	C	1208	NAG	C1-C2-N2-C7
5	A	1213	NAG	C4-C5-C6-O6
5	B	1213	NAG	C4-C5-C6-O6
5	C	1213	NAG	C4-C5-C6-O6
5	A	1216	NAG	C4-C5-C6-O6
5	C	1216	NAG	C4-C5-C6-O6
5	B	1216	NAG	C4-C5-C6-O6
5	A	1201	NAG	C3-C2-N2-C7
5	A	1205	NAG	C3-C2-N2-C7
5	A	1208	NAG	C3-C2-N2-C7
5	B	1201	NAG	C3-C2-N2-C7
5	B	1205	NAG	C3-C2-N2-C7
5	B	1208	NAG	C3-C2-N2-C7
5	C	1201	NAG	C3-C2-N2-C7
5	C	1205	NAG	C3-C2-N2-C7
5	C	1208	NAG	C3-C2-N2-C7
5	B	1210	NAG	C4-C5-C6-O6
5	B	1213	NAG	O5-C5-C6-O6
5	A	1210	NAG	C4-C5-C6-O6
5	A	1213	NAG	O5-C5-C6-O6
5	C	1210	NAG	C4-C5-C6-O6
5	A	1210	NAG	O5-C5-C6-O6
5	B	1210	NAG	O5-C5-C6-O6
5	C	1210	NAG	O5-C5-C6-O6
5	C	1213	NAG	O5-C5-C6-O6
5	A	1205	NAG	C1-C2-N2-C7
5	A	1206	NAG	C1-C2-N2-C7
5	B	1205	NAG	C1-C2-N2-C7
5	B	1206	NAG	C1-C2-N2-C7
5	C	1205	NAG	C1-C2-N2-C7

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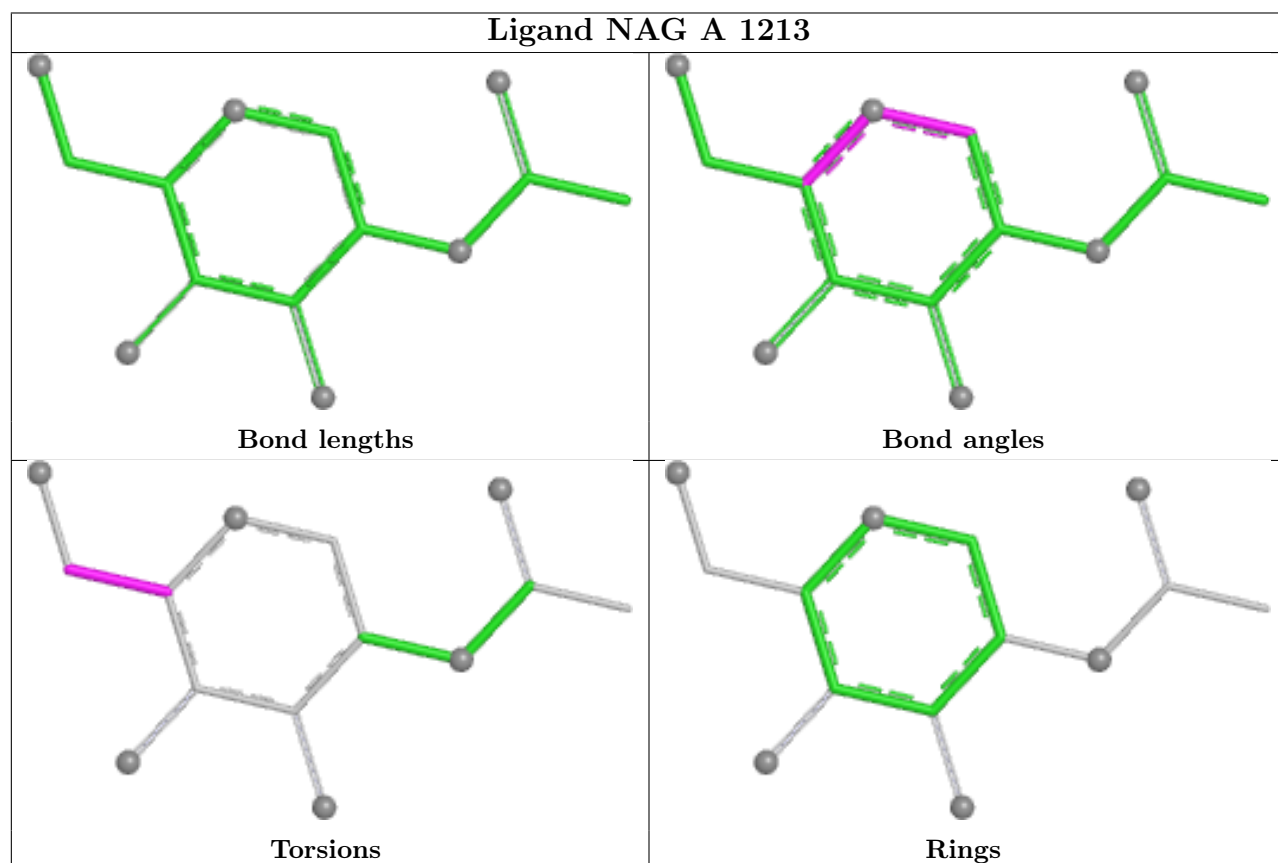
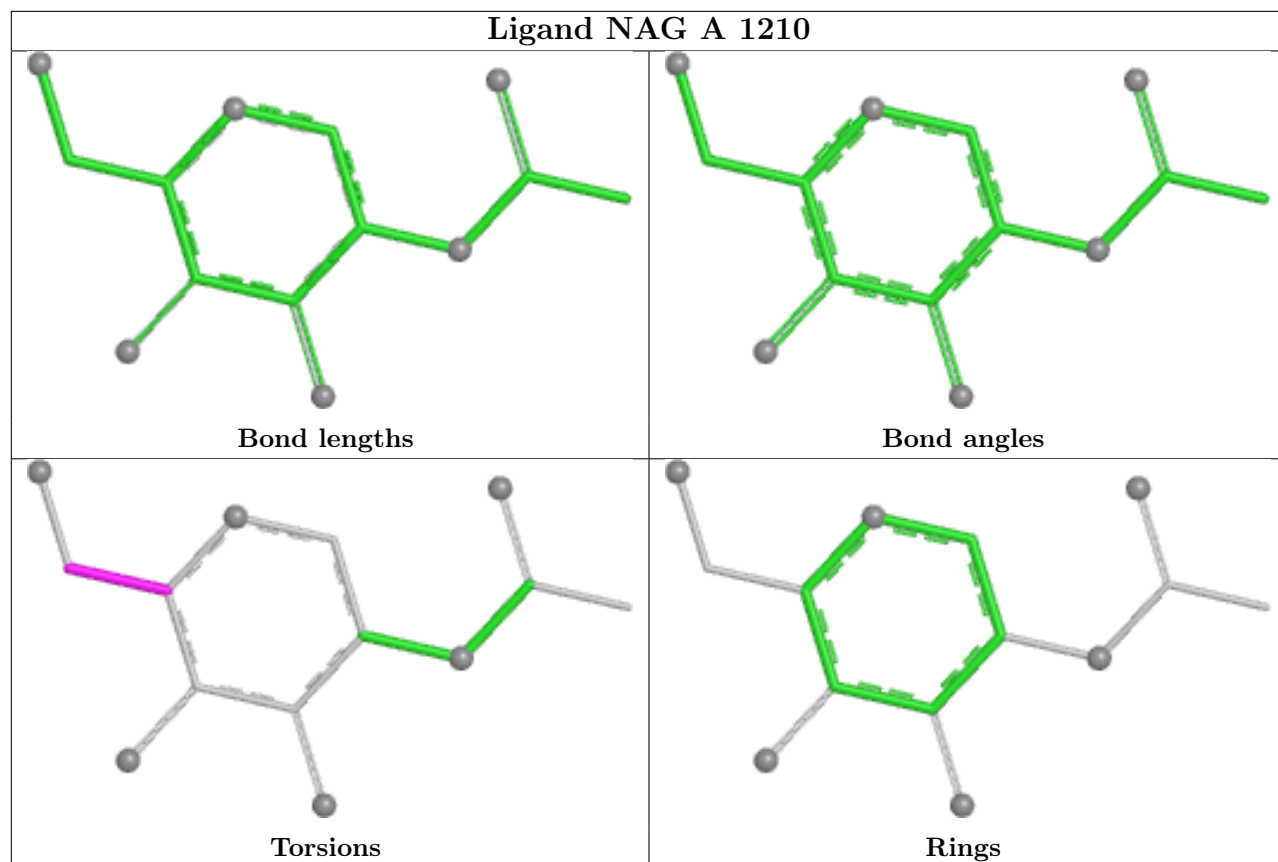
Mol	Chain	Res	Type	Atoms
5	C	1206	NAG	C1-C2-N2-C7

There are no ring outliers.

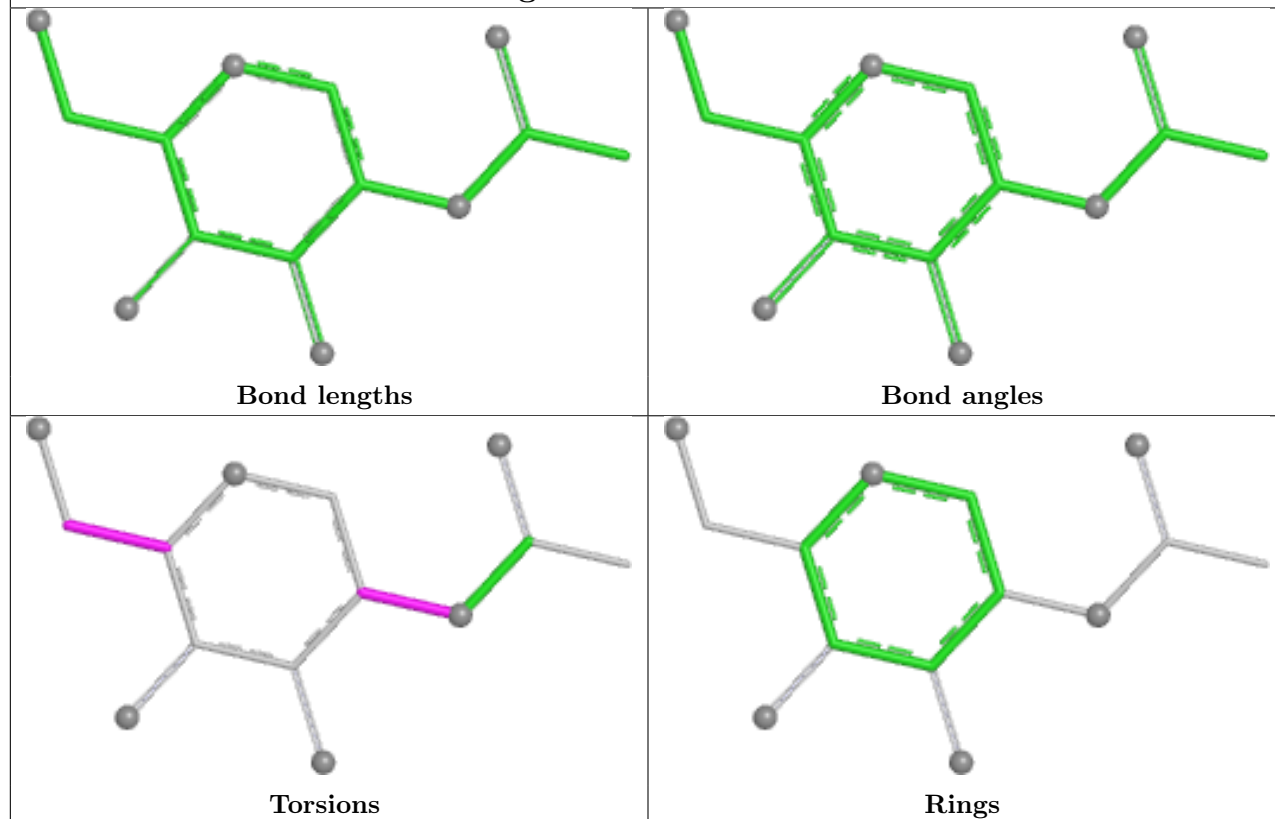
11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1206	NAG	1	0
5	C	1205	NAG	1	0
5	C	1201	NAG	8	0
5	A	1201	NAG	8	0
5	B	1202	NAG	6	0
5	B	1201	NAG	7	0
5	C	1202	NAG	6	0
5	A	1205	NAG	1	0
5	B	1205	NAG	1	0
5	A	1202	NAG	4	0
5	A	1216	NAG	1	0

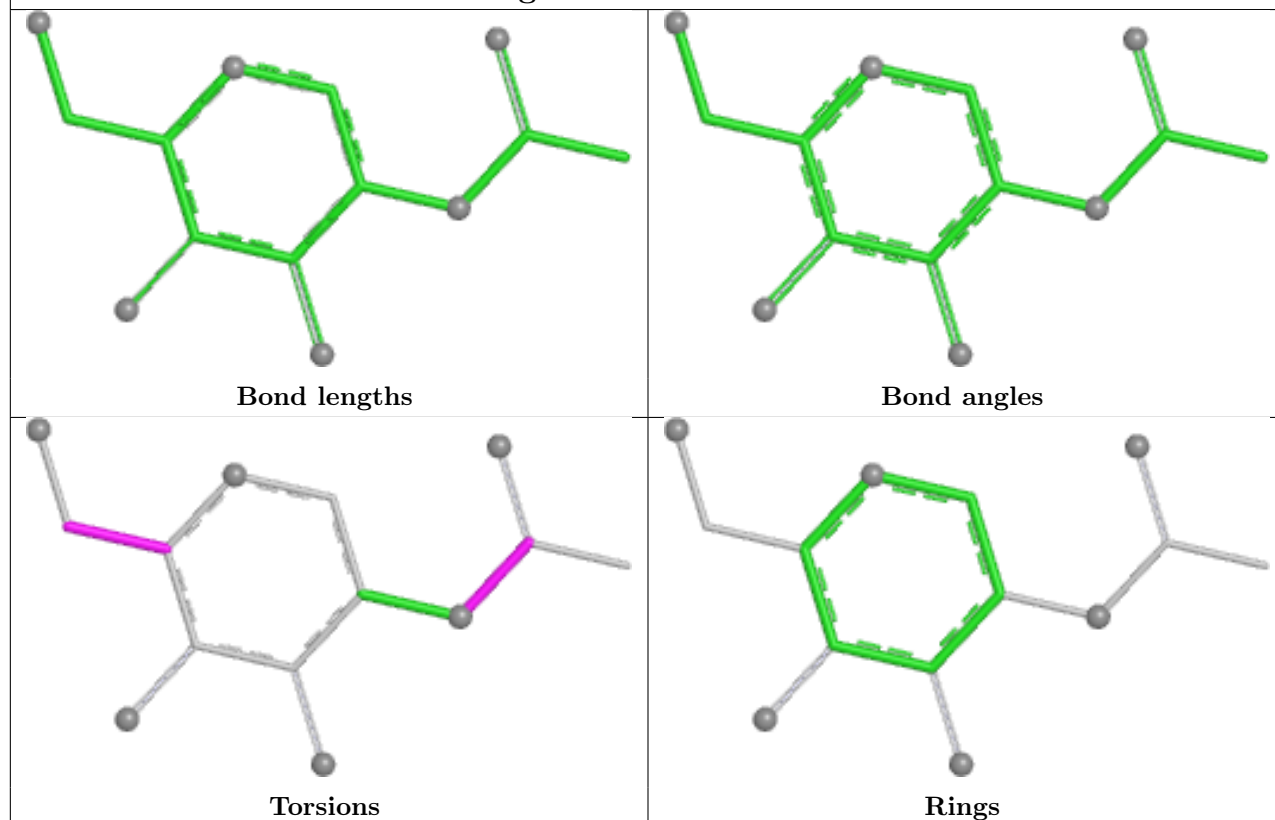
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



