



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:39 AM UTC

PDB ID : 9OZC / pdb_00009ozc
EMDB ID : EMD-71057
Title : Cryo-EM structure of 1:2:1 ROS1/NEL/NICOL holo-complex, conformation 1.
Authors : An, W.D.; Zhang, X.W.; Bai, X.C.
Deposited on : 2025-06-05
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

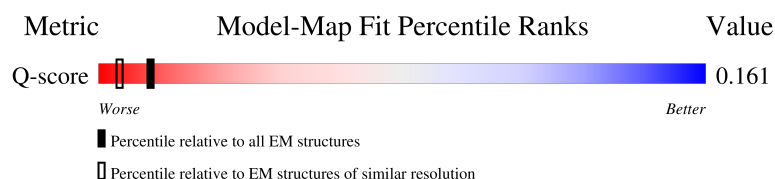
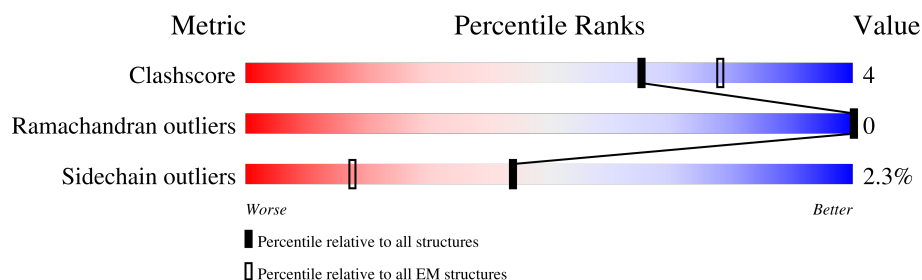
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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




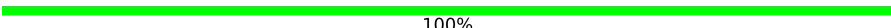
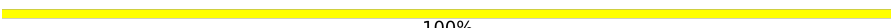
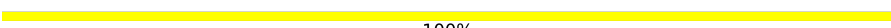
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2311	
2	B	816	
2	C	816	
3	D	95	

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Mol	Chain	Length	Quality of chain
4	E	2	 50%50%
4	F	2	 100%
4	H	2	 100%
5	G	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 50924 atoms, of which 24784 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 Tyrosine-protein kinase receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1612	Total	C	H	N	O	S	0	0
			25483	8324	12543	2113	2451	52		

- Molecule 2 is a protein called Protein NEL.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	785	Total	C	H	N	O	S	0	0
			11698	3710	5615	1076	1194	103		
2	C	793	Total	C	H	N	O	S	0	0
			11815	3749	5670	1089	1204	103		

- Molecule 3 is a protein called NELL2-interacting cell ontogeny regulator 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	60	Total	C	H	N	O	S	0	0
			903	280	446	88	83	6		

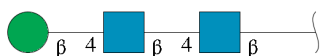
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
4	F	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
4	H	2	Total	C	H	N	O		0	0
			55	16	27	2	10			

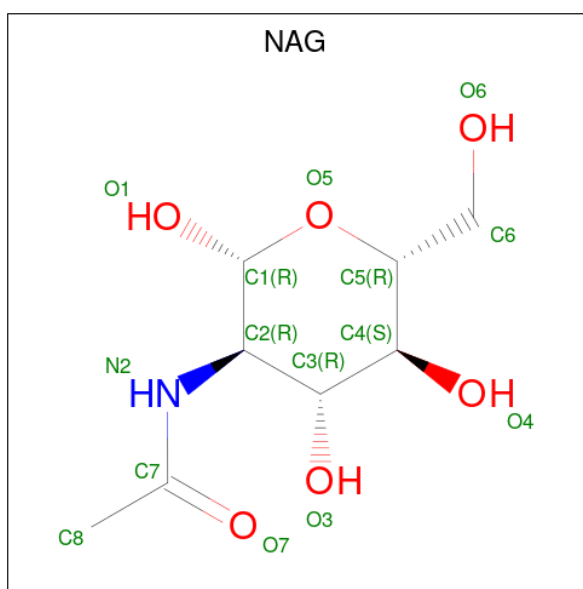
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