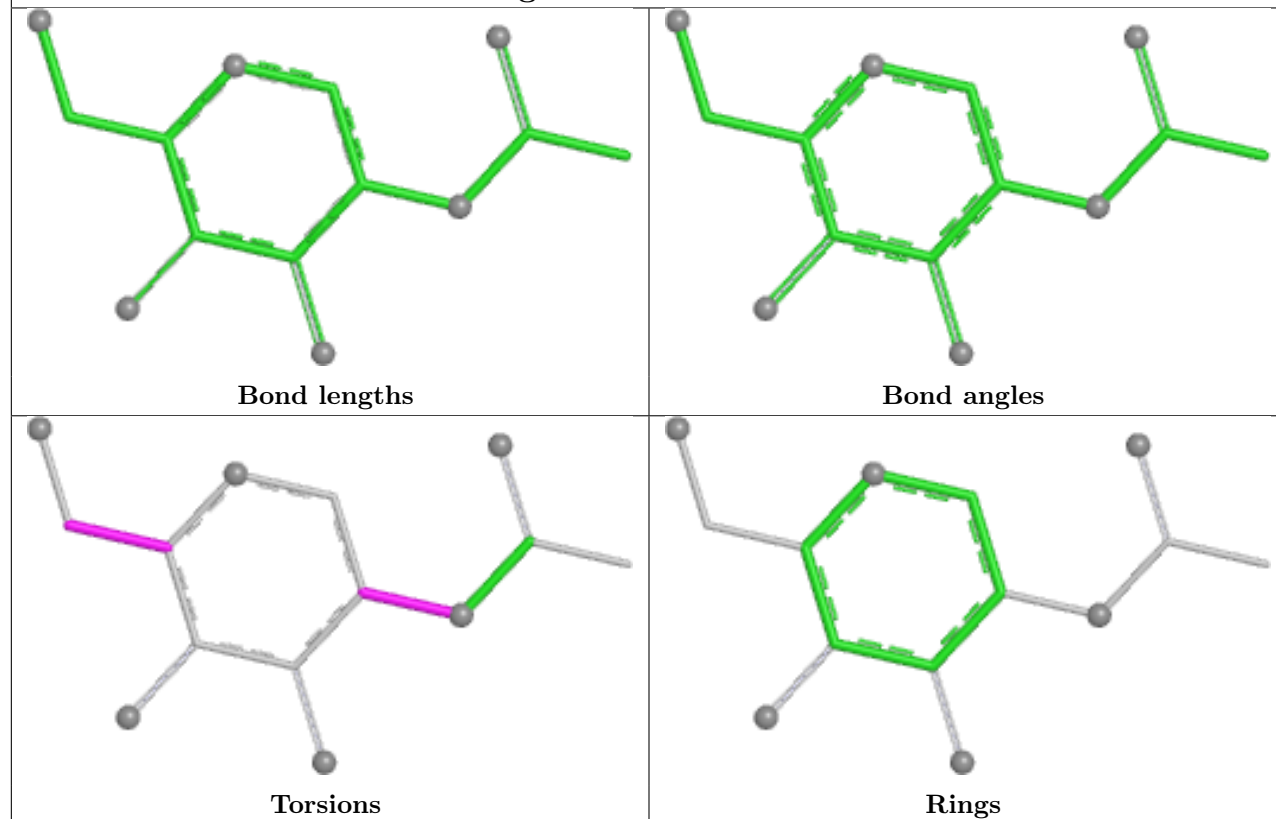
Ligand NAG B 1208



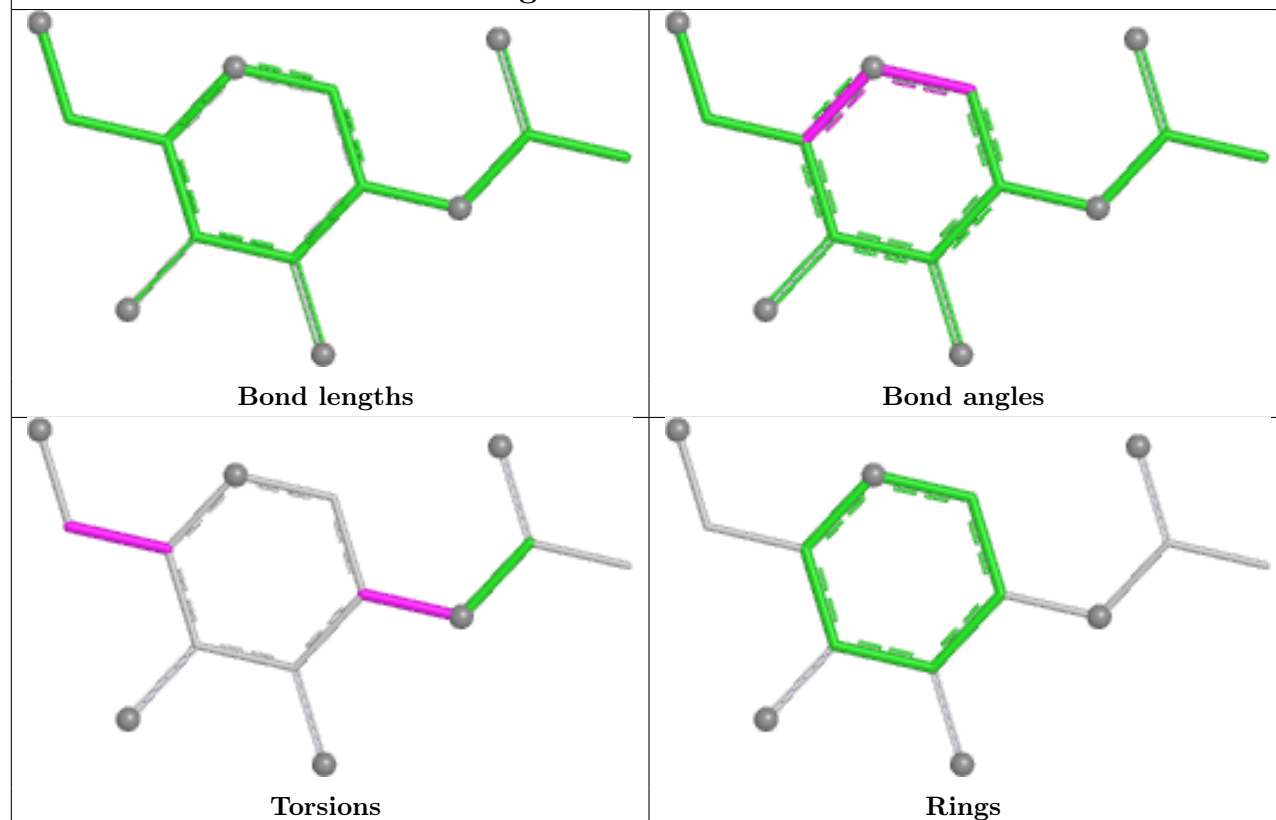
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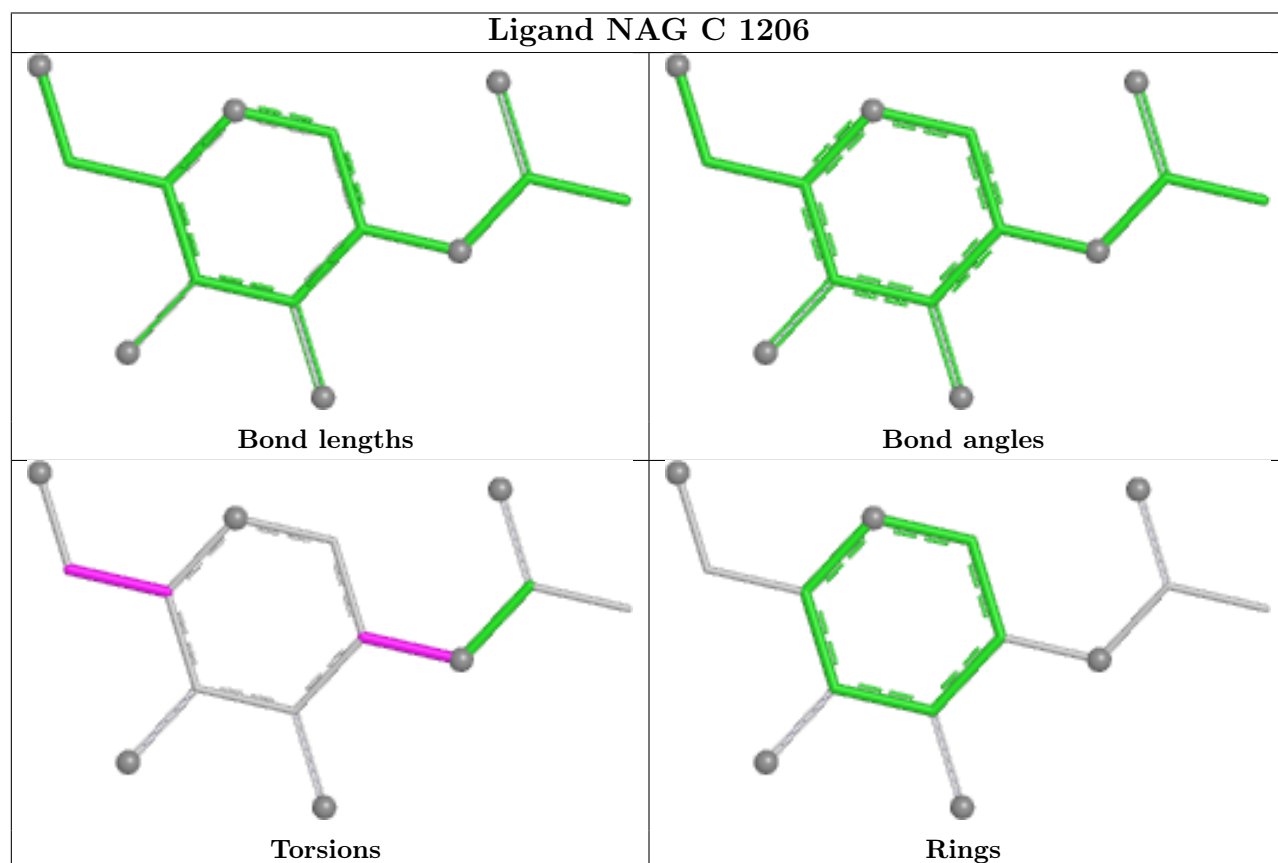
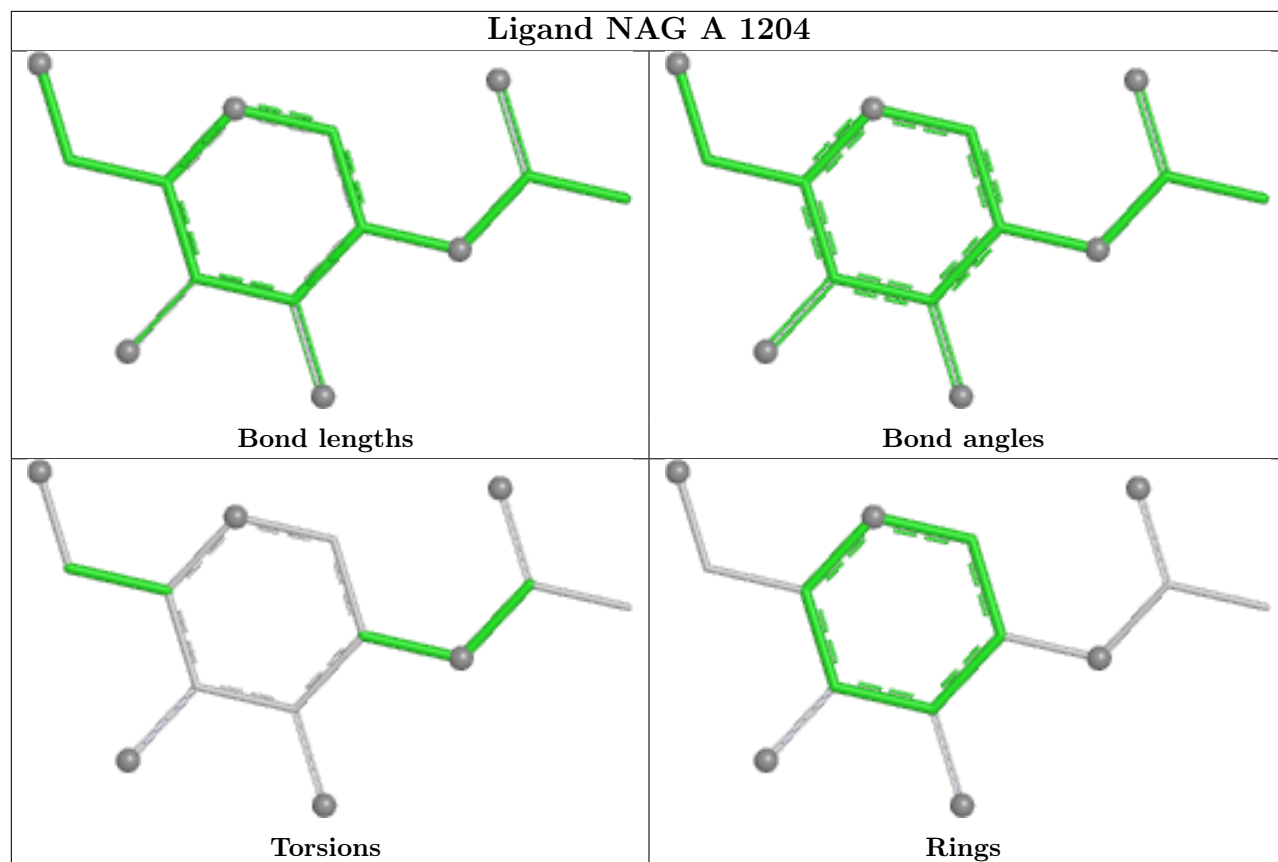


Ligand NAG A 1206

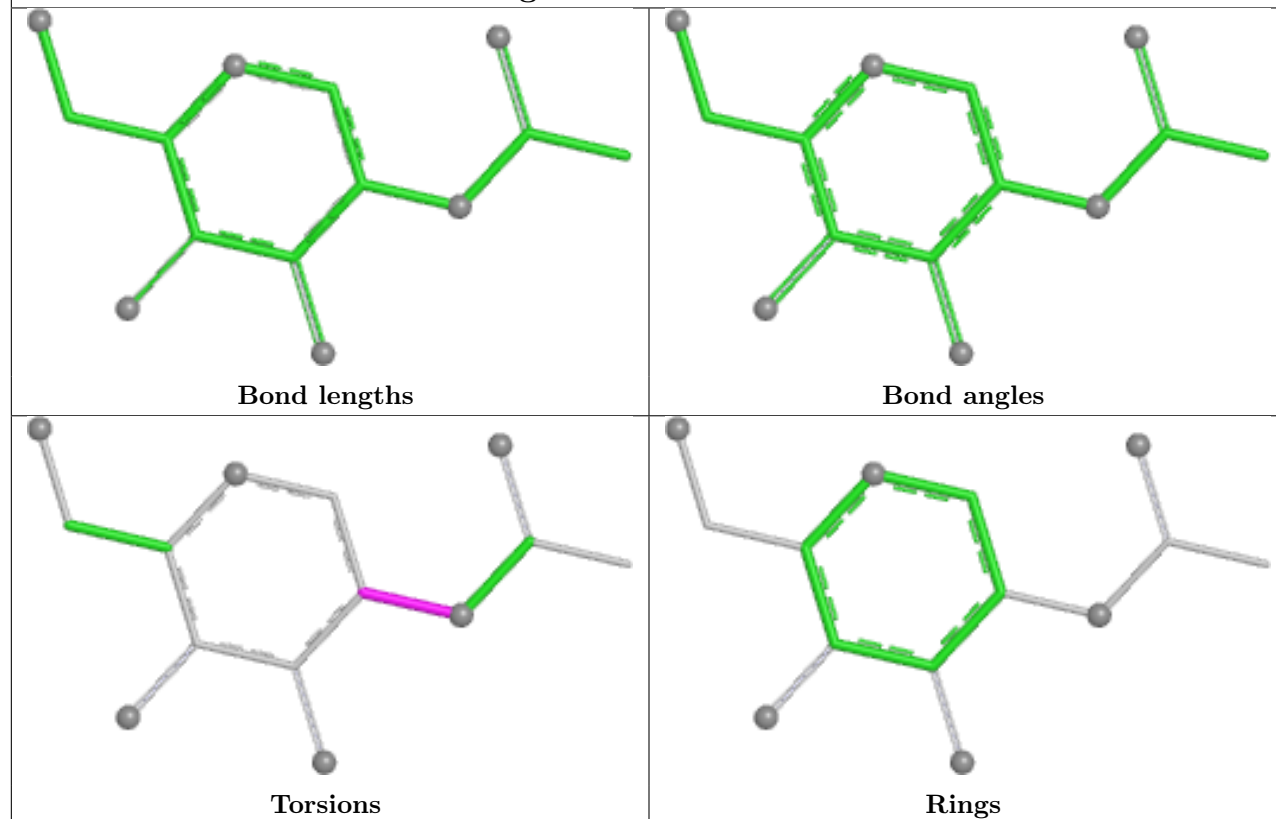


Ligand NAG C 1205

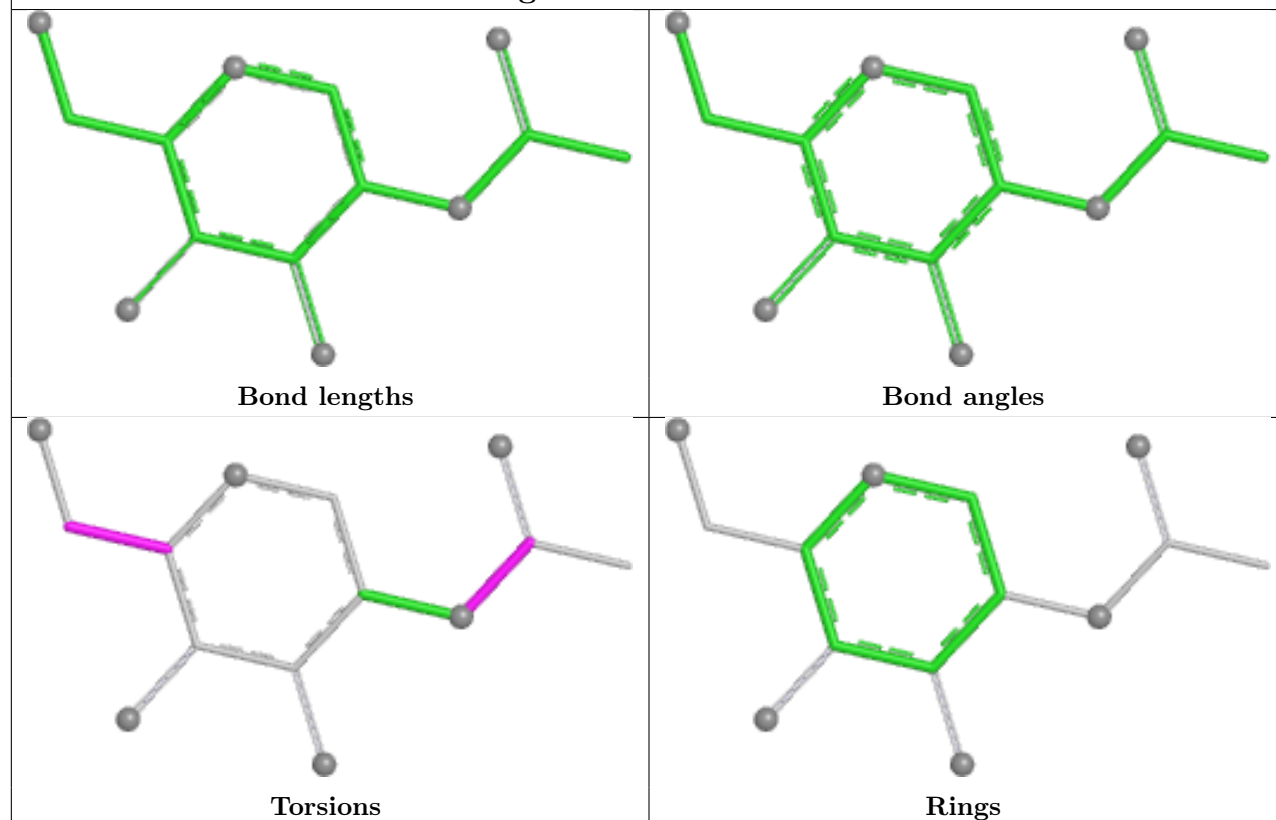




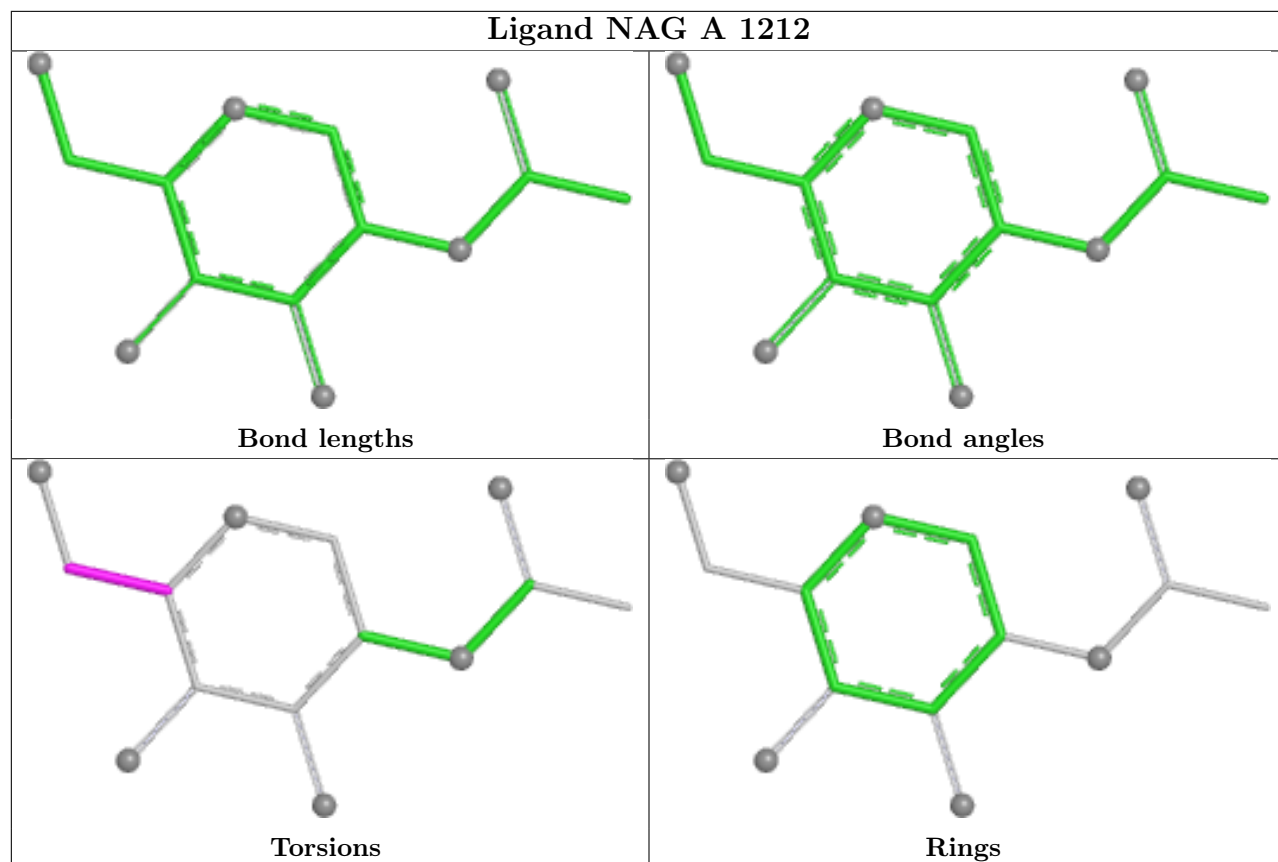
Ligand NAG C 1201



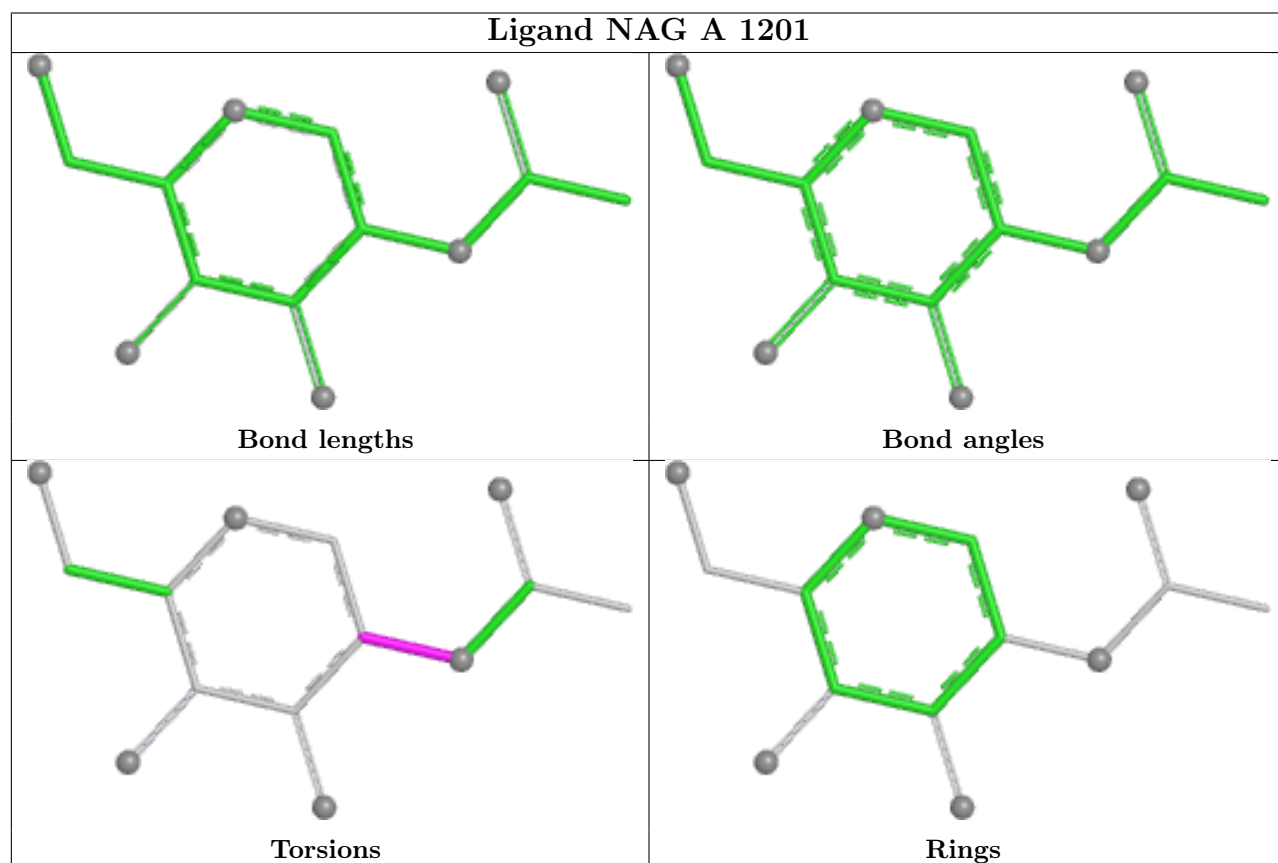
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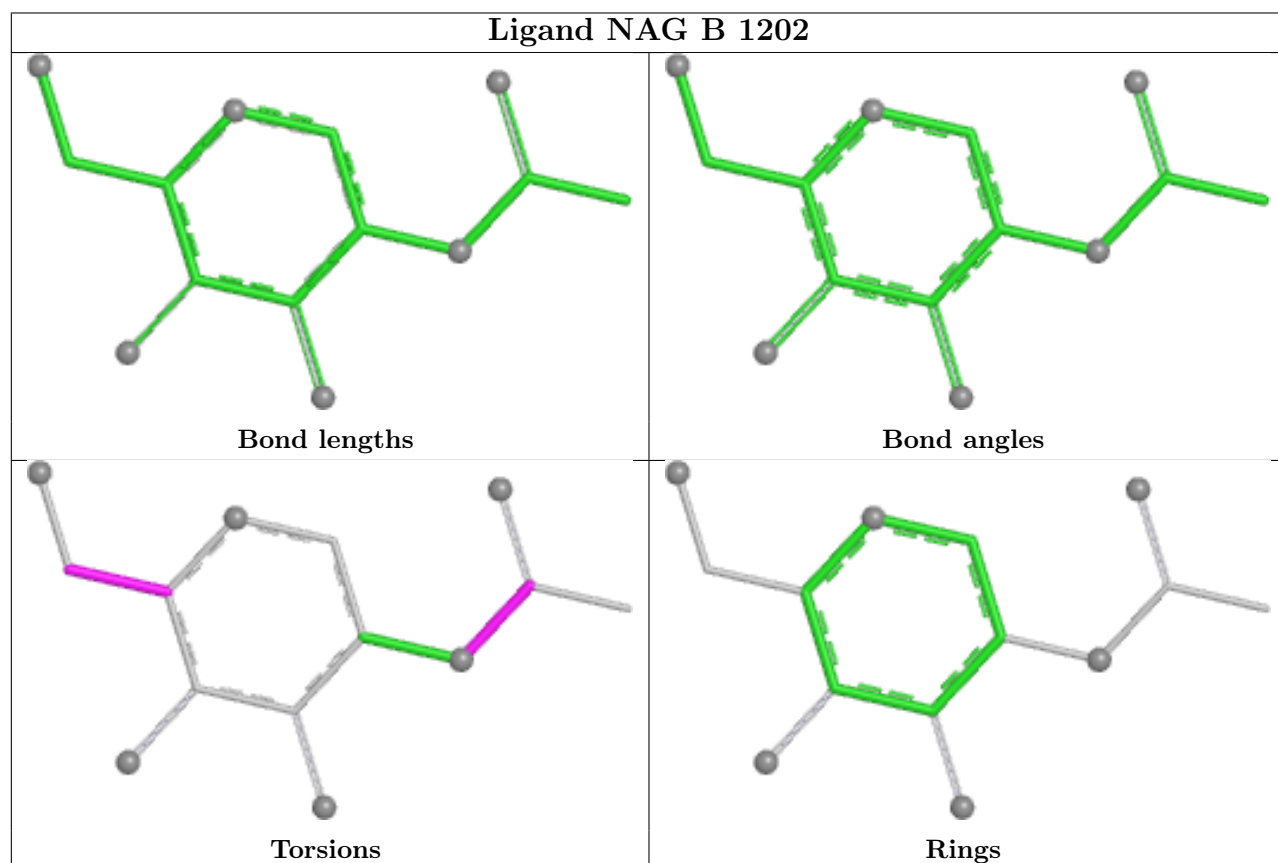
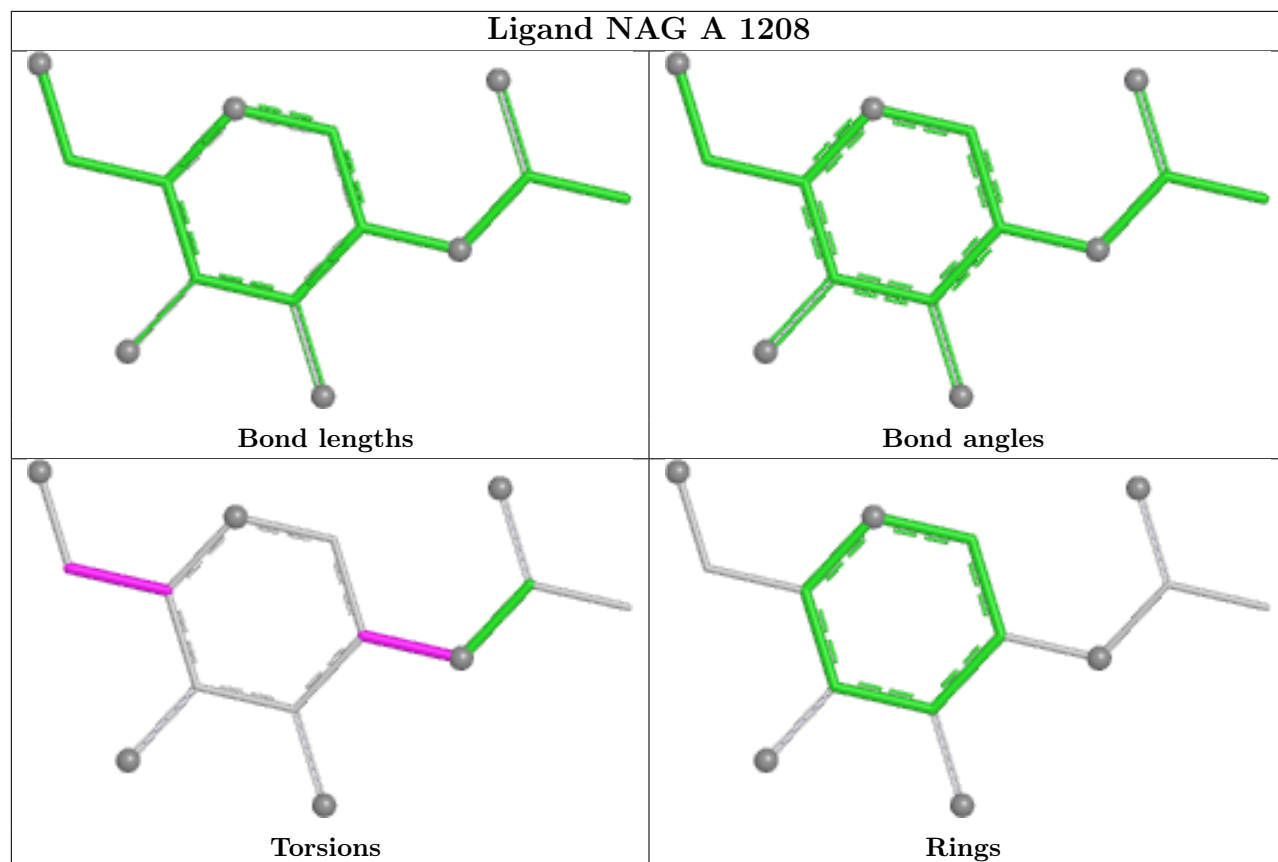