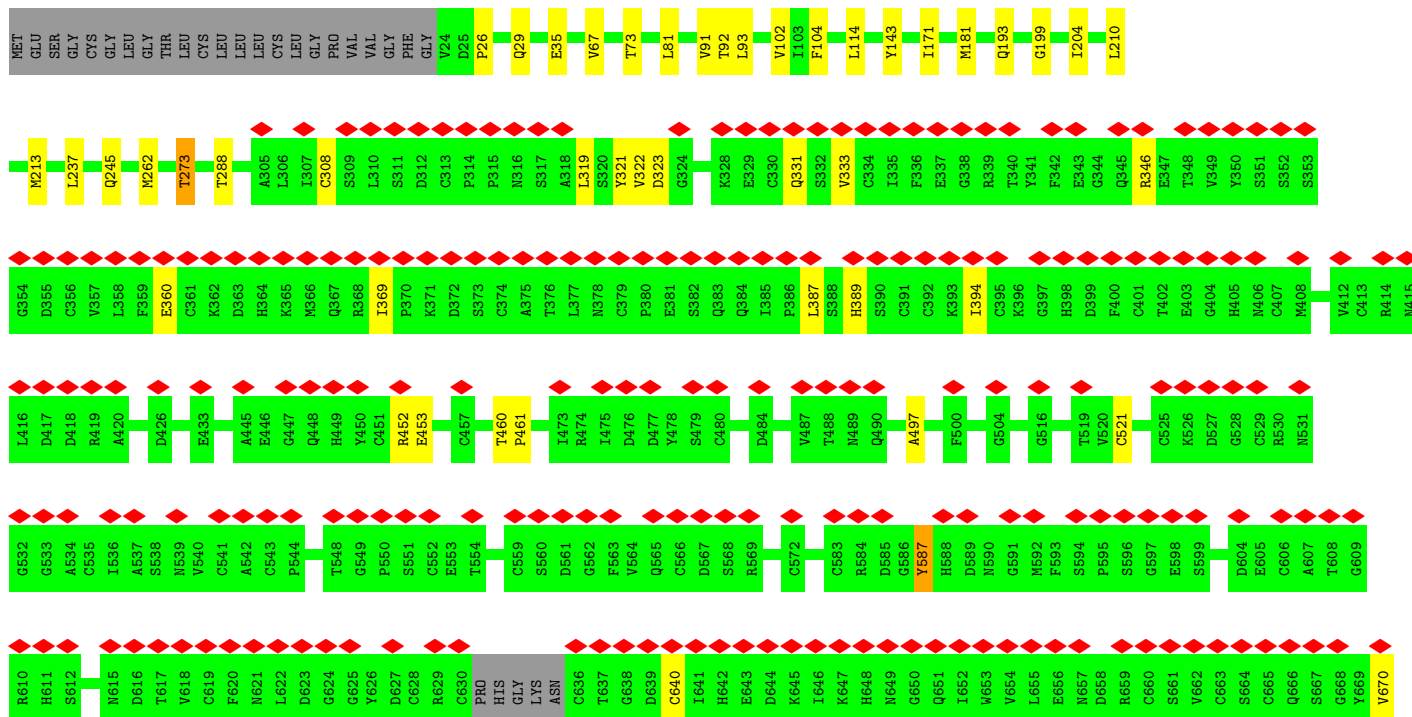
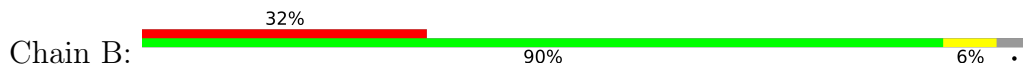
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	