Ligand NAG A 1212

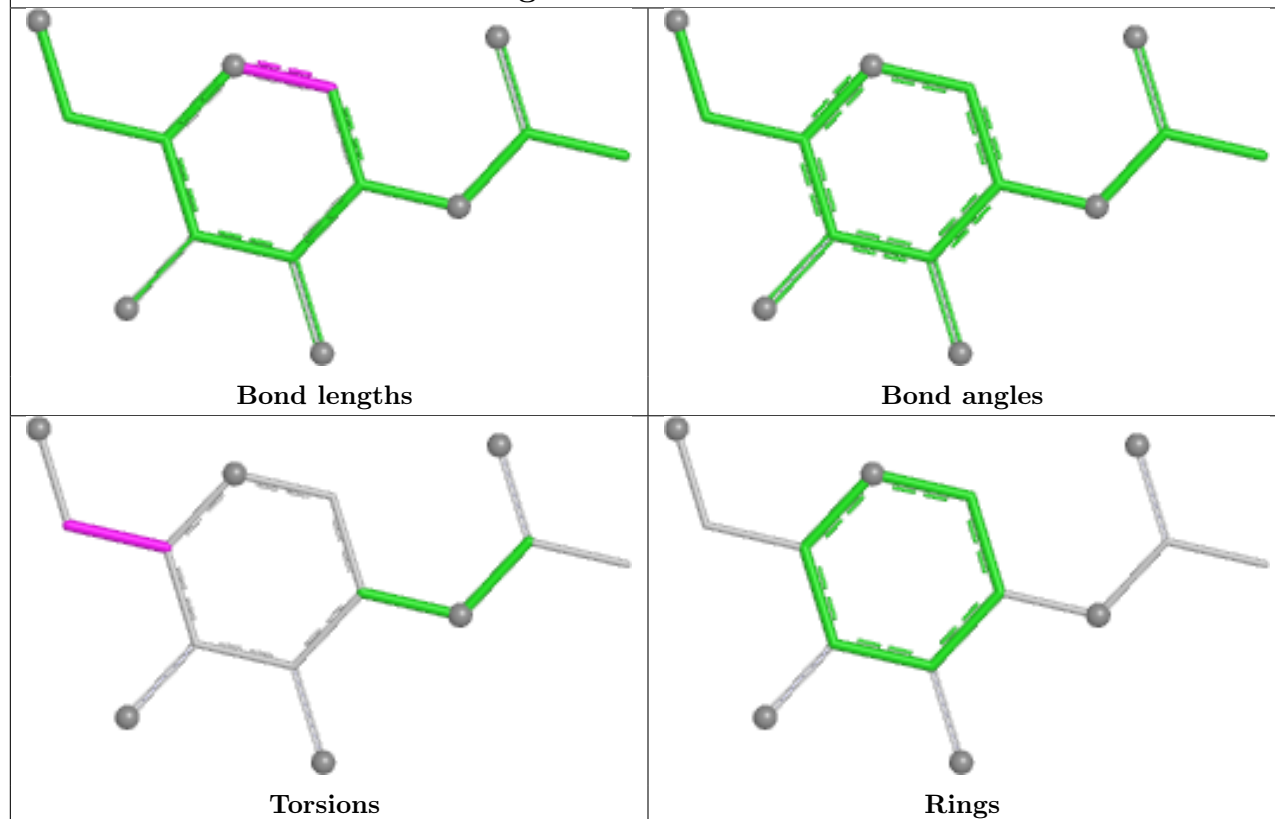


Ligand NAG A 1201

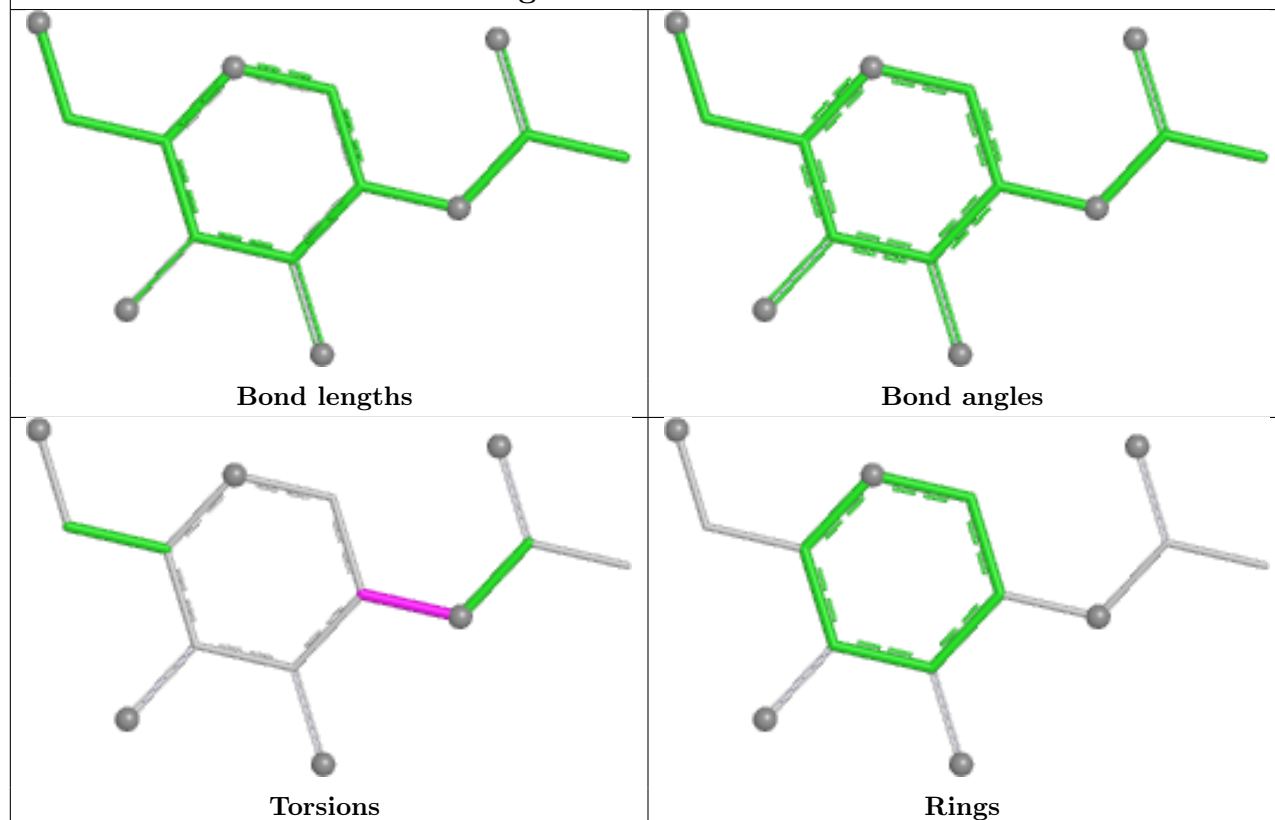




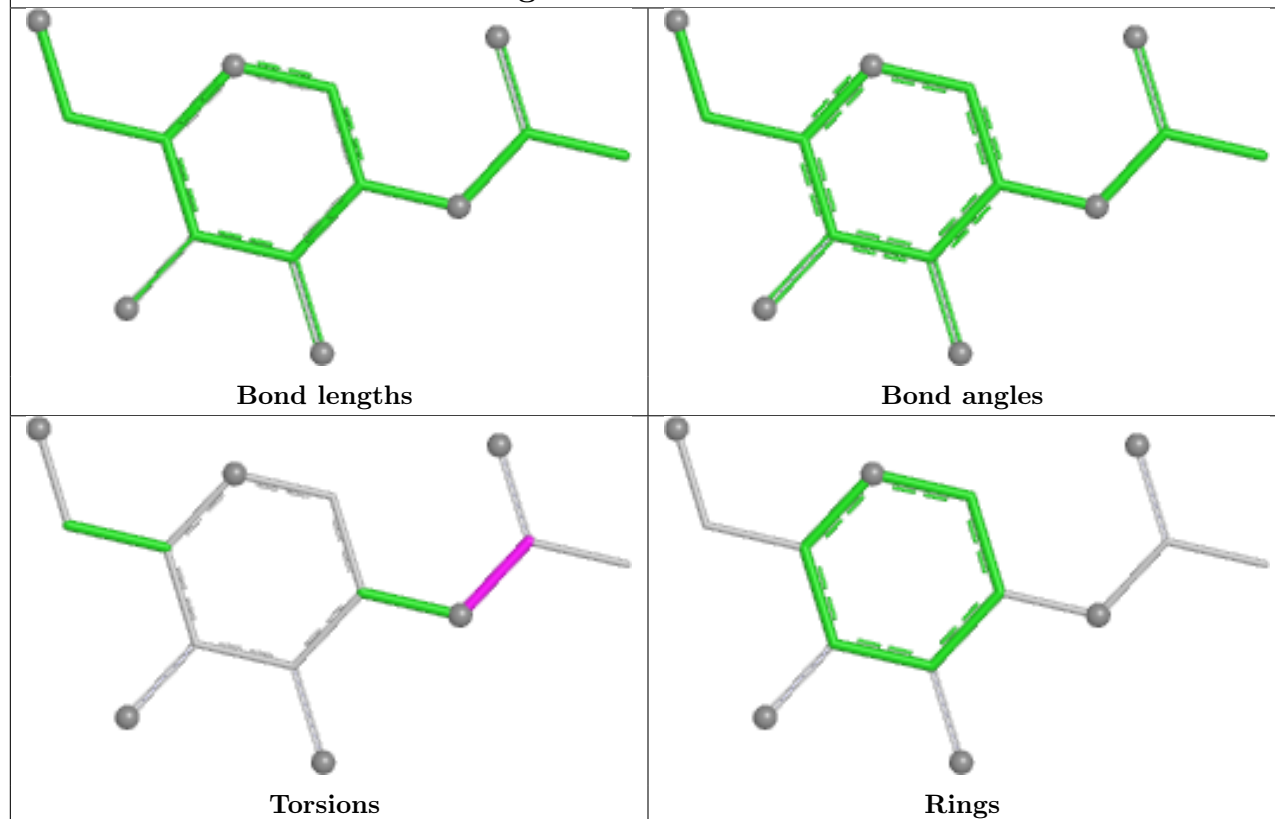
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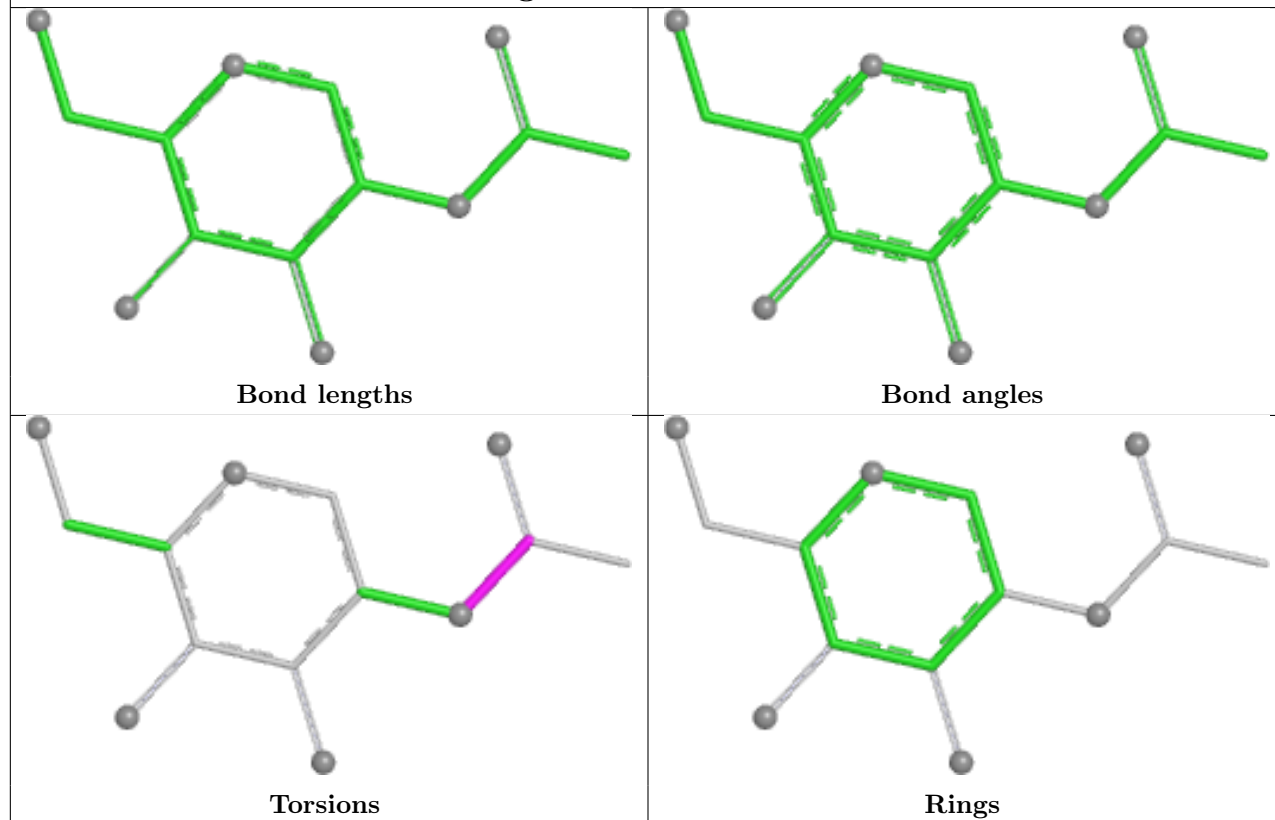
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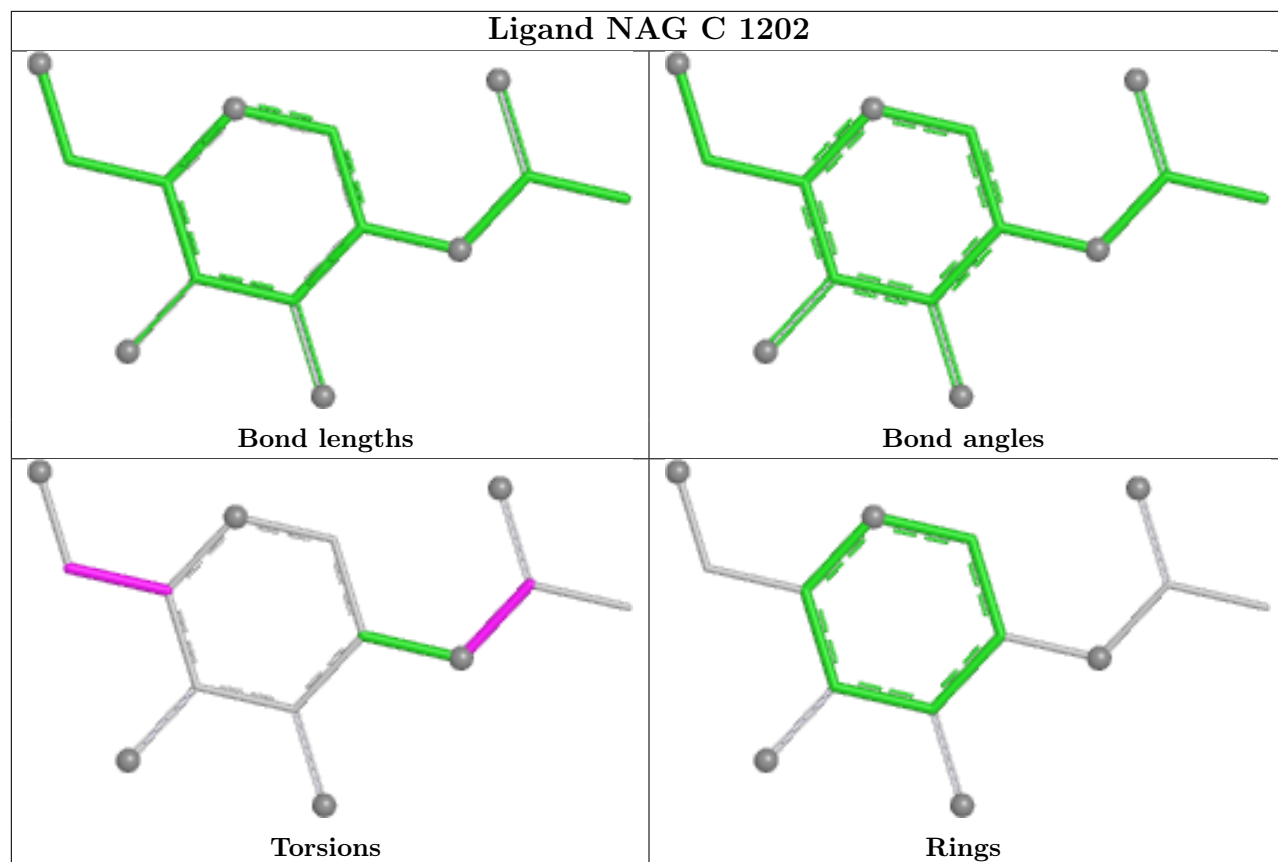
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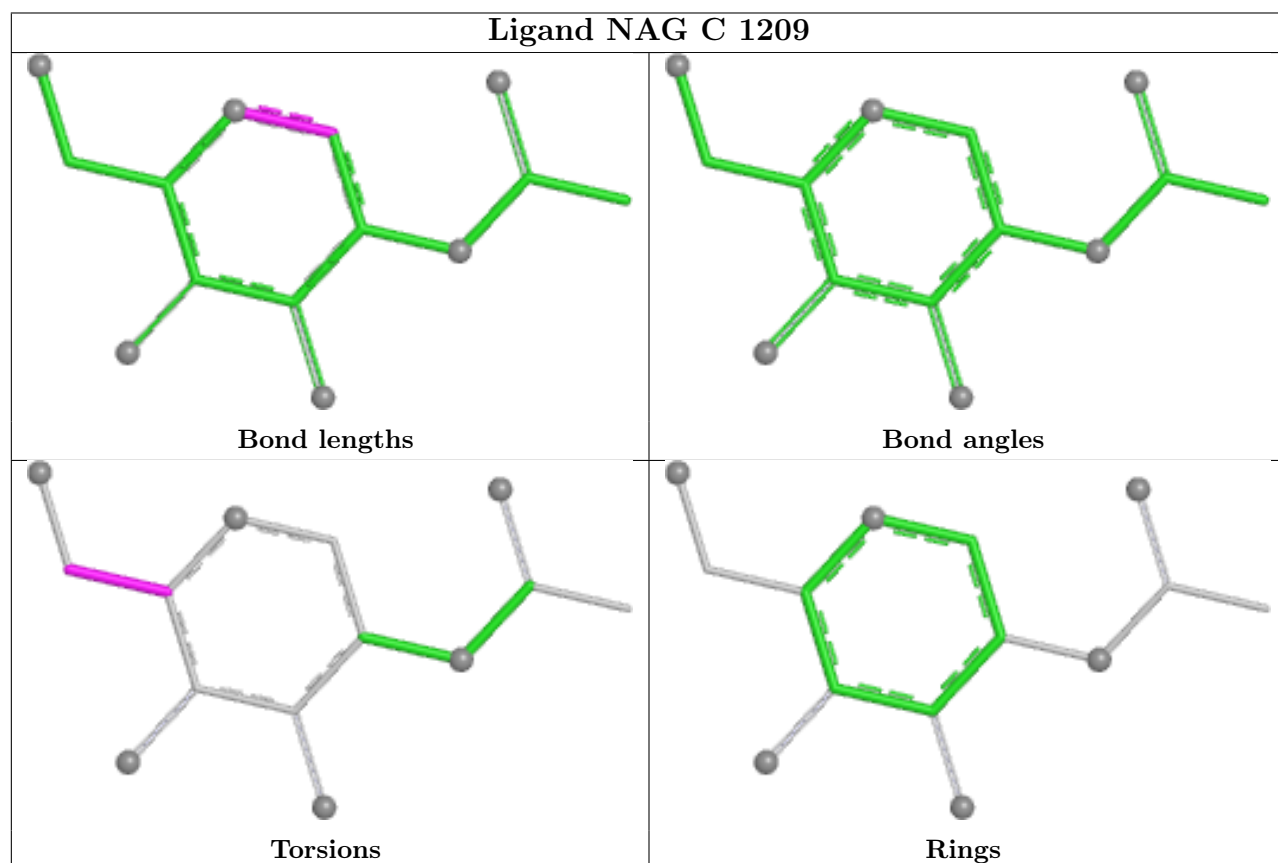
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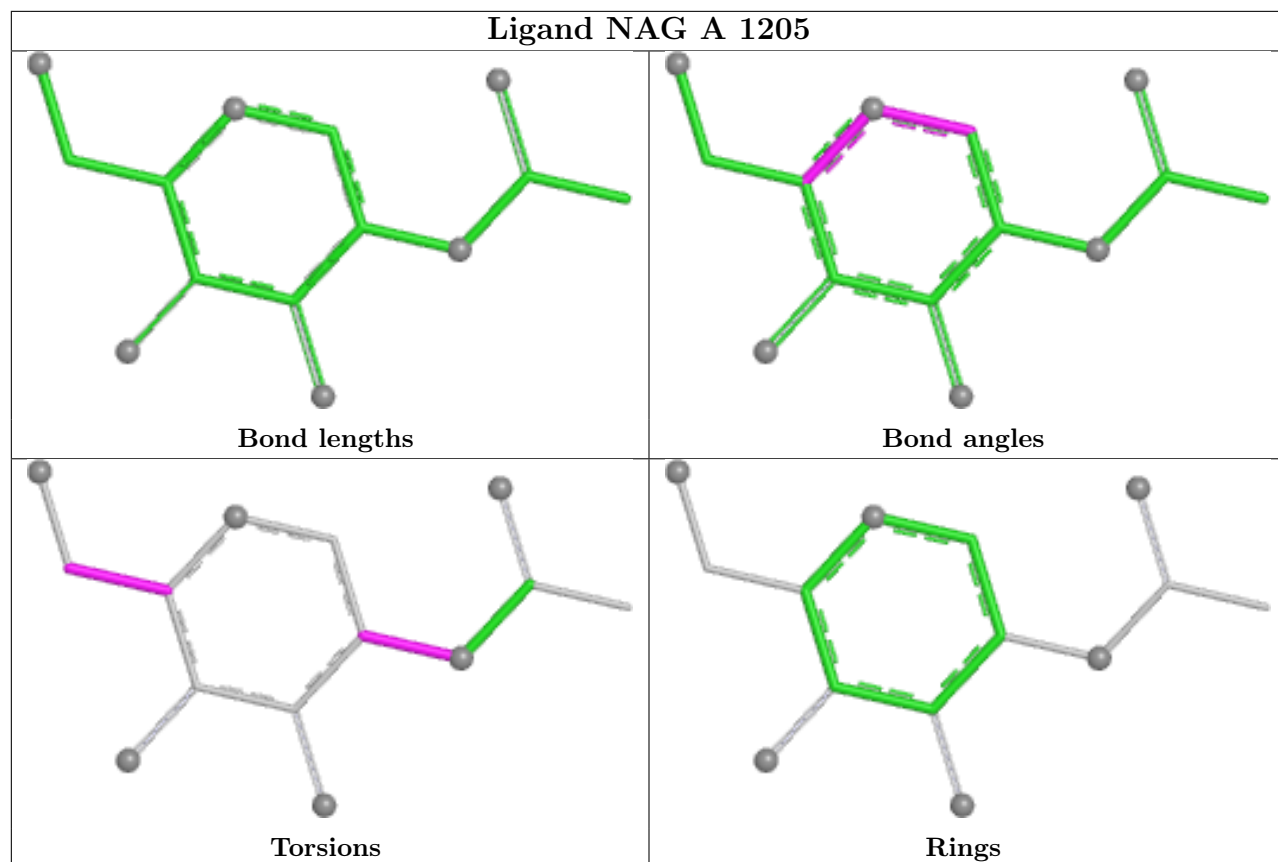
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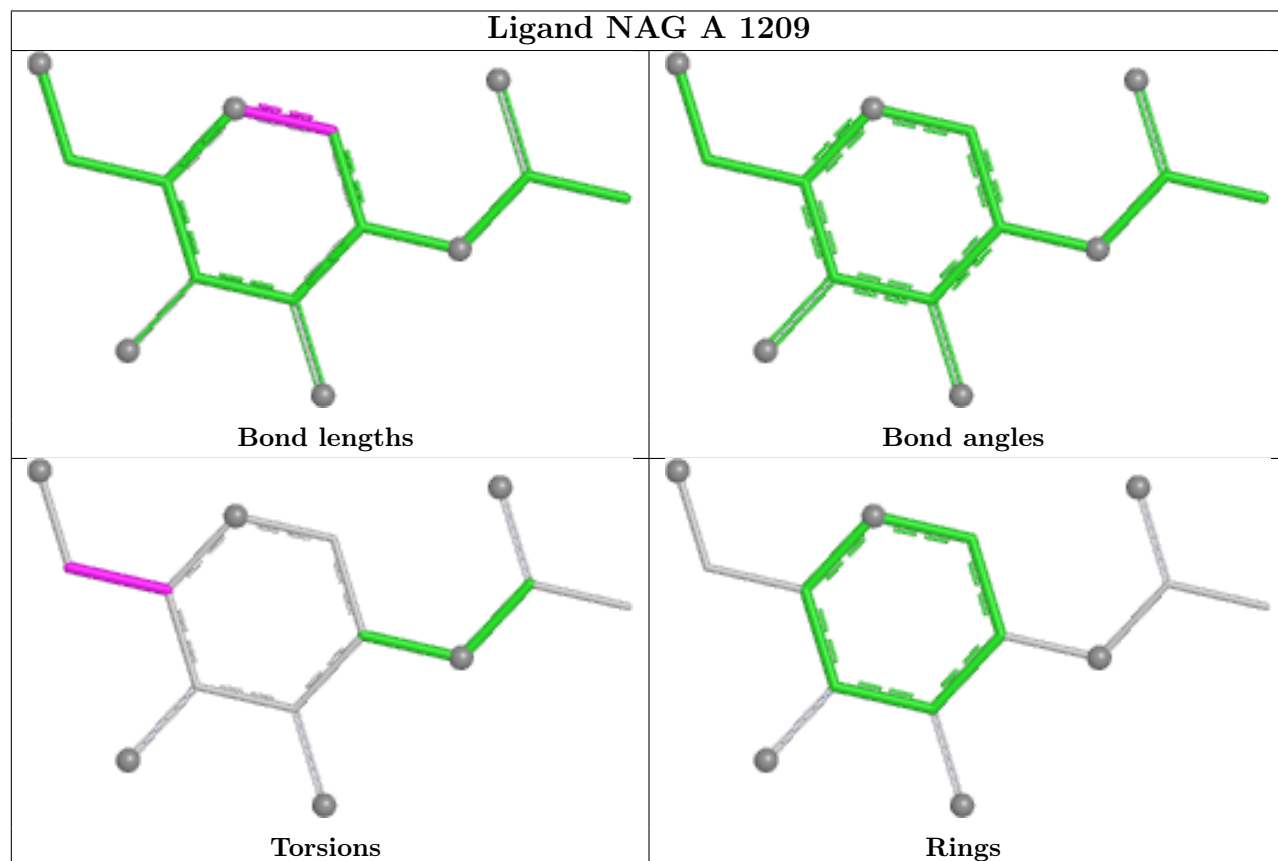
Ligand NAG C 1209