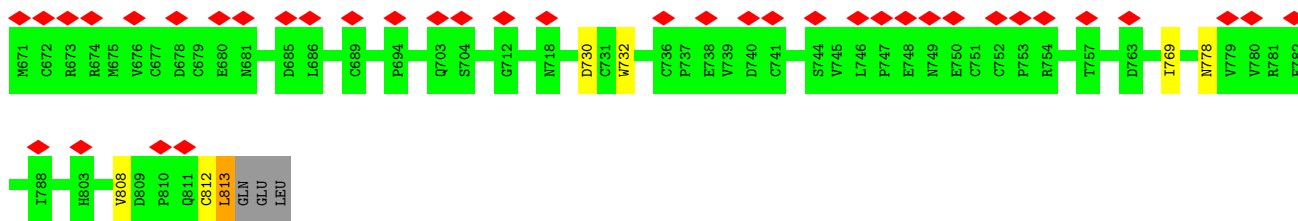
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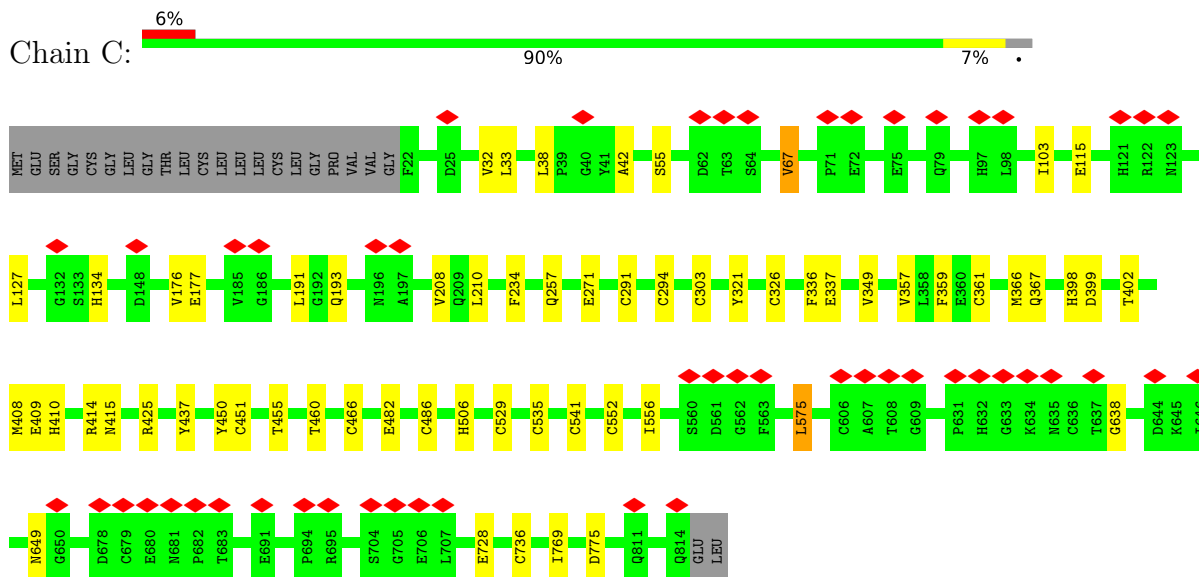
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 2: Protein NEL

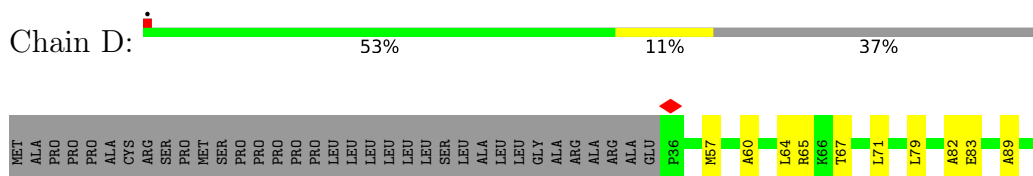




- Molecule 2: Protein NEL



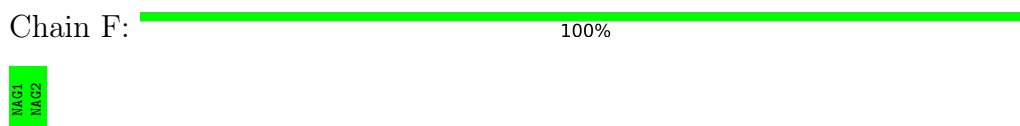
- Molecule 3: NELL2-interacting cell ontogeny regulator 1



- 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

Chain H:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	561.68, 561.68, 561.68	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4042, 1.4042, 1.4042	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/13293	0.41	0/18127
2	B	0.13	0/6209	0.36	0/8399
2	C	0.13	0/6275	0.38	0/8489
3	D	0.18	0/466	0.44	0/629
All	All	0.15	0/26243	0.39	0/35644

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	575	LEU	Peptide

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	12940	12543	12536	140	0
2	B	6083	5615	5612	30	0
2	C	6145	5670	5667	32	0
3	D	457	446	445	9	0
4	E	28	27	25	0	0
4	F	28	27	25	0	0
4	H	28	27	25	0	0
5	G	39	37	34	0	0
6	A	294	294	273	10	0
6	B	28	28	26	1	0
6	C	70	70	65	0	0
All	All	26140	24784	24733	203	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 4.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HB3	1:A:686:LEU:HD11	1.67	0.76
1:A:376:GLY:HA2	6:A:2412:NAG:H81	1.71	0.72
1:A:627:SER:OG	6:A:2406:NAG:H82	1.95	0.67
1:A:1432:ALA:HB3	1:A:1436:LEU:HD11	1.76	0.67
2:B:288:THR:HG23	6:B:2001:NAG:H81	1.76	0.66
1:A:1254:TRP:CE3	6:A:2416:NAG:H82	2.32	0.64
1:A:793:LEU:HB2	1:A:802:LEU:HD11	1.82	0.61
1:A:813:ALA:HB2	1:A:820:TYR:HA	1.84	0.60
1:A:899:ILE:HG23	1:A:904:PHE:O	2.03	0.59
1:A:794:ALA:O	1:A:802:LEU:HD12	2.04	0.58
1:A:487:VAL:HG13	1:A:497:HIS:C	2.30	0.57
1:A:1418:LEU:C	1:A:1418:LEU:HD12	2.30	0.56
1:A:476:LEU:HD12	1:A:477:ILE:H	1.70	0.55
1:A:1242:ILE:HG21	1:A:1489:ILE:HG21	1.88	0.55
2:B:331:GLN:O	2:B:333:VAL:HG13	2.06	0.55
1:A:222:VAL:HG23	1:A:224:TRP:HZ3	1.72	0.54
1:A:1166:THR:HG1	1:A:1173:PHE:HD1	1.53	0.54
1:A:1254:TRP:CD2	6:A:2416:NAG:H82	2.42	0.54
1:A:705:ARG:O	1:A:707:ILE:HG23	2.08	0.54
2:C:294:CYS:HA	2:C:303:CYS:HA	1.89	0.53
2:B:204:ILE:HD12	2:B:204:ILE:N	2.24	0.53
1:A:1057:ILE:HD12	1:A:1152:GLN:HA	1.91	0.52
1:A:1093:TYR:CD2	1:A:1111:VAL:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:CYS:SG	1:A:1486:CYS:O	2.69	0.51
1:A:308:GLN:NE2	6:A:2403:NAG:H82	2.26	0.50
2:C:575:LEU:HD11	2:C:736:CYS:HA	1.93	0.50