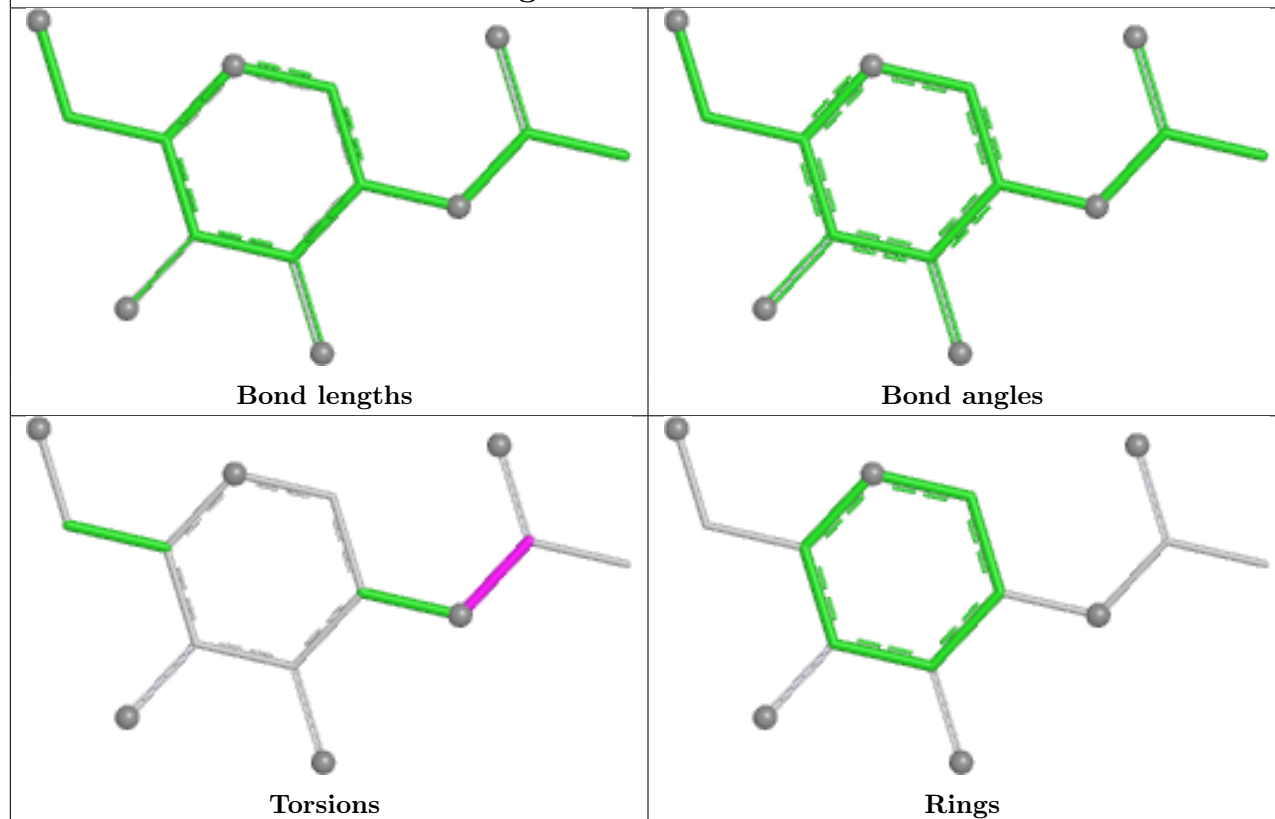
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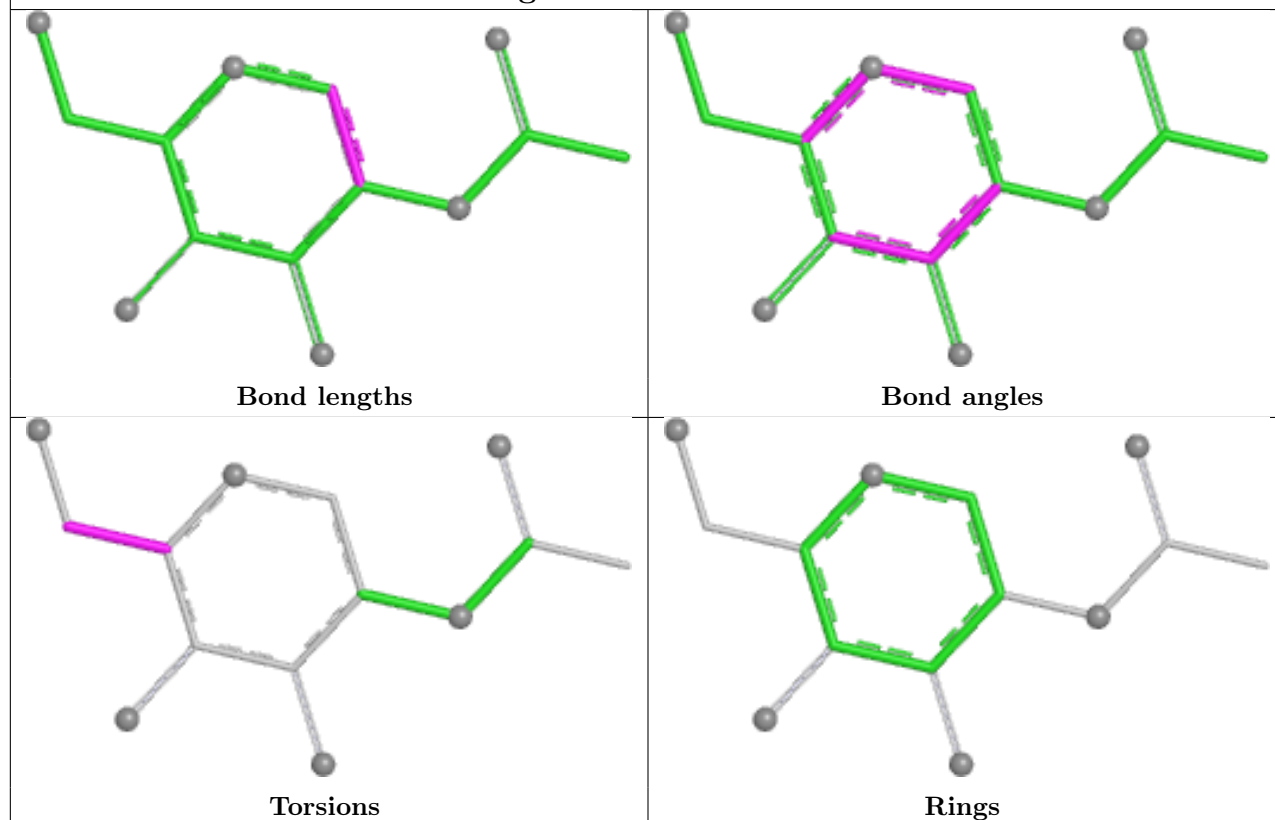
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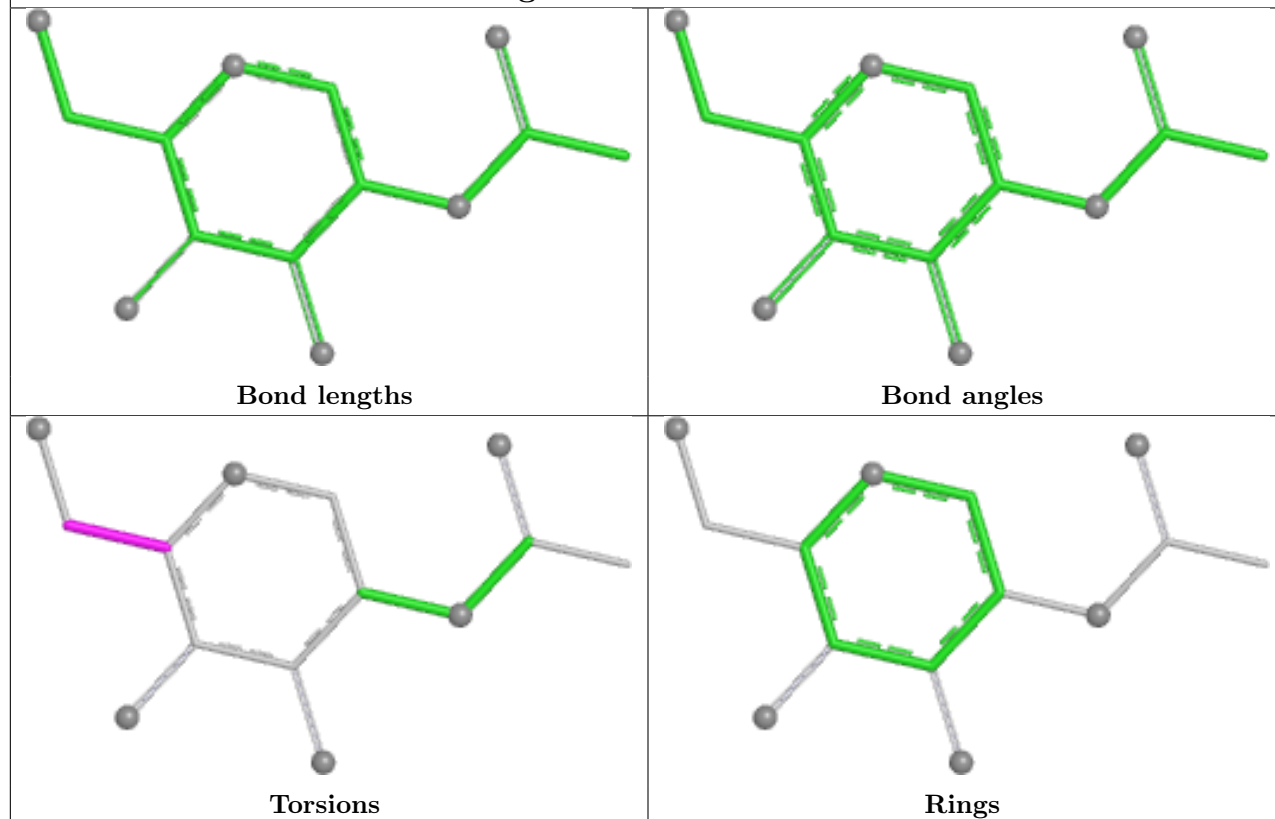
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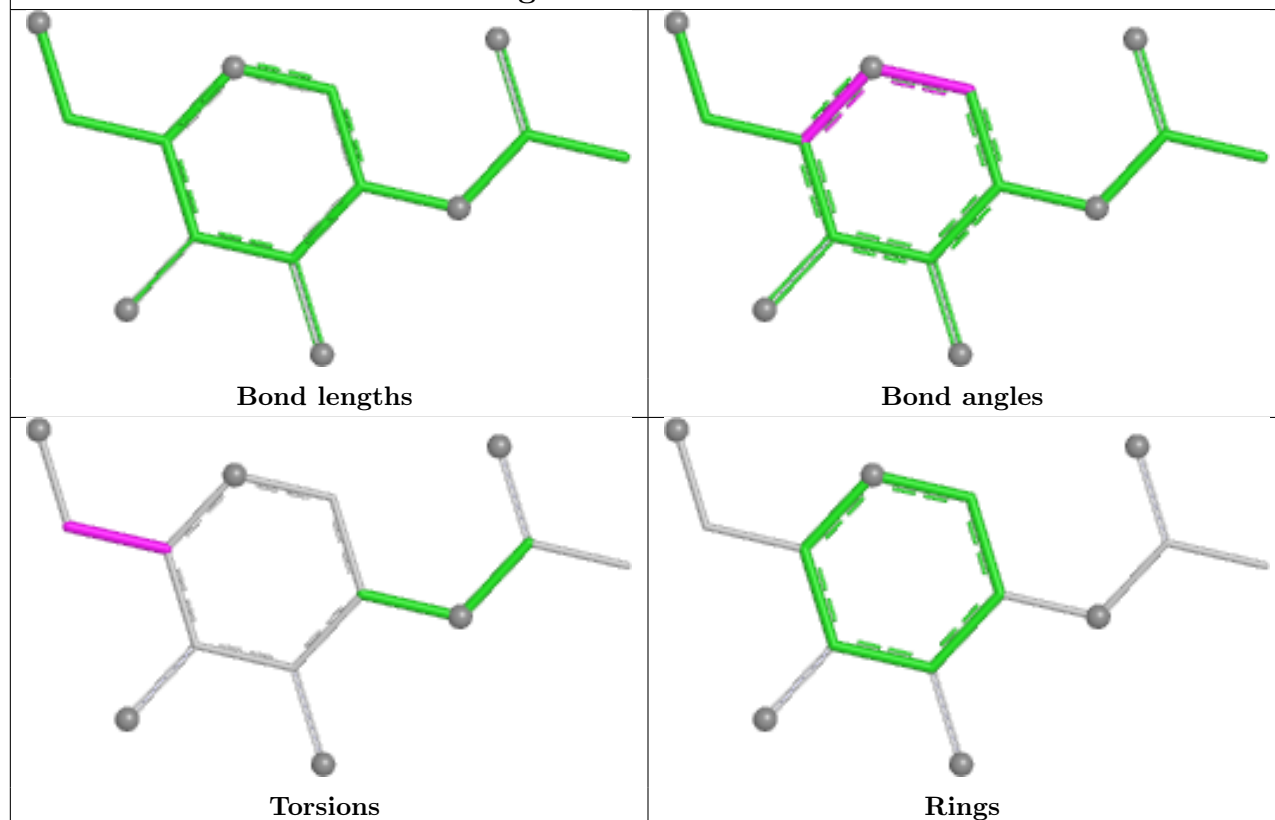
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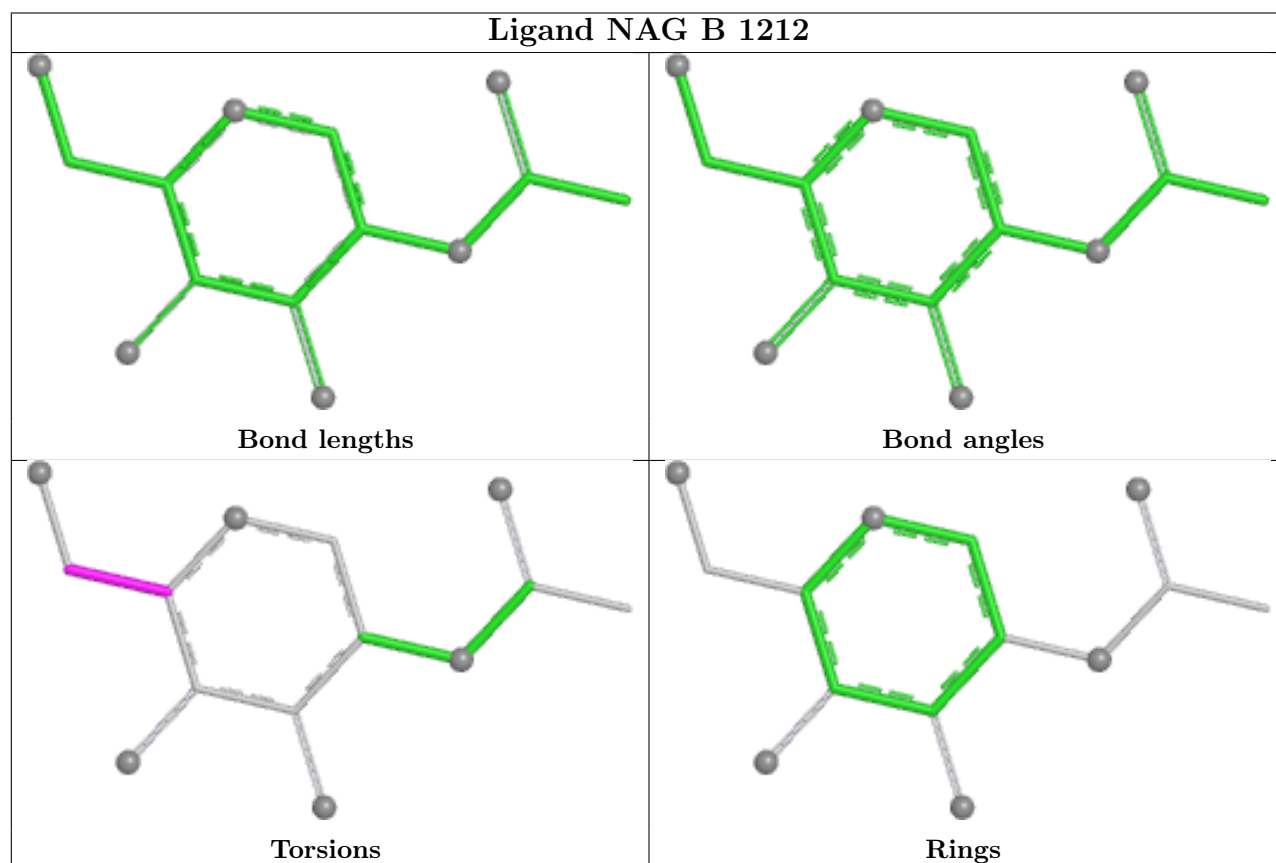
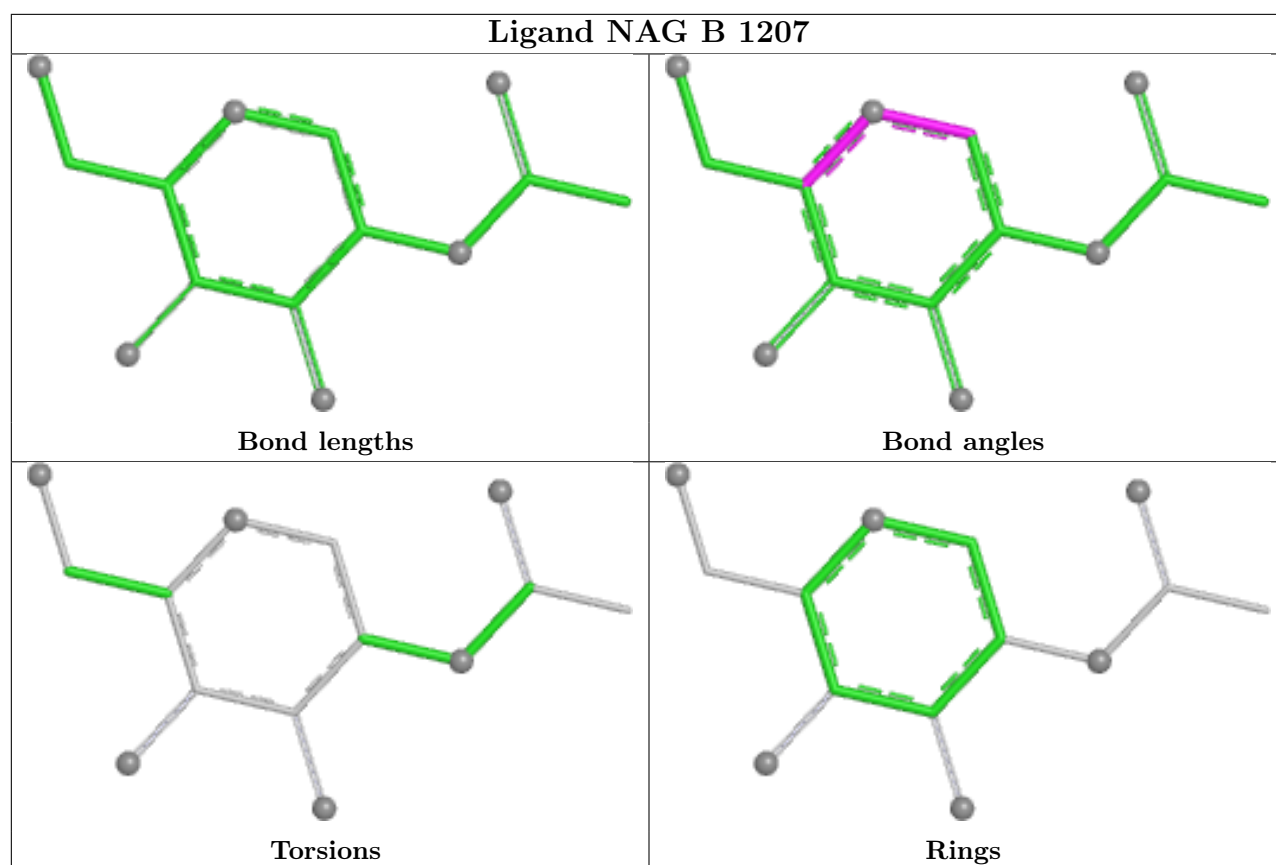