1:A:711:ASP:O	1:A:717:LEU:HD12	2.11	0.50
1:A:468:MET:O	1:A:476:LEU:HD12	2.12	0.50
2:B:35:GLU:HG3	2:B:73:THR:HG23	1.94	0.50
1:A:1399:VAL:HG22	1:A:1400:ASP:O	2.11	0.50
1:A:611:ASP:CG	1:A:652:VAL:HG21	2.37	0.49
1:A:899:ILE:HG23	1:A:904:PHE:C	2.38	0.49
2:B:346:ARG:HB2	2:B:389:HIS:HA	1.95	0.49
2:B:387:LEU:HD21	2:B:394:ILE:HD13	1.95	0.49
1:A:345:VAL:HG12	1:A:358:GLY:HA2	1.94	0.49
2:C:103:ILE:O	2:C:191:LEU:HD12	2.13	0.49
2:B:67:VAL:HG12	2:B:67:VAL:O	2.13	0.49
2:B:81:LEU:HD11	2:B:210:LEU:HD22	1.95	0.48
1:A:1250:MET:O	1:A:1257:THR:HA	2.13	0.48
1:A:91:PHE:O	1:A:95:ARG:HG2	2.13	0.48
1:A:485:ALA:HA	1:A:503:VAL:HG23	1.94	0.48
2:C:67:VAL:HG12	2:C:193:GLN:OE1	2.13	0.48
2:C:176:VAL:HG22	2:C:177:GLU:N	2.29	0.48
1:A:1257:THR:HG21	1:A:1285:ILE:HD12	1.95	0.47
2:C:451:CYS:HB3	2:C:455:THR:HG21	1.96	0.47
2:C:42:ALA:HA	2:C:67:VAL:HA	1.96	0.47
1:A:1630:THR:HG22	1:A:1631:LEU:H	1.79	0.47
1:A:929:LEU:HD23	1:A:930:VAL:H	1.79	0.47
1:A:1336:CYS:HB3	1:A:1378:CYS:O	2.15	0.47
1:A:1166:THR:O	1:A:1172:LEU:HD12	2.14	0.47
2:C:359:PHE:HA	2:C:367:GLN:O	2.14	0.47
1:A:1114:VAL:HG22	1:A:1115:LYS:N	2.29	0.47
1:A:753:ALA:HB2	1:A:793:LEU:HD11	1.97	0.47
2:B:808:VAL:HG13	3:D:79:LEU:HD23	1.97	0.46
2:C:769:ILE:HG23	3:D:57:MET:HE2	1.96	0.46
1:A:514:GLU:HA	1:A:514:GLU:OE1	2.15	0.46
2:B:26:PRO:HA	2:B:29:GLN:HB3	1.97	0.46
1:A:116:ALA:HA	1:A:126:LEU:HD23	1.97	0.46
1:A:717:LEU:HD13	1:A:731:MET:SD	2.55	0.46
2:C:176:VAL:HG22	2:C:177:GLU:H	1.80	0.46
1:A:846:LEU:O	1:A:860:ARG:HA	2.15	0.46
1:A:164:VAL:HG12	1:A:165:LYS:N	2.31	0.46
1:A:1597:PRO:O	1:A:1598:ASN:HB2	2.15	0.46
1:A:392:PHE:CE2	1:A:409:ALA:HB3	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG12	2:B:92:THR:N	2.30	0.46
1:A:476:LEU:HD12	1:A:477:ILE:N	2.29	0.45
3:D:67:THR:O	3:D:71:LEU:HG	2.16	0.45
2:B:245:GLN:HG2	3:D:64:LEU:HD21	1.98	0.45
1:A:260:TYR:CG	1:A:261:SER:N	2.84	0.45
1:A:479:PHE:CD2	1:A:508:MET:HB3	2.51	0.45
2:B:360:GLU:HB3	2:B:369:ILE:HD12	1.99	0.45
1:A:1574:VAL:HG21	1:A:1661:SER:HB3	1.98	0.45
1:A:1256:GLU:HB2	1:A:1280:LYS:HG2	1.98	0.45