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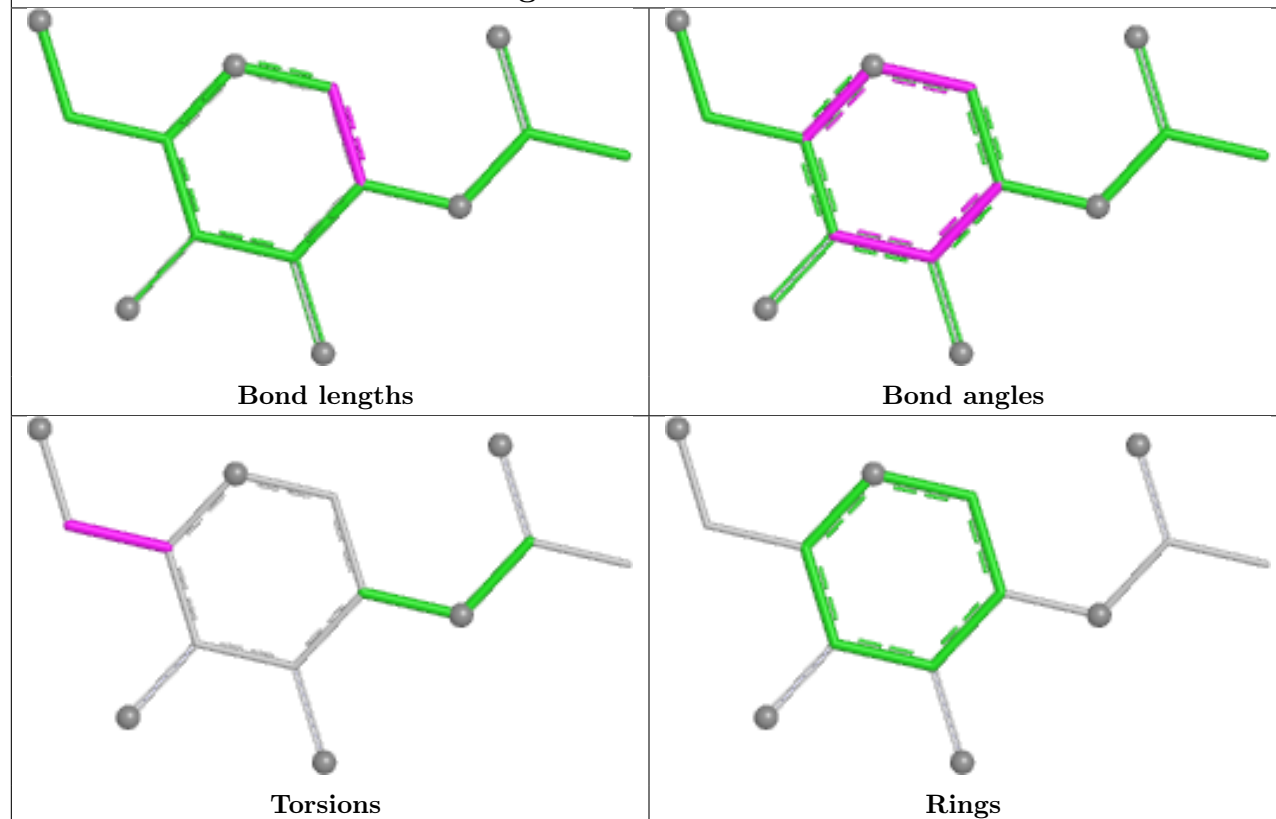


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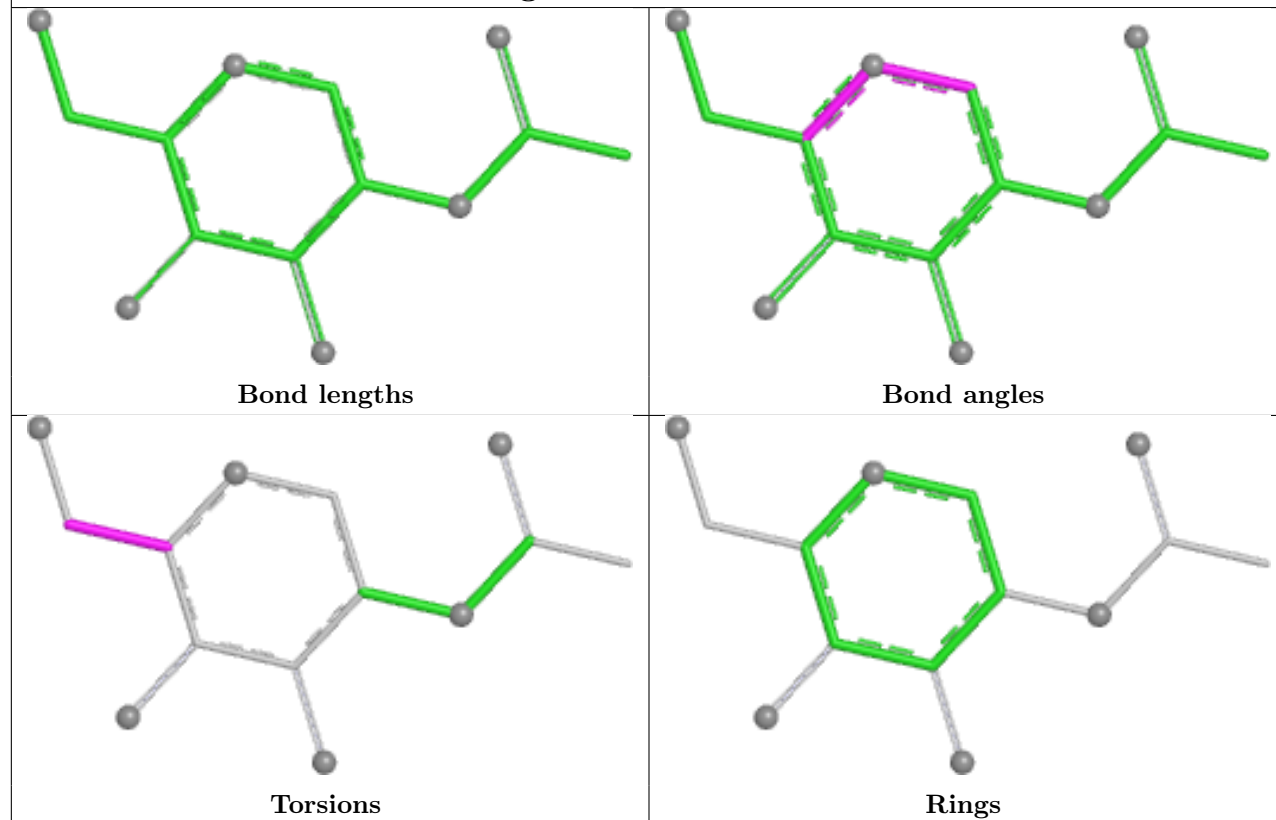




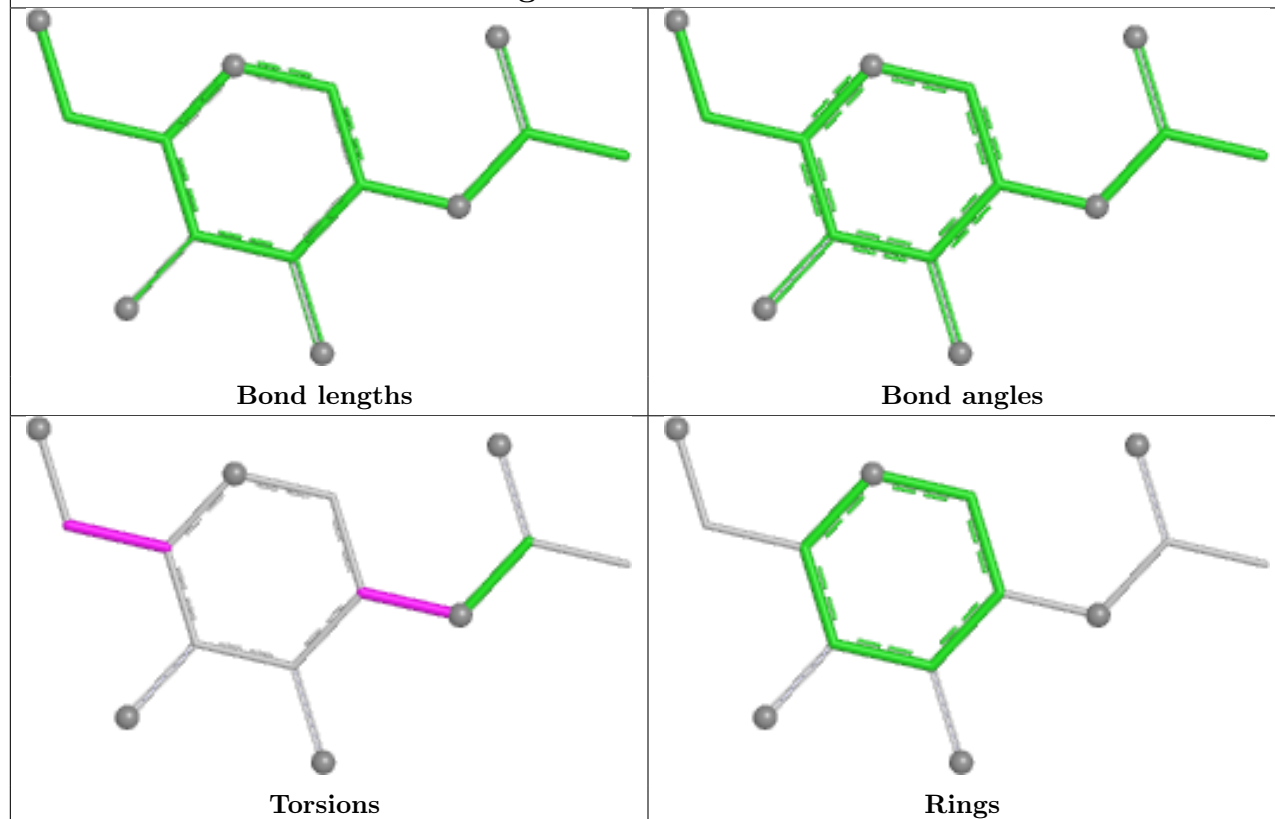
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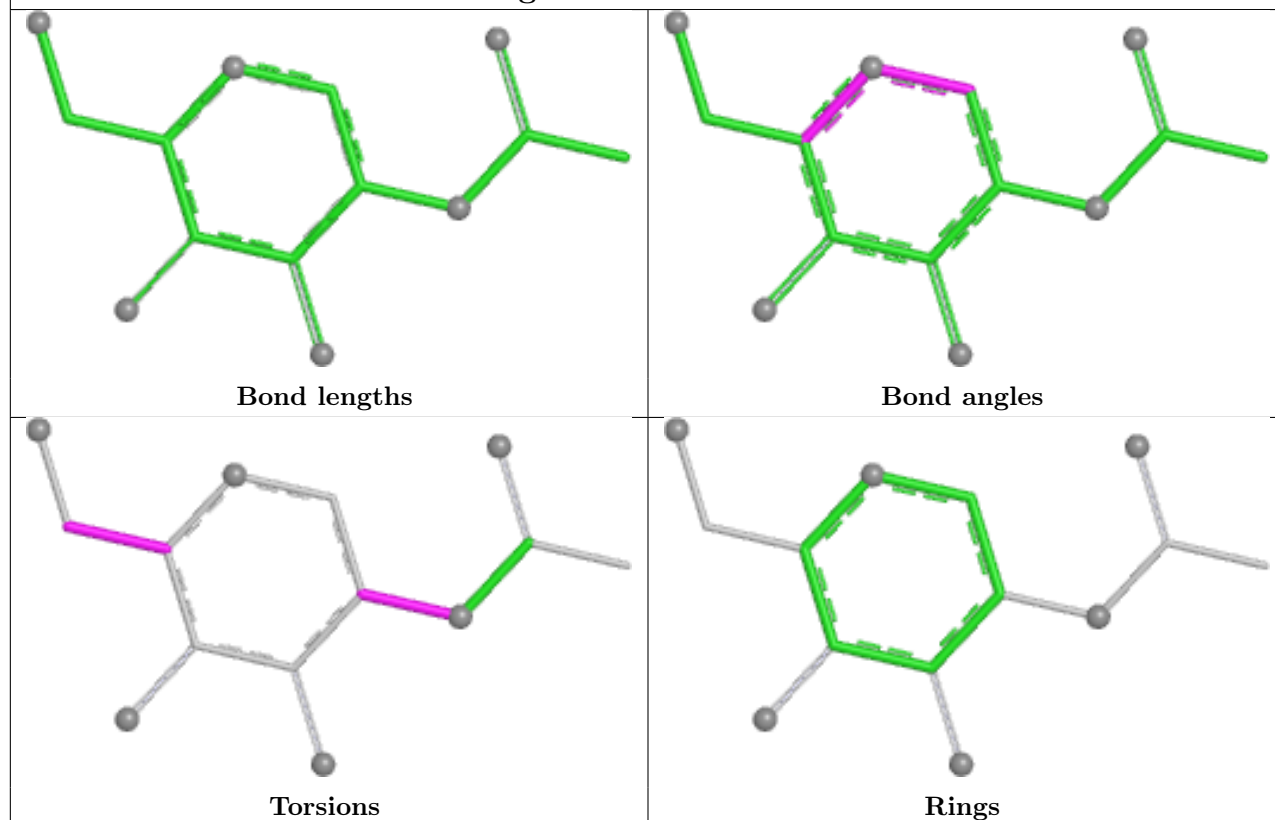
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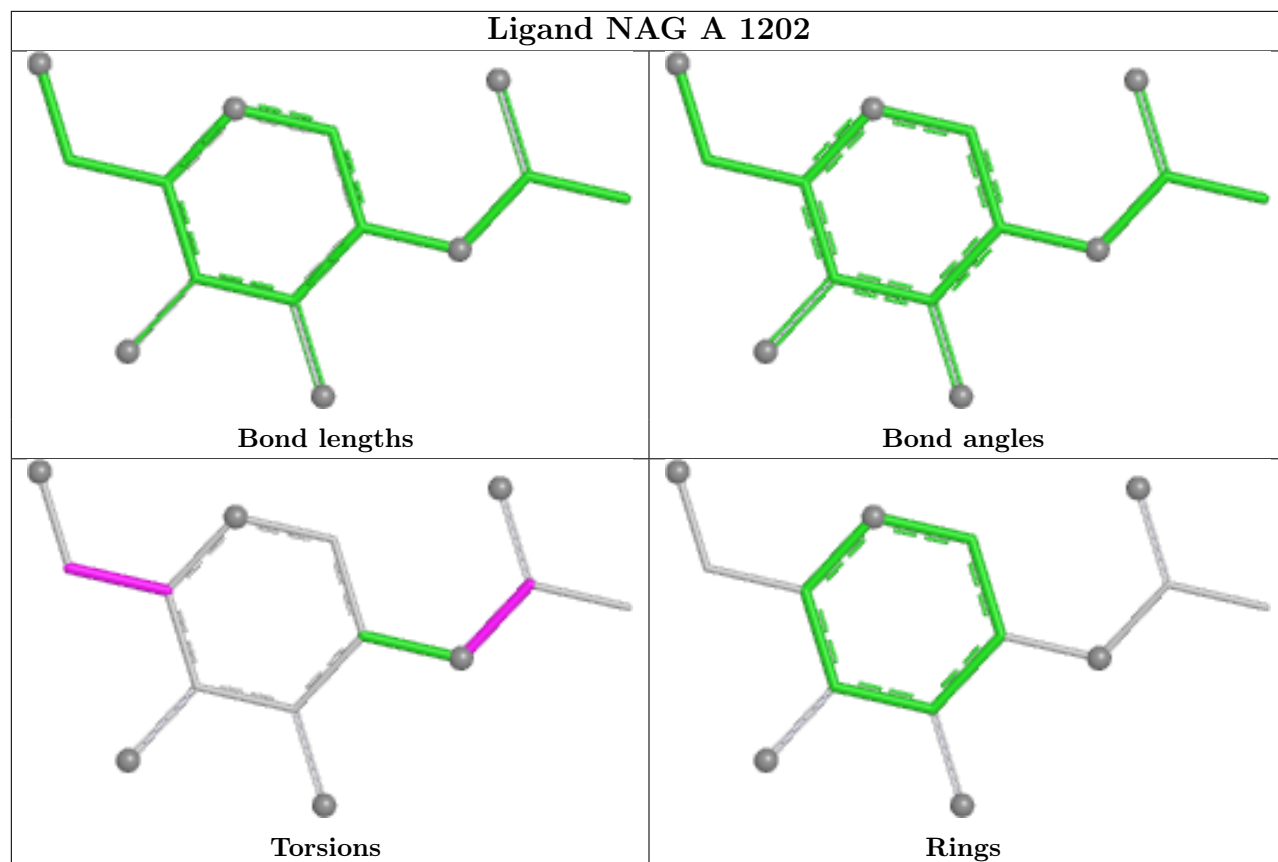
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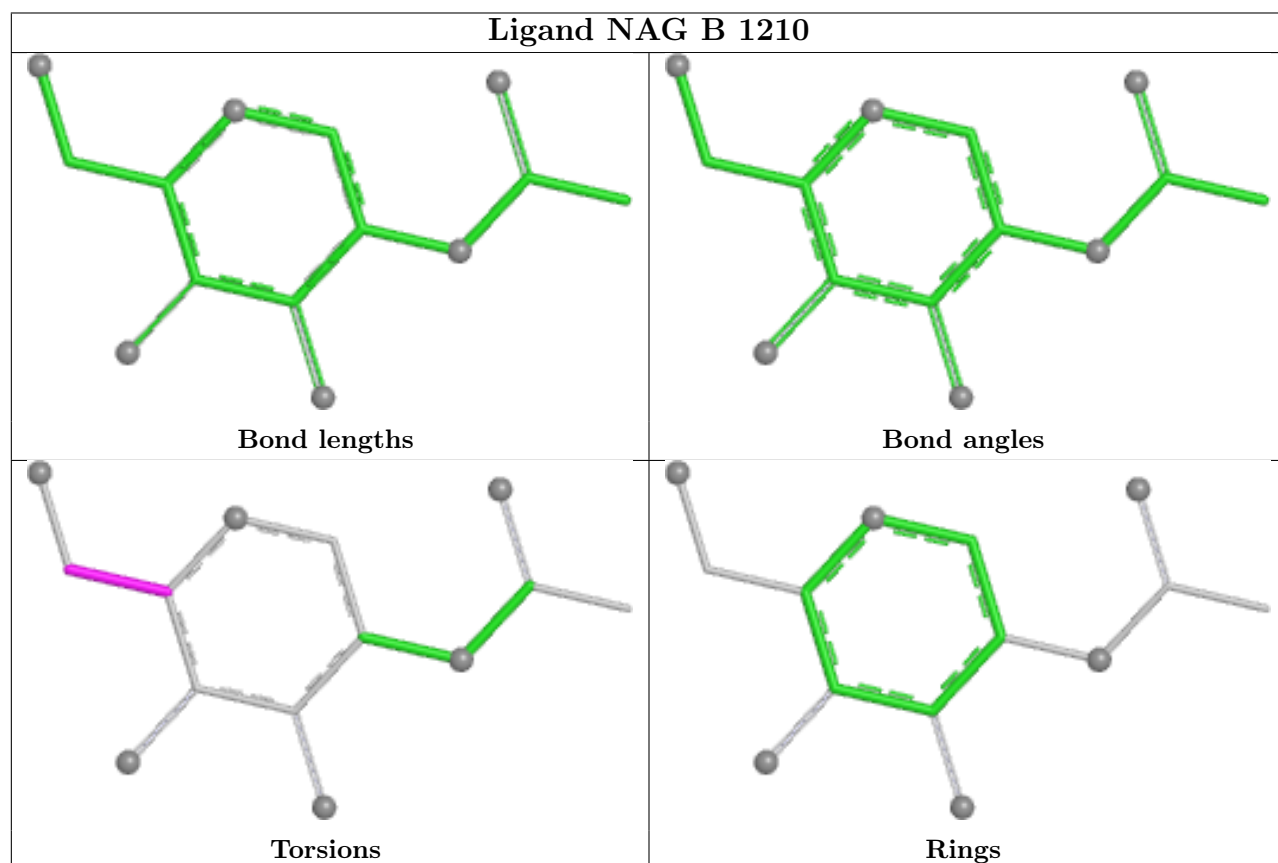
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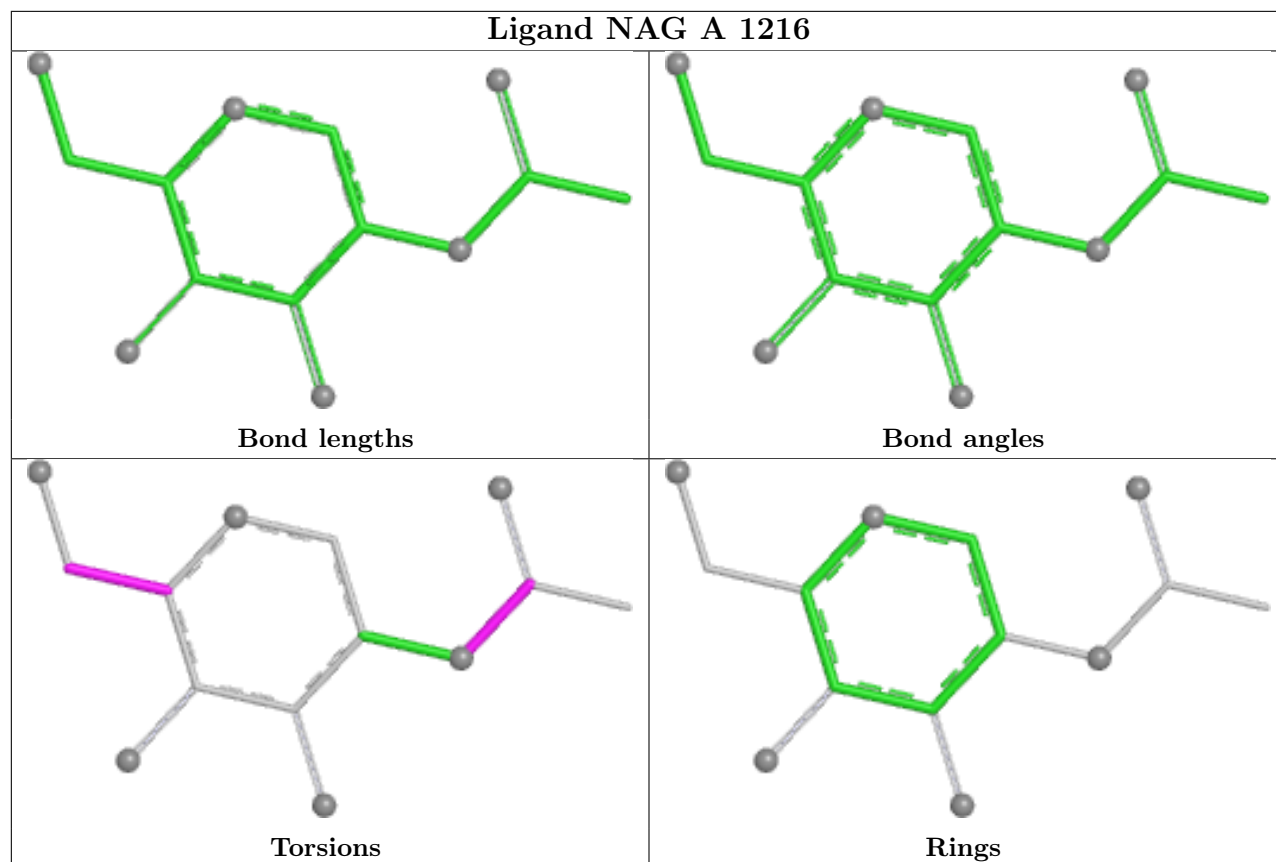
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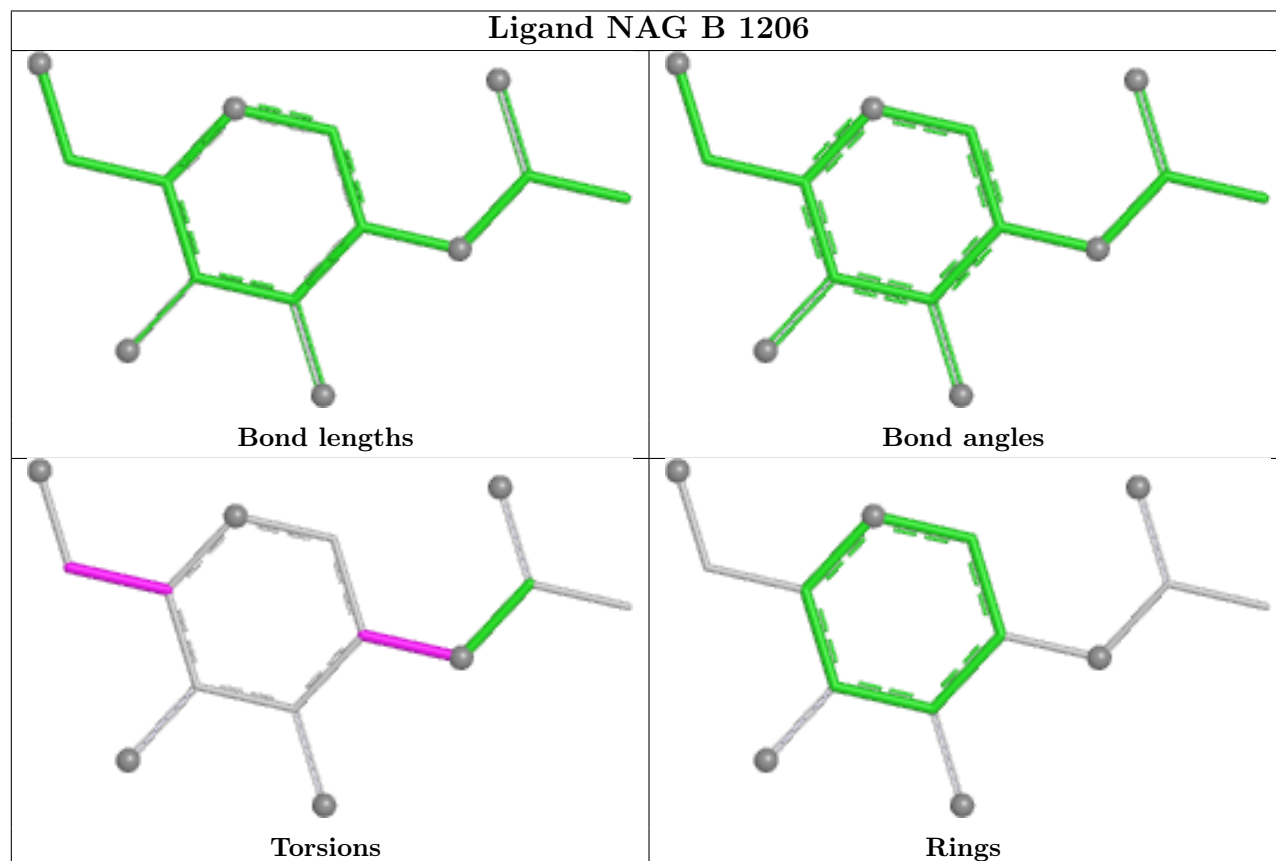
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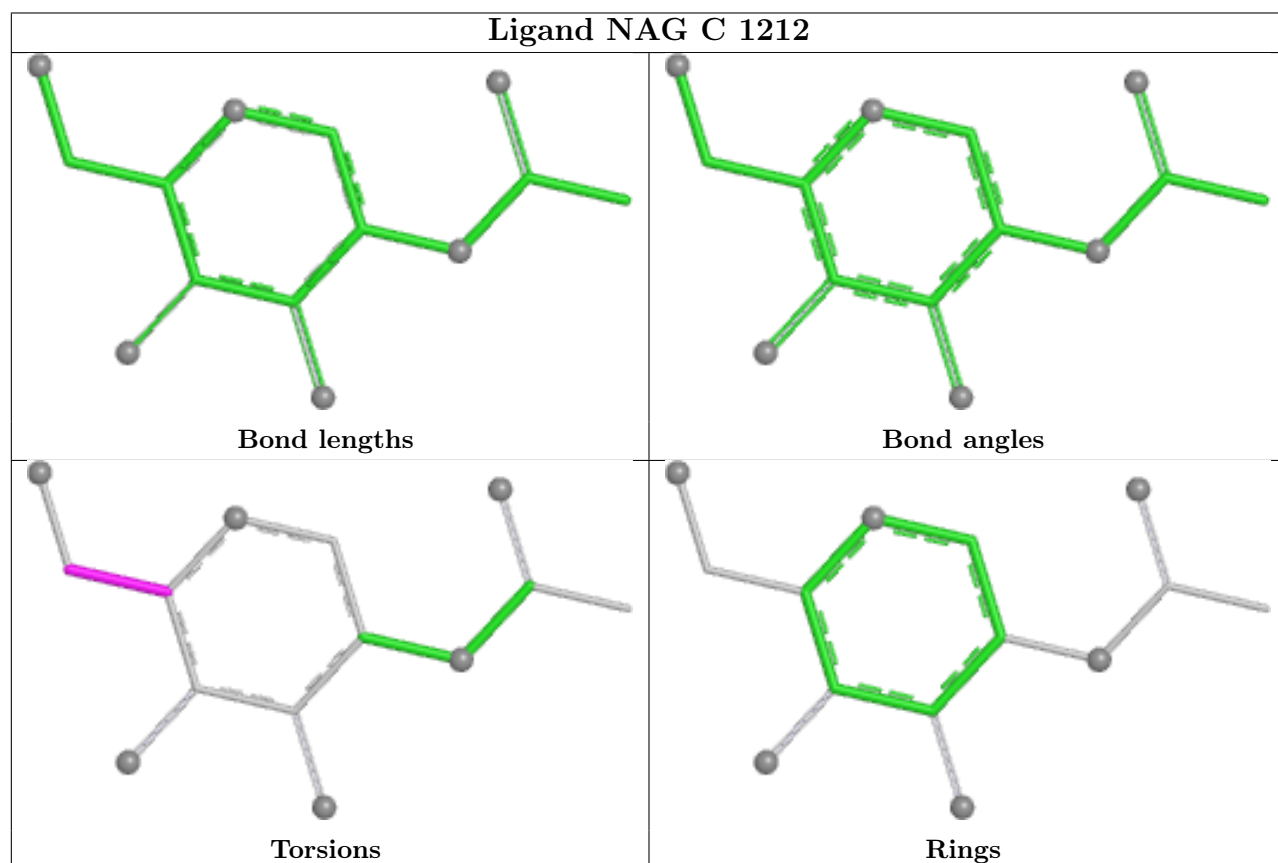
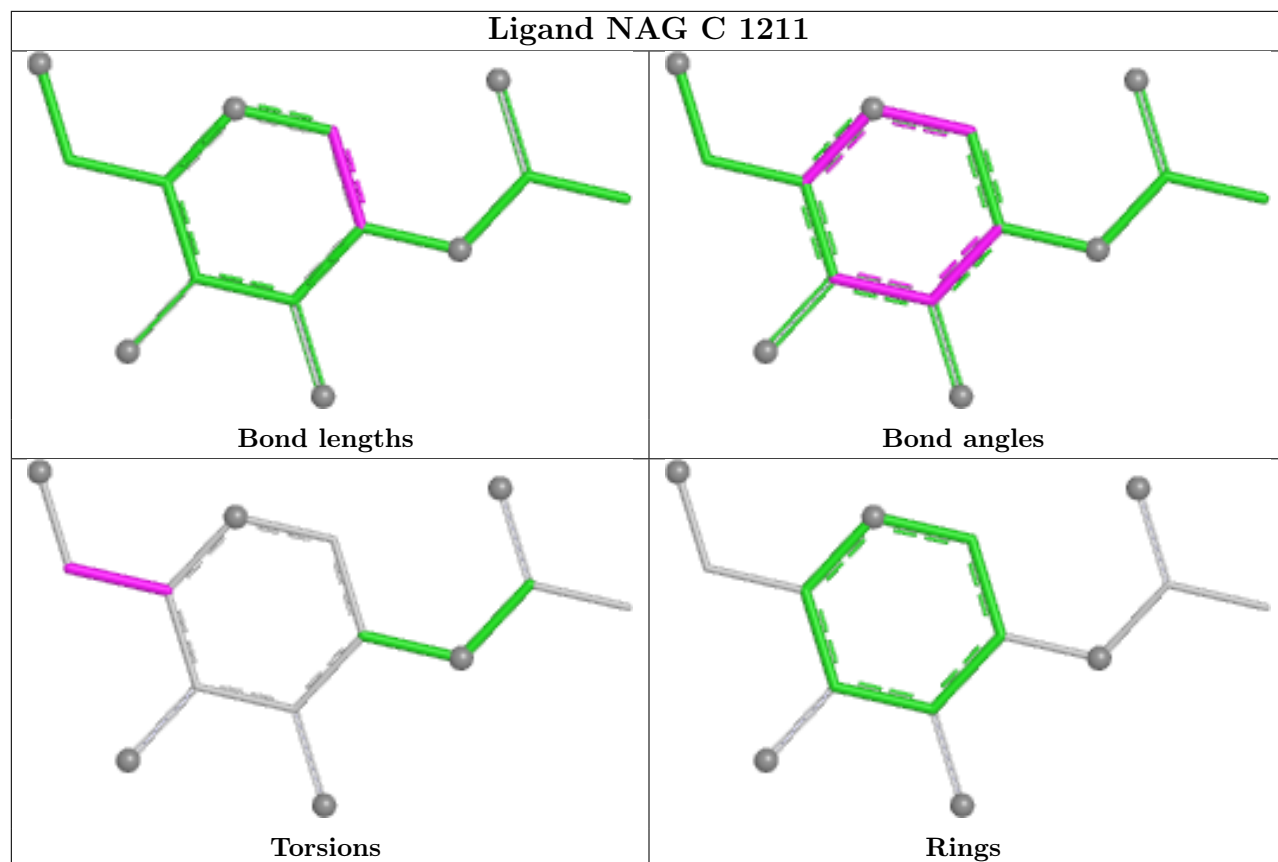


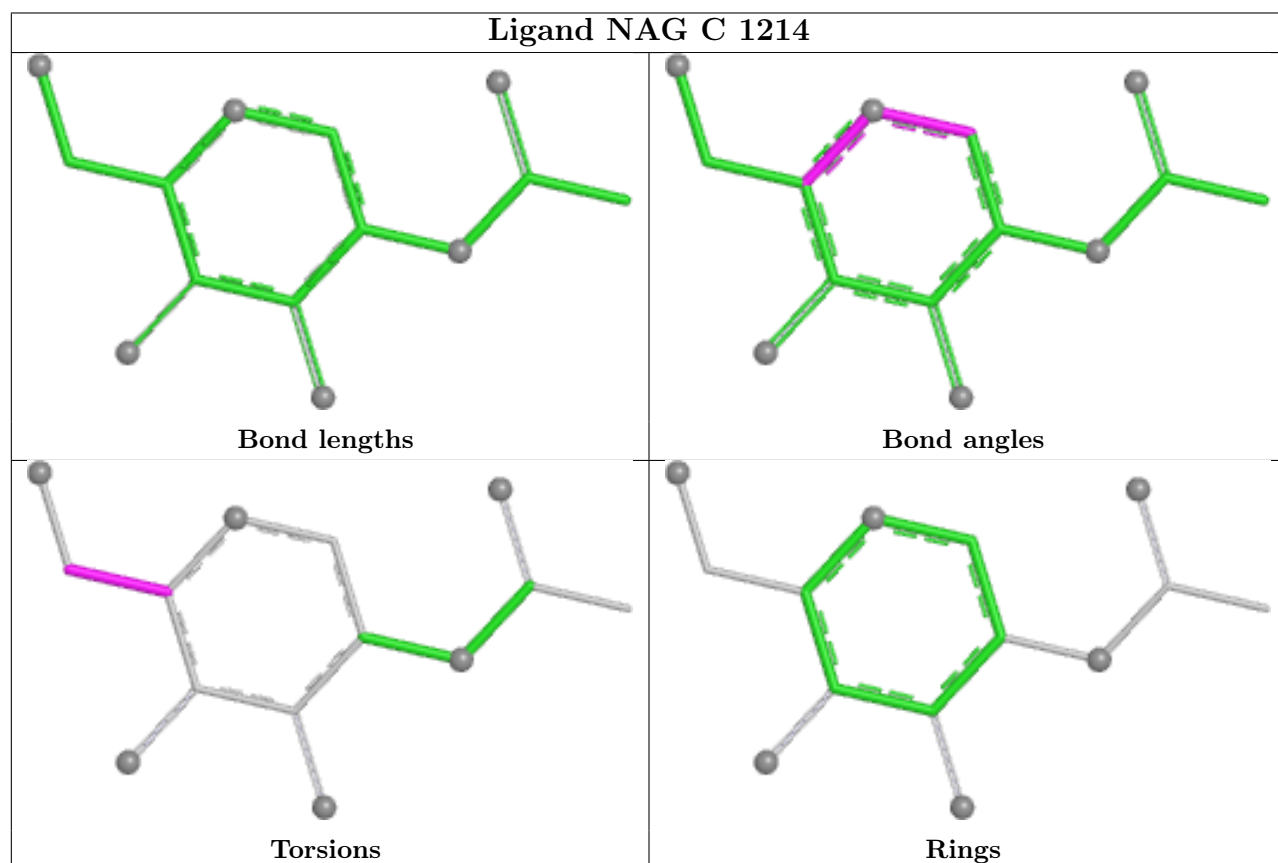
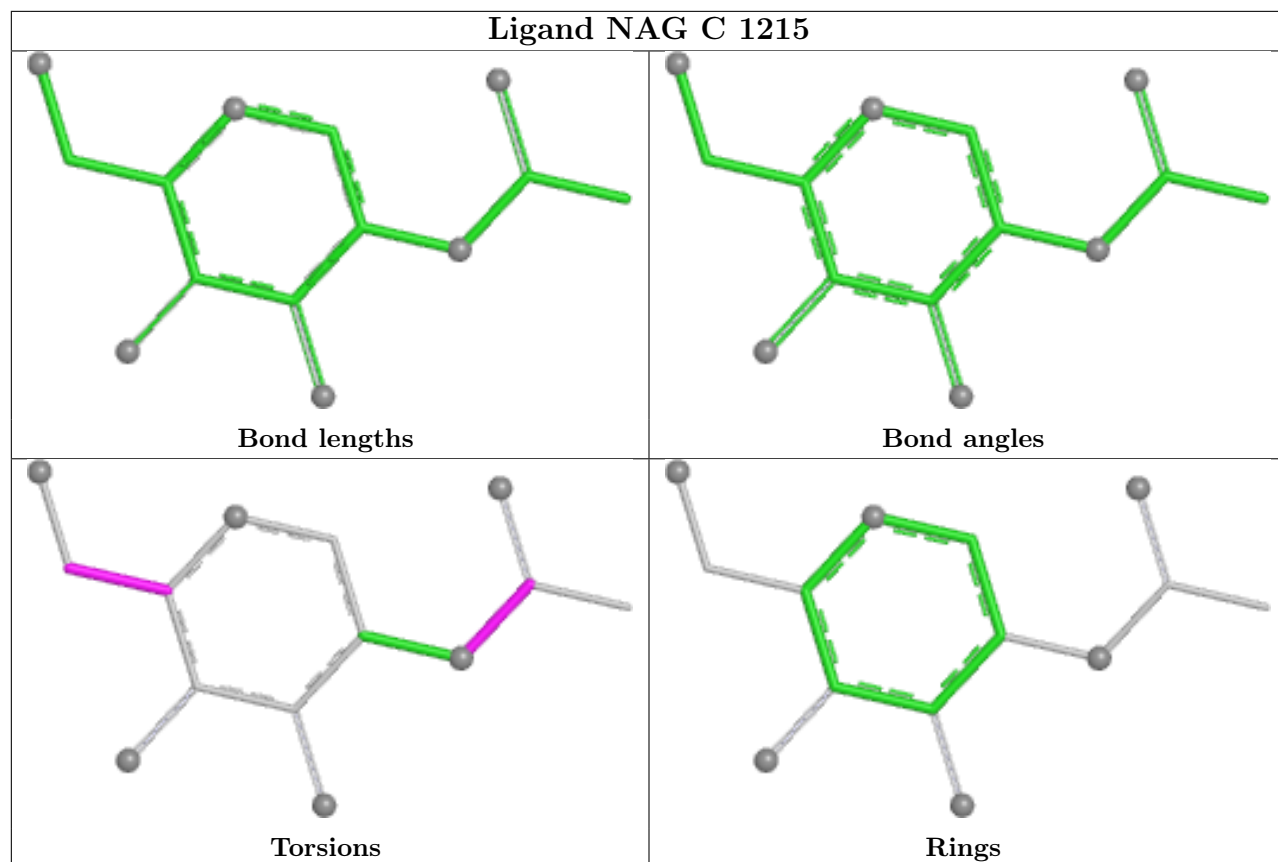
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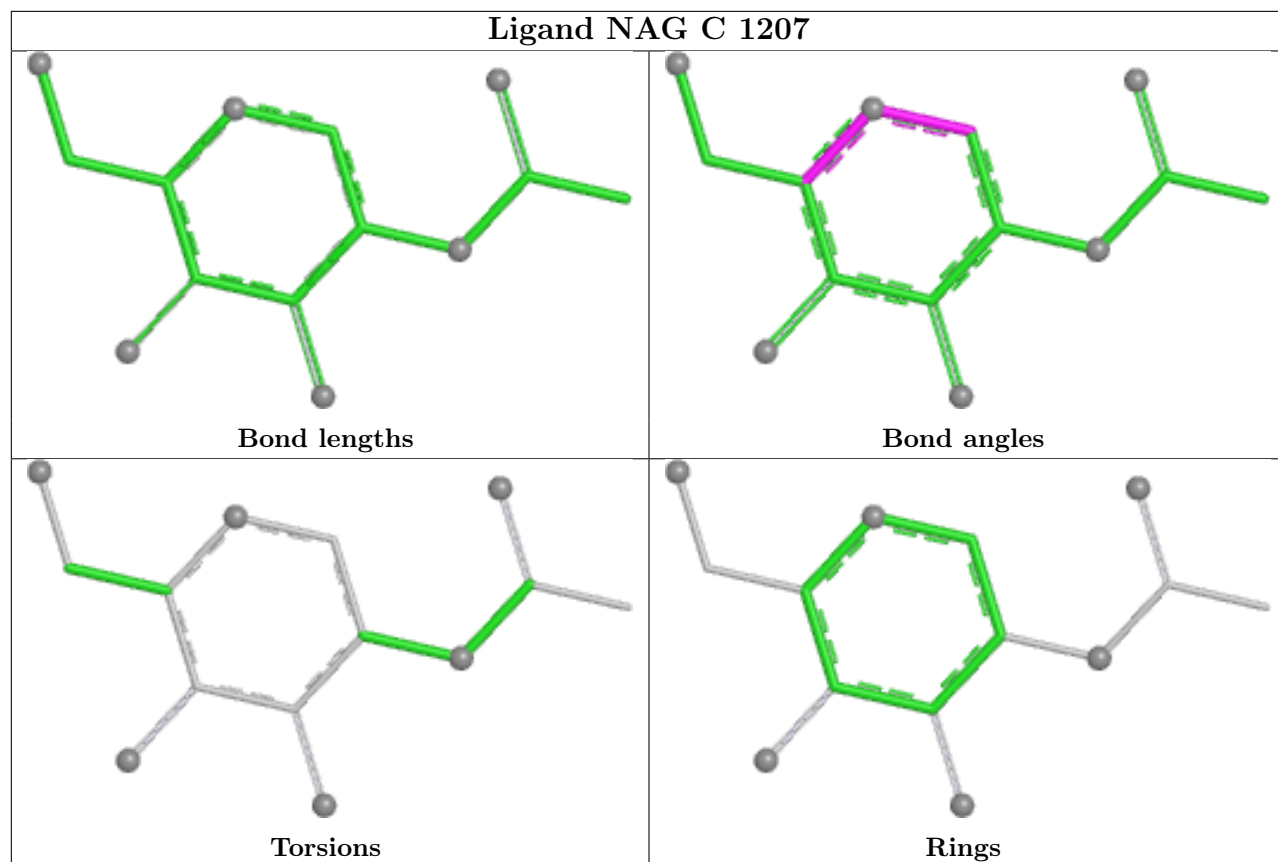
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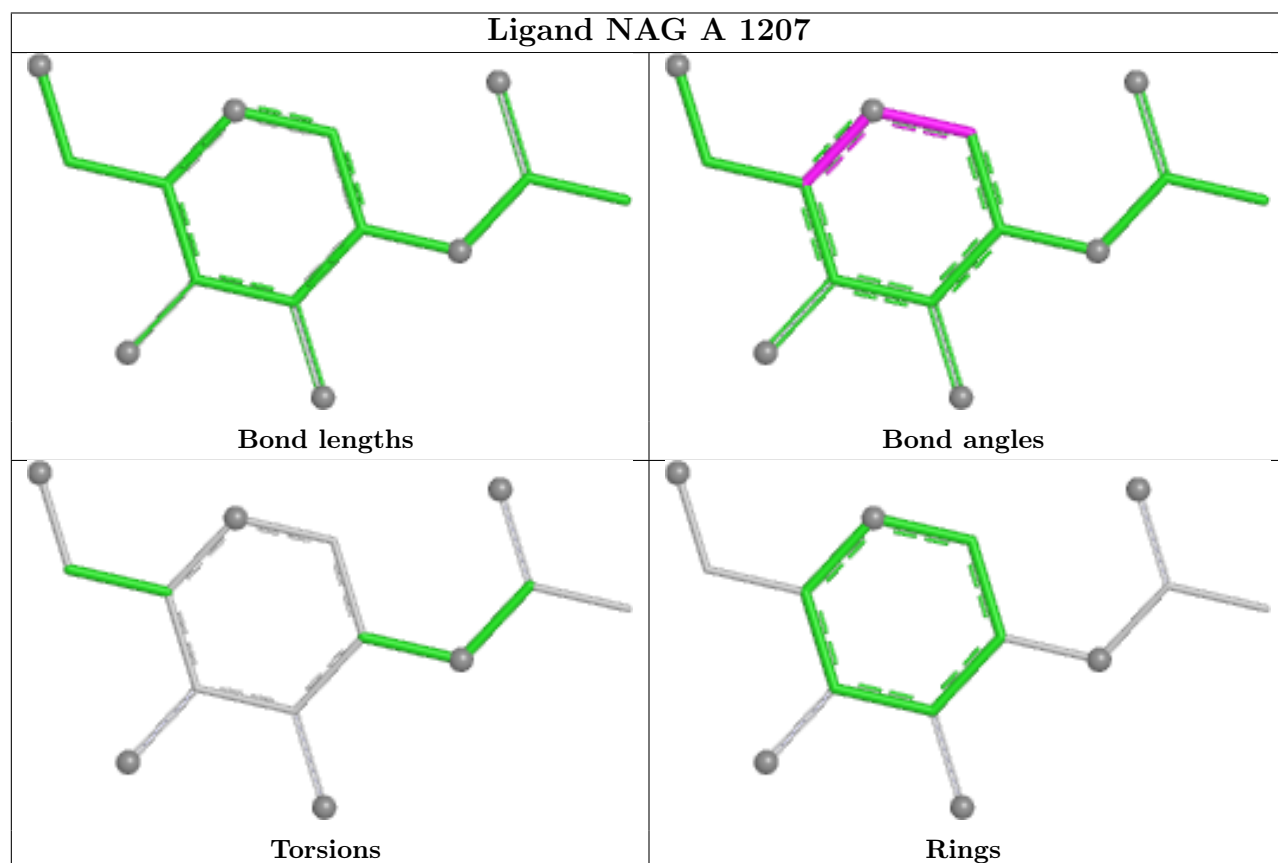