1:A:1485:LEU:O	1:A:1486:CYS:C	2.59	0.45
1:A:1544:VAL:HG12	1:A:1545:ALA:N	2.32	0.45
1:A:310:LEU:HD23	1:A:325:LEU:HD22	1.98	0.45
1:A:332:HIS:HA	6:A:2403:NAG:H81	1.98	0.45
2:B:273:THR:HG23	3:D:89:ALA:HB2	1.99	0.45
2:B:460:THR:O	2:B:461:PRO:C	2.59	0.45
2:C:115:GLU:O	2:C:127:LEU:HD12	2.16	0.45
1:A:793:LEU:HD12	1:A:794:ALA:N	2.32	0.45
1:A:450:ASP:C	1:A:451:THR:HG1	2.24	0.44
1:A:154:THR:O	1:A:155:GLU:HG3	2.17	0.44
1:A:957:PHE:HA	1:A:969:ILE:O	2.17	0.44
1:A:300:LYS:HG2	1:A:563:ALA:HA	2.00	0.44
1:A:773:LYS:HD2	1:A:780:MET:HB3	2.00	0.44
2:C:775:ASP:C	2:C:775:ASP:OD1	2.60	0.44
3:D:60:ALA:O	3:D:64:LEU:HG	2.17	0.44
1:A:392:PHE:C	1:A:392:PHE:CD1	2.94	0.44
1:A:716:THR:C	1:A:731:MET:HE2	2.42	0.44
1:A:1257:THR:HG21	1:A:1285:ILE:CG1	2.48	0.44
2:B:262:MET:HE3	3:D:82:ALA:HB2	2.00	0.44
2:C:337:GLU:O	2:C:337:GLU:CG	2.64	0.44
1:A:383:VAL:HG22	1:A:390:MET:HE2	1.99	0.44
1:A:605:TRP:CZ2	1:A:607:ASN:HB3	2.53	0.44
1:A:1356:ILE:HD12	1:A:1356:ILE:H	1.82	0.44
1:A:1242:ILE:HD11	1:A:1449:PRO:HD3	2.00	0.44
1:A:1397:LEU:HD12	1:A:1405:TYR:O	2.16	0.44
2:B:245:GLN:HG3	3:D:64:LEU:HD11	2.00	0.44
2:C:349:VAL:HB	2:C:357:VAL:HG13	1.99	0.43
1:A:968:ILE:C	1:A:969:ILE:HD13	2.43	0.43
1:A:1247:PHE:CD1	1:A:1297:LEU:HD22	2.53	0.43
1:A:1252:THR:O	6:A:2415:NAG:H82	2.18	0.43
2:B:452:ARG:O	2:B:453:GLU:C	2.60	0.43
1:A:646:GLU:HA	1:A:664:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TYR:CD1	2:B:171:ILE:HD13	2.53	0.43
2:C:408:MET:O	2:C:409:GLU:C	2.62	0.43
1:A:313:ARG:HH21	1:A:543:VAL:HG13	1.84	0.43
1:A:1253:SER:HB3	1:A:1256:GLU:HB3	2.00	0.43
1:A:364:ASP:CG	1:A:366:SER:HG	2.26	0.43
1:A:770:ILE:HG22	1:A:771:TYR:N	2.33	0.43
1:A:1093:TYR:O	1:A:1134:PHE:HA	2.18	0.43
1:A:1194:ASP:HB3	1:A:1237:ILE:HG22	2.00	0.43
1:A:1541:ALA:HB1	1:A:1561:GLU:CD	2.44	0.43
1:A:246:HIS:CG	1:A:247:GLU:N	2.87	0.43
1:A:1247:PHE:CD1	1:A:1261:PHE:HB3	2.53	0.43
1:A:720:SER:OG	1:A:752:LEU:HD11	2.19	0.43
1:A:1166:THR:HG22	1:A:1438:ILE:HG22	2.00	0.43
2:B:193:GLN:HA	2:B:199:GLY:O	2.18	0.43
2:C:32:VAL:HG11	2:C:191:LEU:HD13	1.99	0.43
1:A:1167:PHE:CZ	1:A:1437:LYS:HB2	2.54	0.43
1:A:1426:HIS:CG	1:A:1427:SER:N	2.87	0.43
2:C:361:CYS:HA	2:C:366:MET:HA	2.01	0.43
1:A:726:VAL:HB	1:A:743:VAL:HG11	2.01	0.42
1:A:1499:PHE:N	1:A:1499:PHE:CD1	2.87	0.42
1:A:141:GLN:HA	1:A:152:ARG:O	2.19	0.42
1:A:1073:VAL:HG12	1:A:1074:GLU:N	2.33	0.42
1:A:726:VAL:O	1:A:743:VAL:HG22	2.18	0.42
1:A:929:LEU:HD23	1:A:930:VAL:N	2.34	0.42
1:A:959:ILE:HG23	1:A:966:PHE:CD2	2.54	0.42
1:A:154:THR:O	1:A:155:GLU:CG	2.67	0.42
1:A:399:HIS:HB3	1:A:409:ALA:CB	2.49	0.42
1:A:1254:TRP:CZ2	6:A:2417:NAG:H5	2.54	0.42
1:A:1299:TRP:CE2	1:A:1310:PHE:HB2	2.53	0.42
2:C:67:VAL:HG13	2:C:191:LEU:O	2.19	0.42
2:C:450:TYR:C	2:C:466:CYS:SG	3.02	0.42
1:A:891:TYR:CG	1:A:892:TYR:N	2.87	0.42
1:A:802:LEU:HB2	1:A:815:LEU:HD23	2.02	0.42
1:A:812:SER:HB3	1:A:823:LEU:HD11	2.01	0.42
1:A:1451:LYS:HD3	1:A:1454:LEU:HD12	2.02	0.42
2:B:812:CYS:O	2:B:813:LEU:C	2.62	0.42
1:A:143:LYS:HD2	1:A:151:TRP:CD2	2.55	0.42
1:A:347:TYR:HA	1:A:356:VAL:HA	2.02	0.42
2:B:640:CYS:HB3	2:B:670:VAL:HG23	2.00	0.42
2:C:486:CYS:SG	2:C:506:HIS:HB2	2.59	0.42
2:C:33:LEU:HD13	2:C:38:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:VAL:CG2	1:A:390:MET:HE2	2.49	0.42
1:A:834:VAL:HA	1:A:850:VAL:HG22	2.01	0.42
1:A:1541:ALA:HB1	1:A:1561:GLU:HG2	2.02	0.42
2:C:336:PHE:CD2	2:C:366:MET:HE1	2.54	0.42
1:A:1002:HIS:N	1:A:1003:PRO:CD	2.82	0.42
1:A:1461:GLU:HB3	1:A:1560:ARG:H	1.85	0.42
1:A:1325:TYR:CG	1:A:1330:GLU:HA	2.54	0.41
1:A:1409:GLU:HA	1:A:1414:THR:HG22	2.03	0.41
2:B:93:LEU:HD23	2:B:93:LEU:H	1.84	0.41
1:A:341:VAL:HG21	1:A:564:ALA:HA	2.02	0.41
1:A:1114:VAL:HG22	1:A:1115:LYS:H	1.85	0.41
1:A:1256:GLU:HG2	1:A:1257:THR:N	2.36	0.41
1:A:1572:GLU:O	1:A:1573:GLY:C	2.62	0.41
1:A:450:ASP:O	1:A:451:THR:OG1	2.37	0.41
2:C:337:GLU:O	2:C:337:GLU:HG3	2.19	0.41
1:A:1133:ARG:HG2	1:A:1152:GLN:HB3	2.01	0.41
1:A:1195:ILE:HG12	1:A:1206:TYR:HB3	2.02	0.41
2:C:33:LEU:HD23	2:C:208:VAL:H	1.86	0.41
1:A:1168:SER:CB	1:A:1436:LEU:HD12	2.51	0.41
1:A:1247:PHE:CE1	1:A:1297:LEU:HD22	2.55	0.41
2:C:414:ARG:CZ	2:C:414:ARG:HA	2.50	0.41