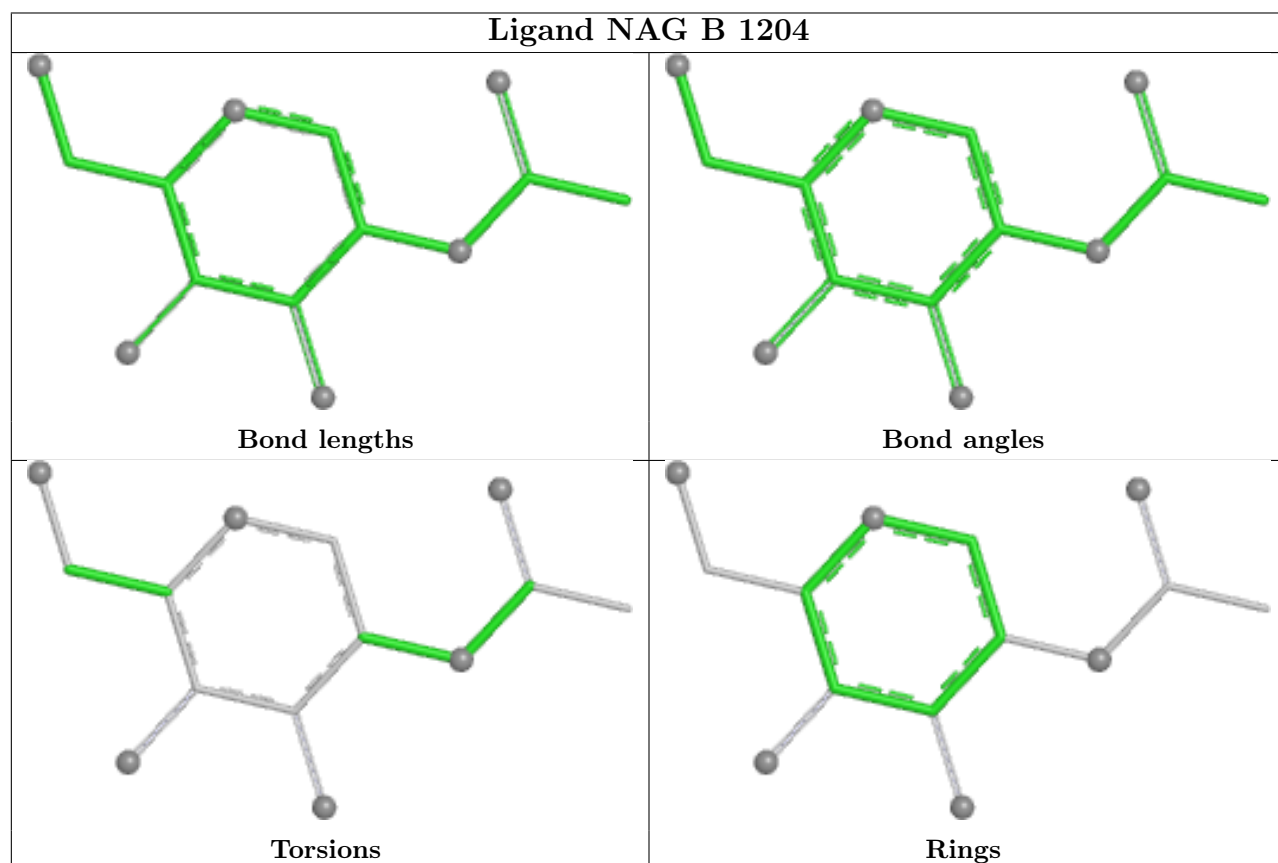
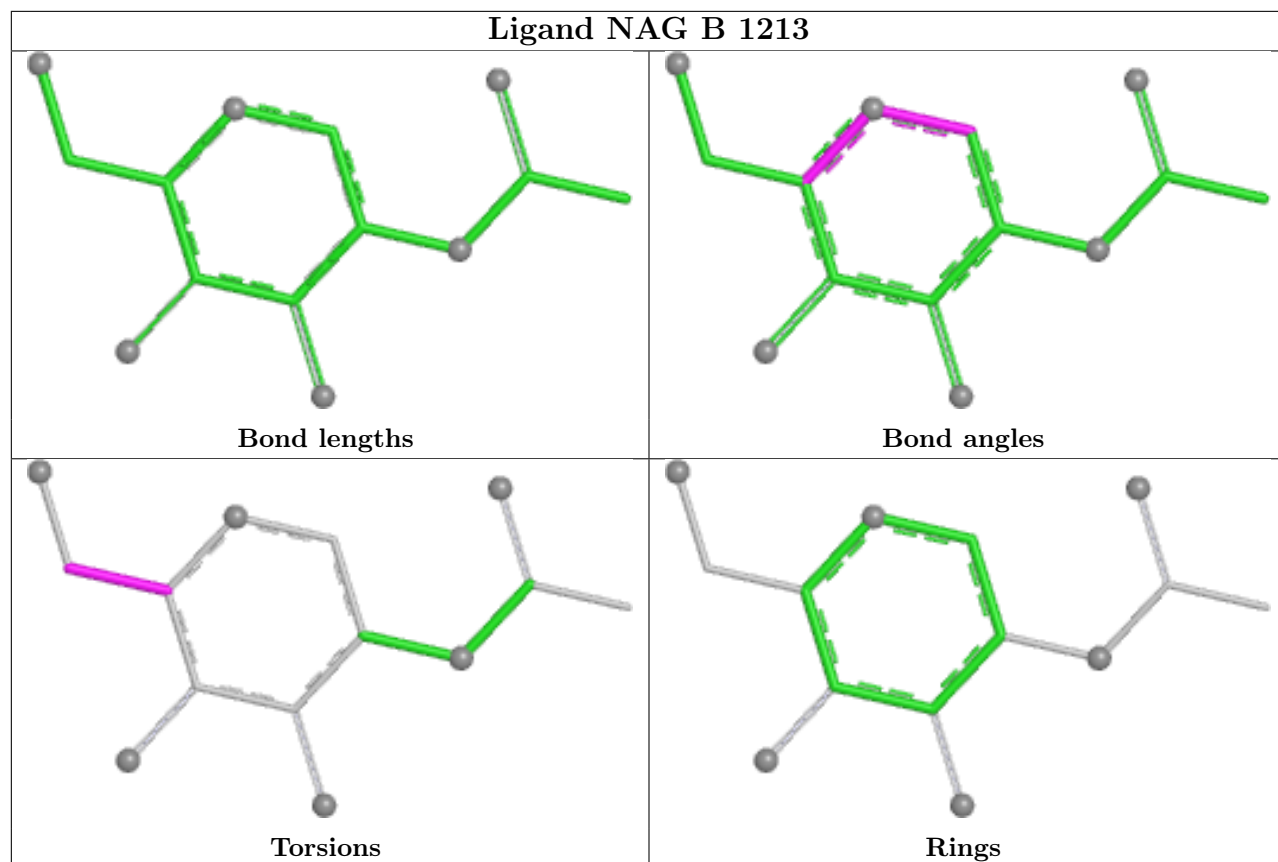


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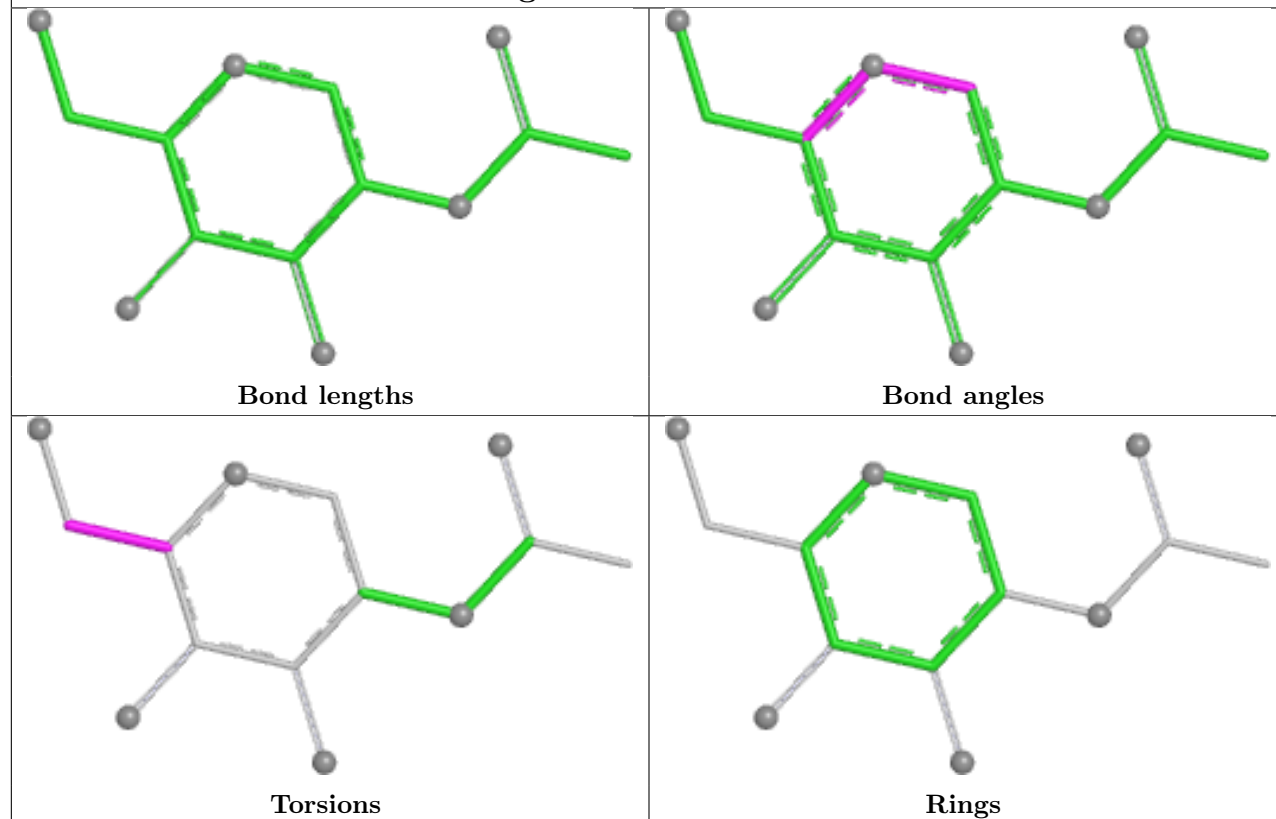


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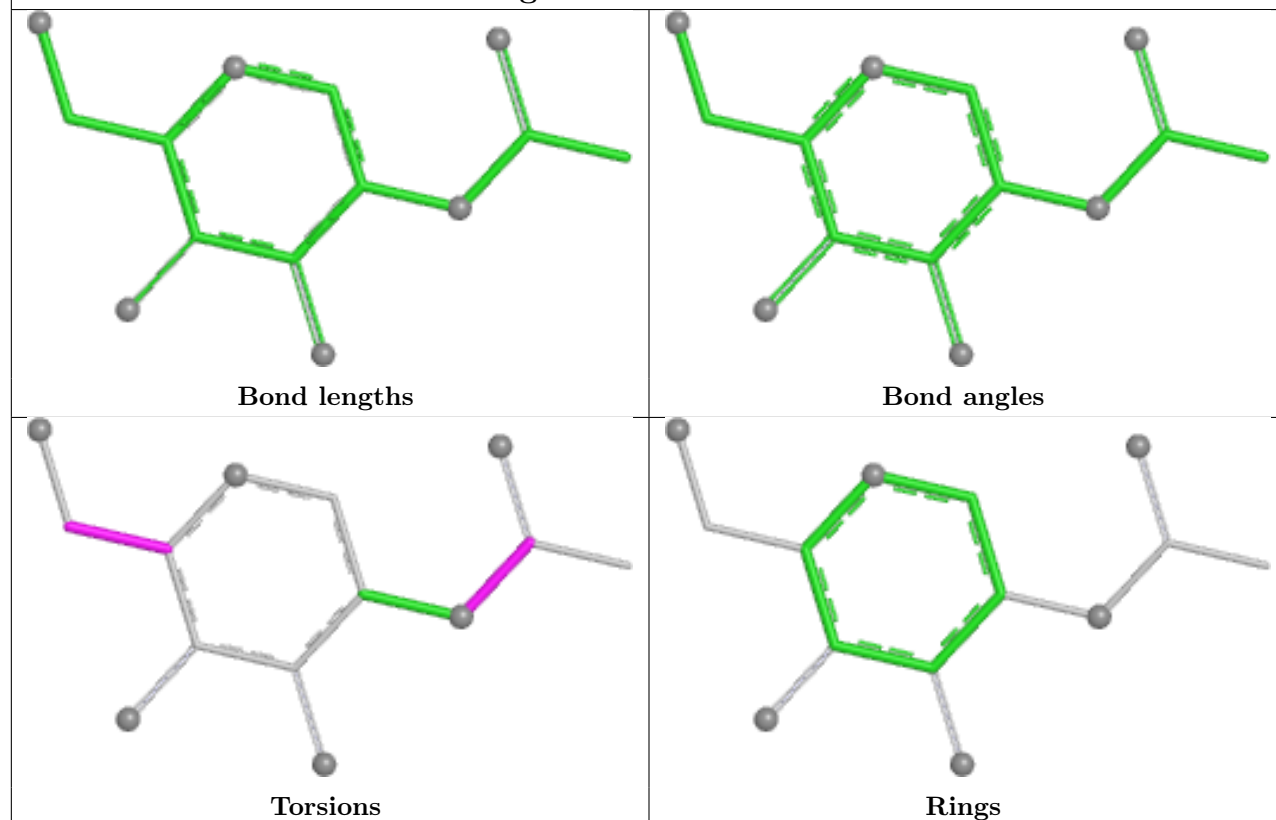


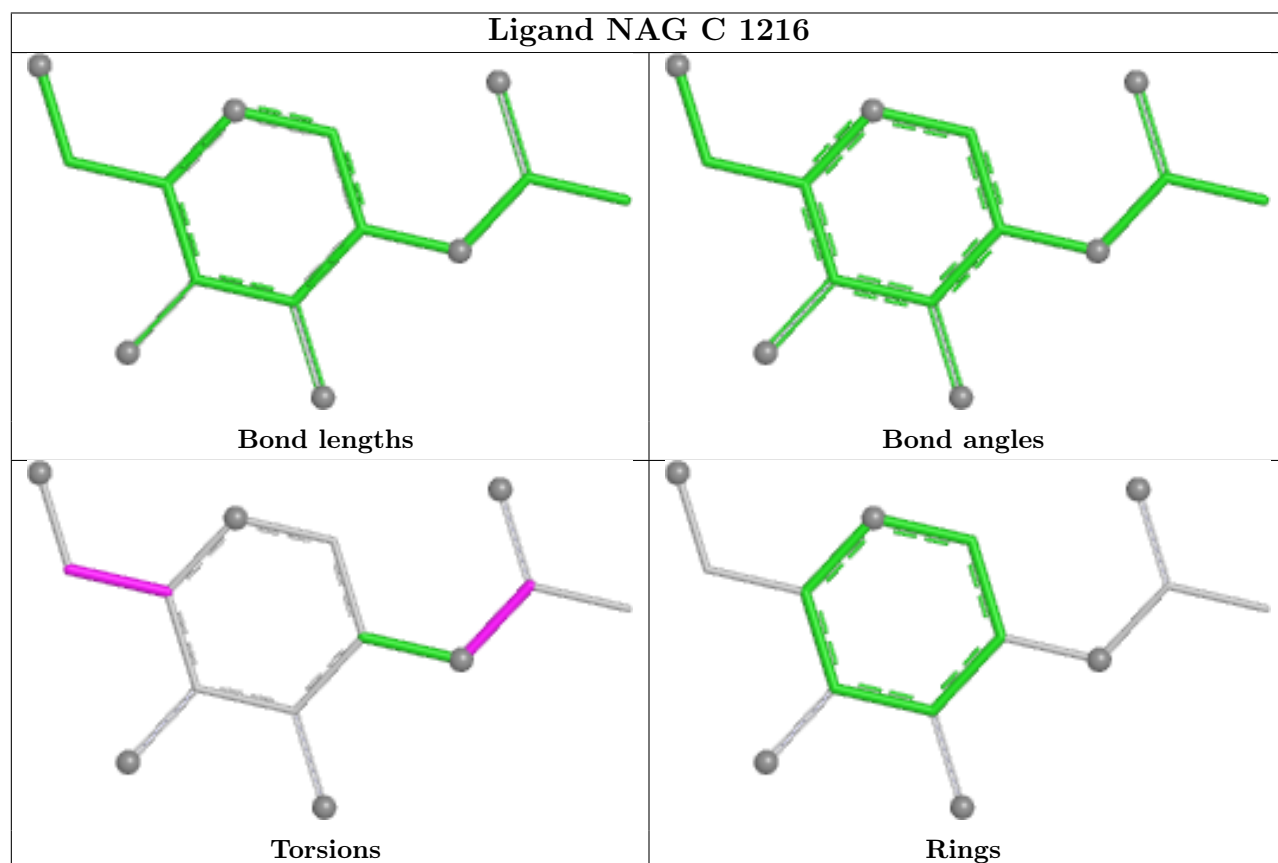
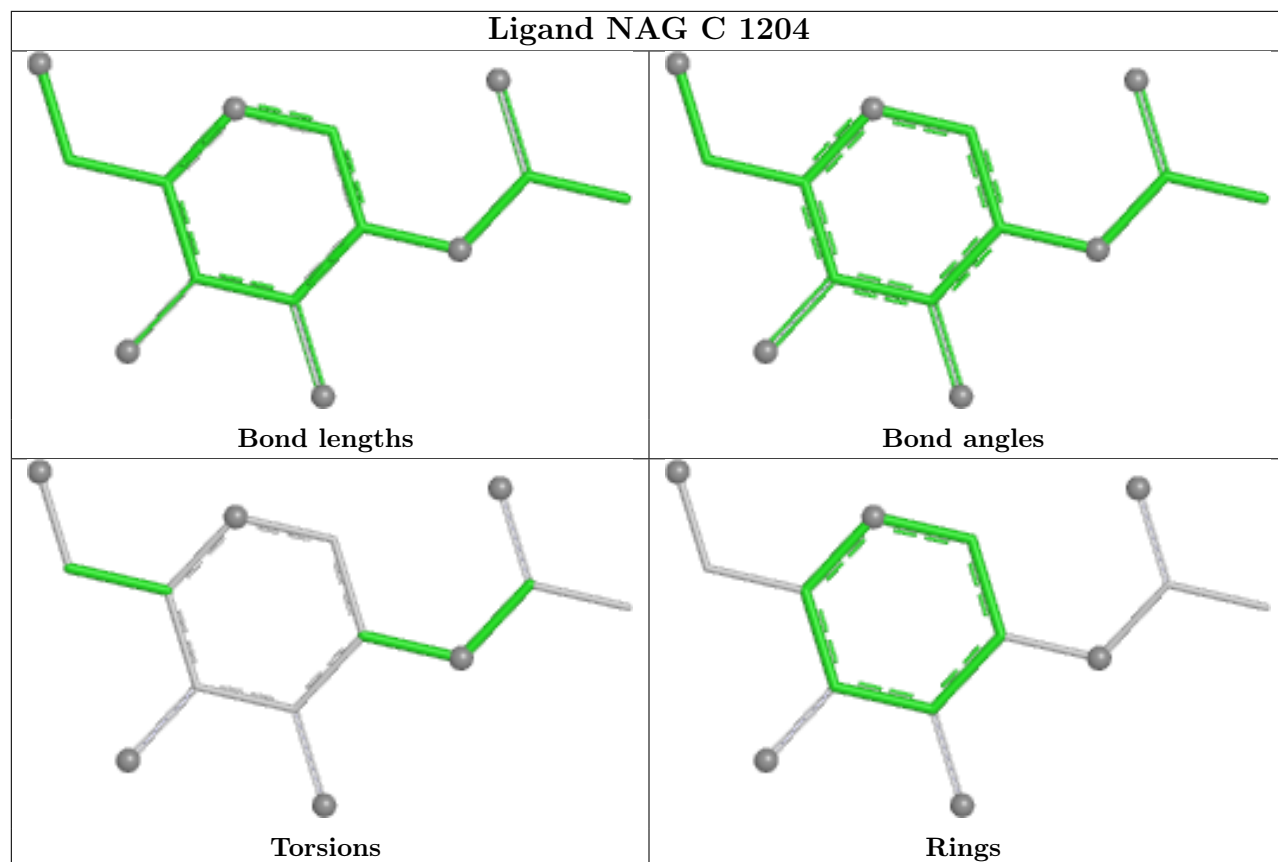


Ligand NAG A 1214



Ligand NAG B 1215





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-30496. These allow visual inspection of the internal detail of the map and identification of artifacts.

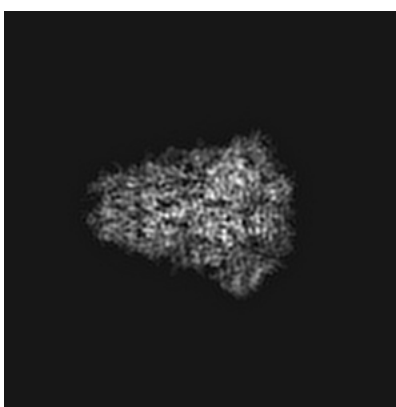
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

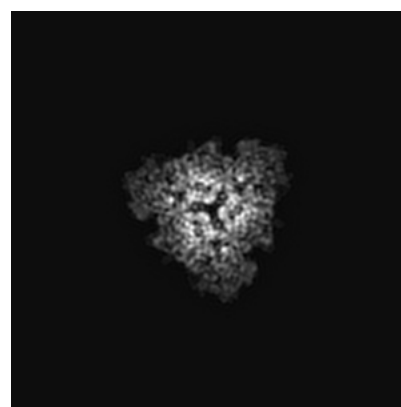
6.1.1 Primary map



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: 100



Y Index: 100



Z Index: 100

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: 89



Y Index: 105

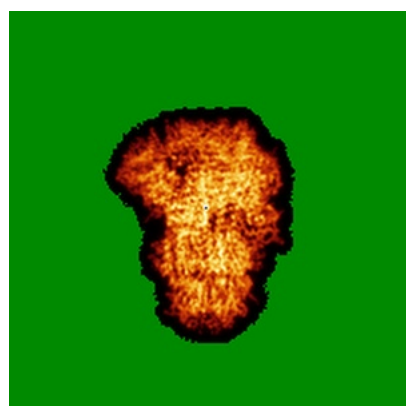


Z Index: 110

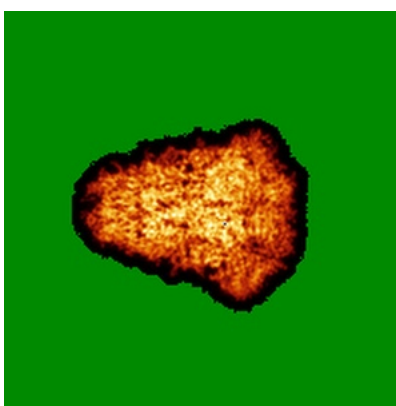
The images above show the largest variance slices of the map in three orthogonal directions.

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

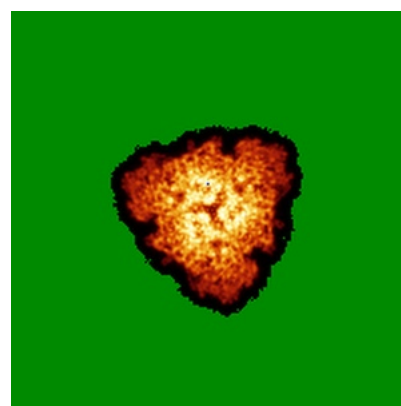
6.4.1 Primary map



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

This section was not generated.

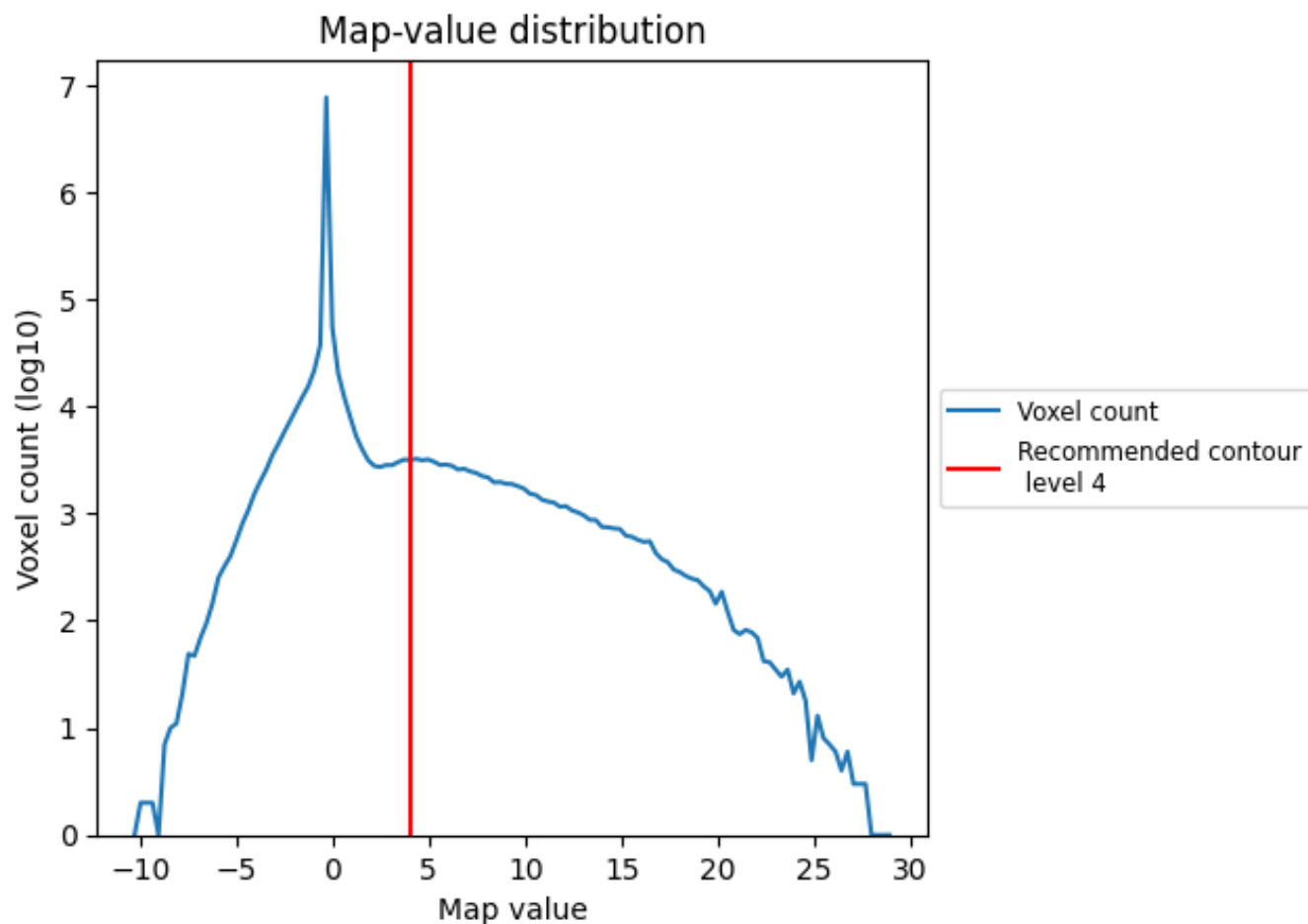
6.6 Mask visualisation

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

7 Map analysis [i](#)

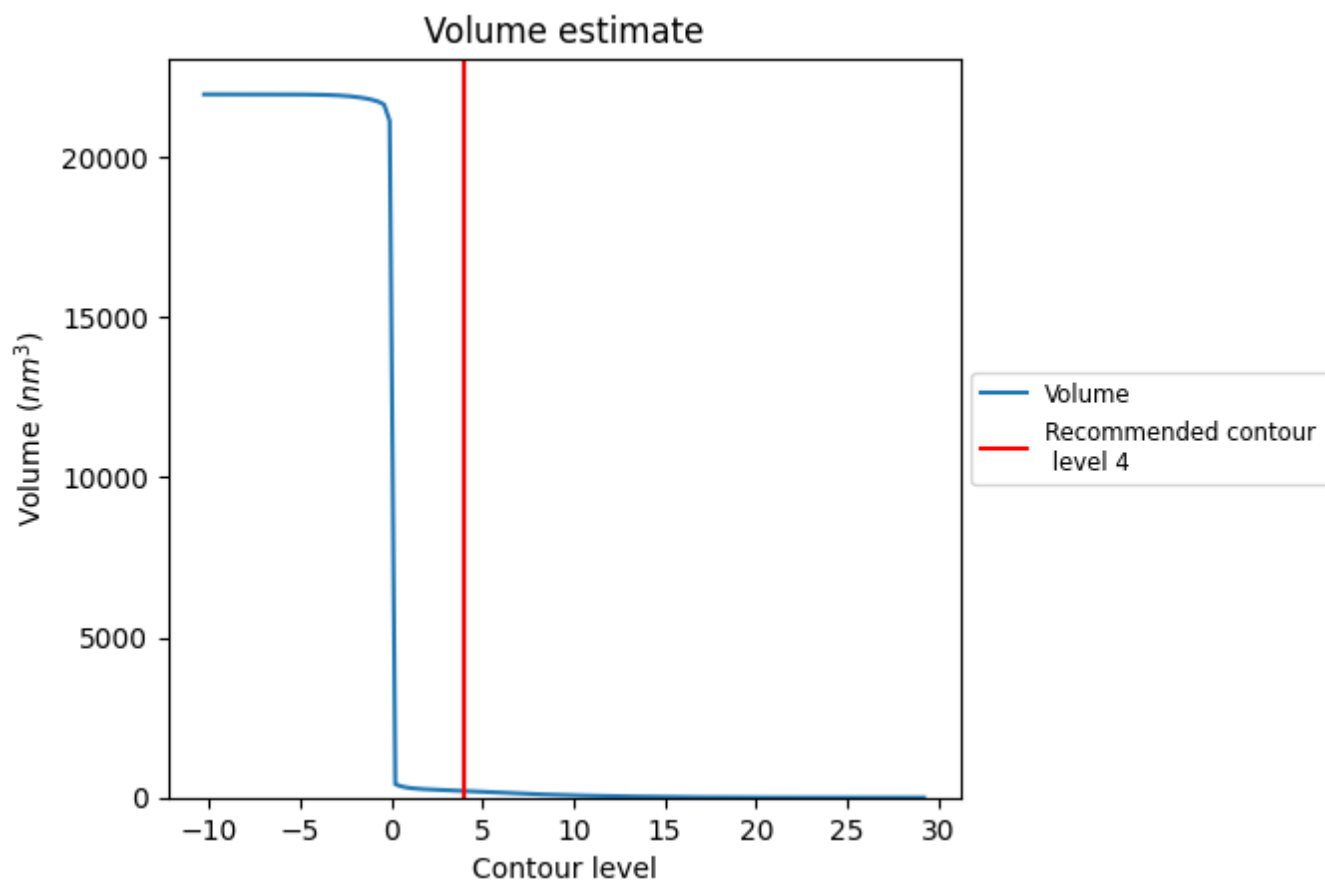
This section contains the results of statistical analysis of the map.

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.

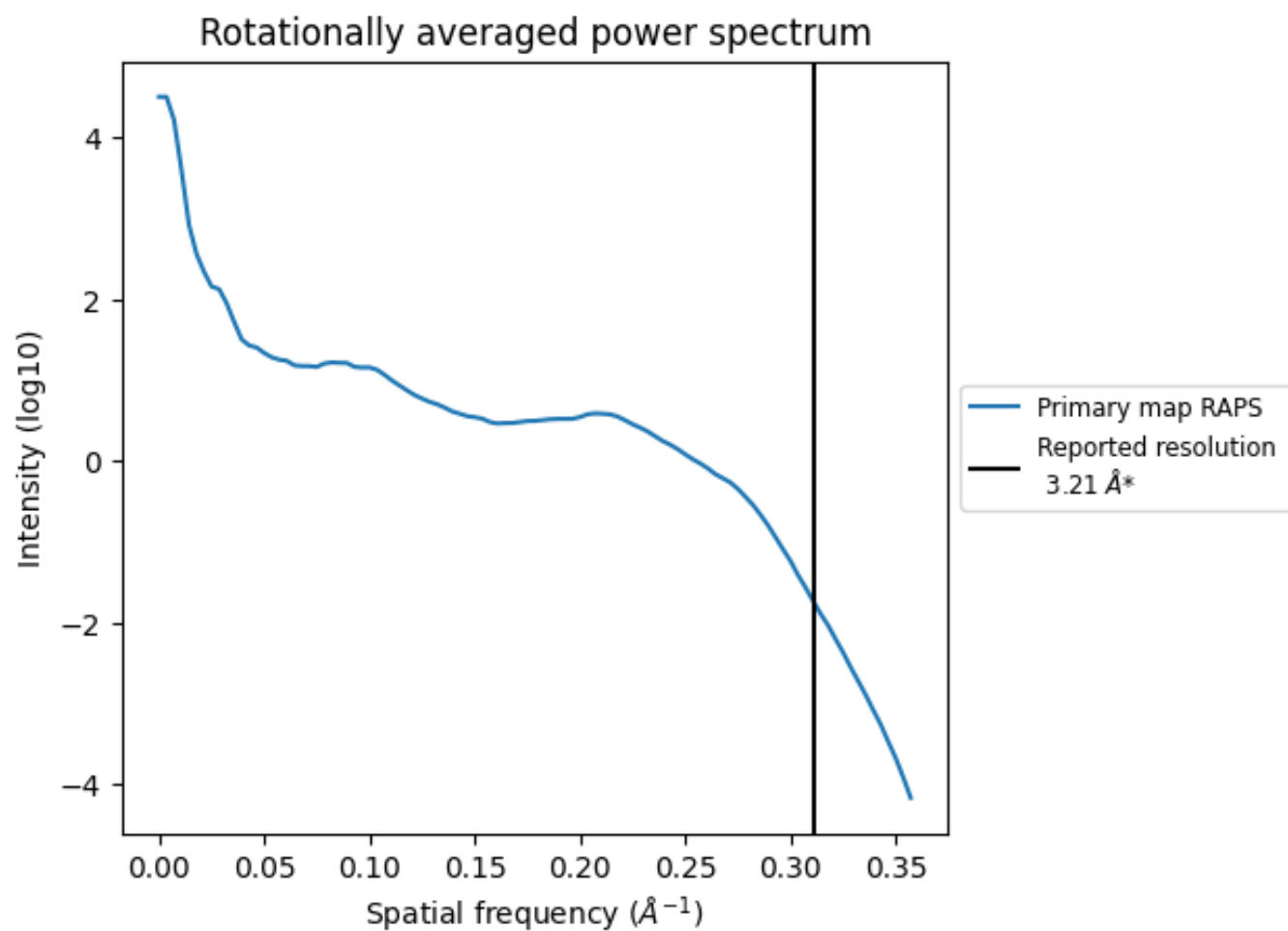
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm³; this corresponds to an approximate mass of 184 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 0.312 Å⁻¹

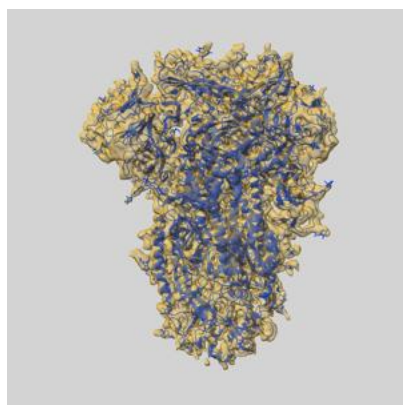
8 Fourier-Shell correlation

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

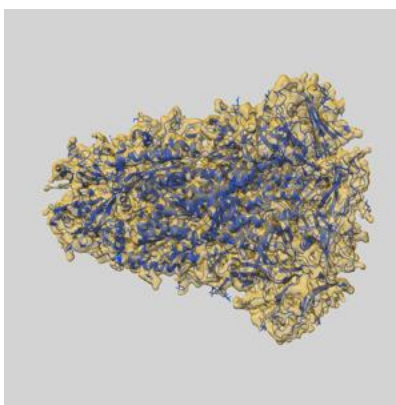
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30496 and PDB model 7CYC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

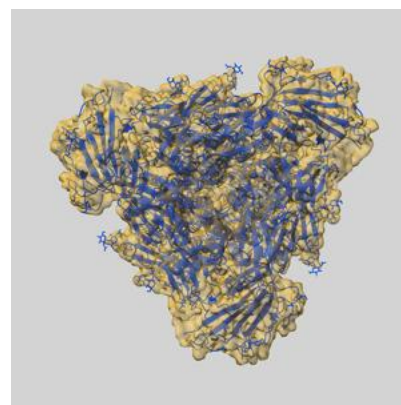
9.1 Map-model overlay [i](#)



X



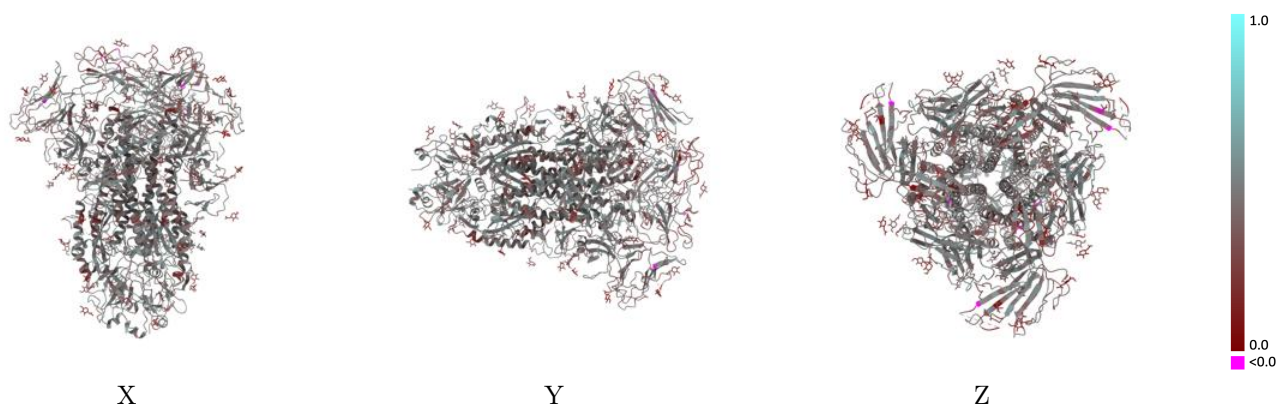
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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](#)

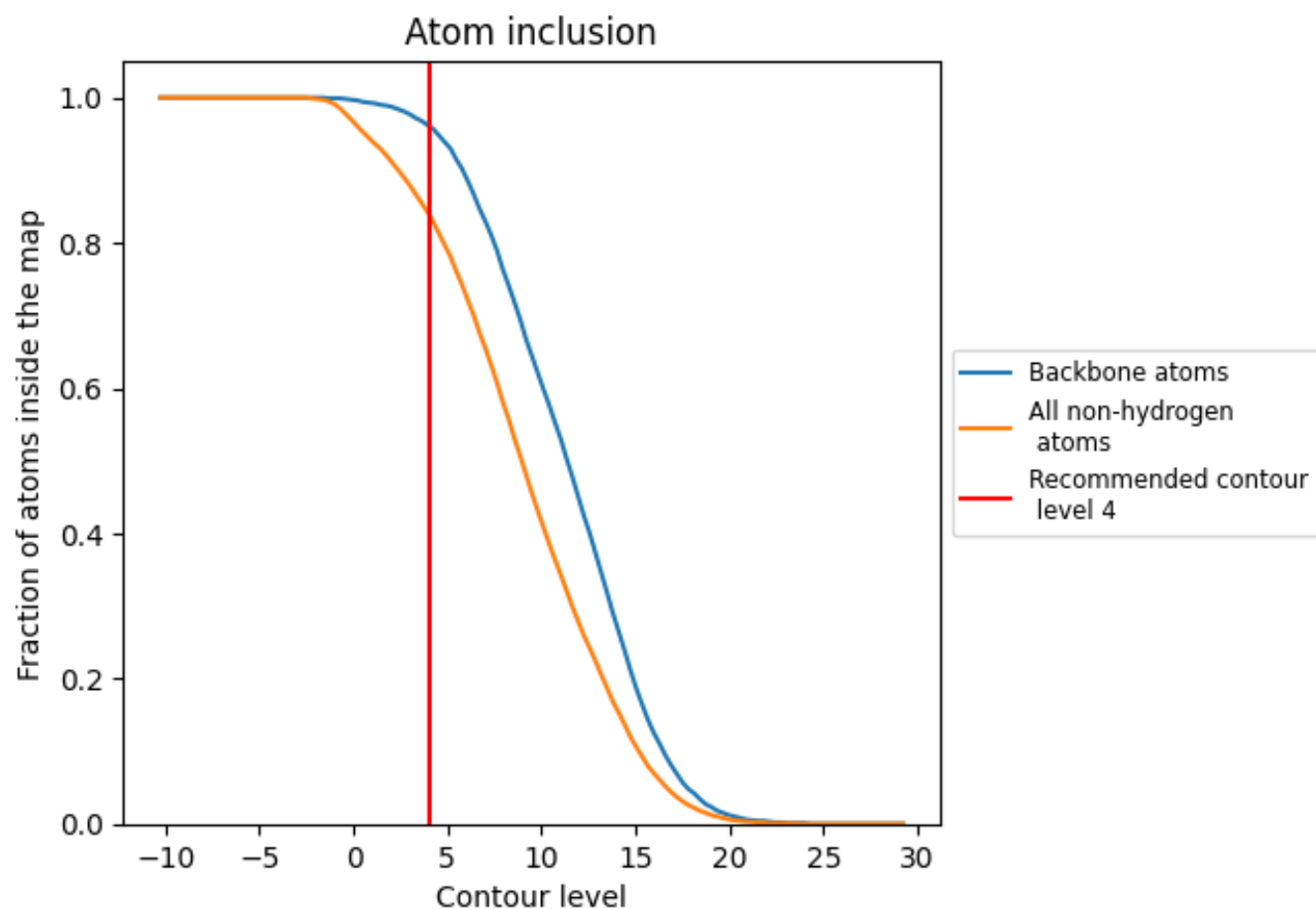


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.4240
A	 0.8460	 0.4280
B	 0.8450	 0.4270
C	 0.8480	 0.4260
D	 0.5420	 0.3230
E	 0.6150	 0.3120
F	 0.4290	 0.1820
G	 0.7440	 0.4220
H	 0.5540	 0.3310
I	 0.5380	 0.2800
J	 0.3930	 0.1950
K	 0.7690	 0.4430
L	 0.5900	 0.3190
M	 0.5380	 0.2550
N	 0.3930	 0.2380
O	 0.7950	 0.4320