1:A:337:ILE:CG2	1:A:338:SER:N	2.83	0.41
1:A:339:VAL:HG22	1:A:340:ASN:N	2.36	0.41
1:A:686:LEU:HD12	1:A:687:TRP:H	1.85	0.41
1:A:956:SER:HB3	6:A:2407:NAG:H82	2.02	0.41
2:C:638:GLY:HA3	2:C:649:ASN:HB2	2.03	0.41
1:A:681:VAL:HG22	1:A:686:LEU:HA	2.03	0.41
2:C:291:CYS:SG	2:C:437:TYR:CG	3.13	0.41
2:C:399:ASP:HB3	2:C:402:THR:HG23	2.03	0.41
1:A:95:ARG:HD2	1:A:95:ARG:N	2.36	0.41
1:A:98:ASP:O	1:A:102:VAL:HG23	2.20	0.41
1:A:1242:ILE:HB	1:A:1292:PRO:HB3	2.02	0.41
1:A:1394:ILE:HA	1:A:1407:THR:O	2.21	0.41
2:B:104:PHE:CE2	2:B:210:LEU:HD21	2.55	0.41
2:B:322:VAL:HG12	2:B:323:ASP:N	2.35	0.41
1:A:173:TYR:O	1:A:194:SER:HA	2.21	0.41
1:A:688:LYS:HB2	1:A:700:LEU:HD11	2.03	0.41
1:A:1457:LEU:HB3	1:A:1481:THR:O	2.21	0.41
2:B:273:THR:CG2	3:D:89:ALA:HB2	2.51	0.41
1:A:469:ILE:HG12	1:A:476:LEU:HD13	2.02	0.40
1:A:1097:LEU:HD23	6:A:2414:NAG:H62	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:LEU:HD21	2:C:234:PHE:CD1	2.55	0.40
1:A:1242:ILE:HD12	1:A:1292:PRO:HB2	2.03	0.40
1:A:1298:TYR:HA	1:A:1311:TYR:HA	2.03	0.40
1:A:538:SER:C	1:A:539:PHE:CD1	2.99	0.40
1:A:1095:GLN:O	1:A:1132:VAL:HA	2.22	0.40
2:B:587:TYR:CD1	2:B:587:TYR:N	2.89	0.40
2:C:398:HIS:CG	2:C:399:ASP:N	2.89	0.40
1:A:762:TYR:CE2	1:A:815:LEU:HD22	2.57	0.40
1:A:1011:TYR:CG	1:A:1012:LYS:N	2.90	0.40
1:A:295:VAL:HG22	1:A:296:LYS:N	2.37	0.40
1:A:498:THR:HG21	1:A:501:ALA:HA	2.02	0.40
1:A:1413:TYR:HB2	1:A:1432:ALA:O	2.21	0.40
2:B:114:LEU:HB2	2:B:181:MET:SD	2.61	0.40
2:B:497:ALA:HB2	2:B:521:CYS:SG	2.61	0.40
2:C:399:ASP:OD1	2:C:415:ASN:HA	2.21	0.40
2:C:410:HIS:H	2:C:425:ARG:NH2	2.19	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	1600/2311 (69%)	1494 (93%)	106 (7%)	0	100	100
2	B	781/816 (96%)	738 (94%)	43 (6%)	0	100	100
2	C	791/816 (97%)	744 (94%)	47 (6%)	0	100	100
3	D	58/95 (61%)	55 (95%)	3 (5%)	0	100	100
All	All	3230/4038 (80%)	3031 (94%)	199 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1456/2058 (71%)	1419 (98%)	37 (2%)	42	62
2	B	702/726 (97%)	690 (98%)	12 (2%)	53	68
2	C	708/726 (98%)	692 (98%)	16 (2%)	44	64
3	D	47/75 (63%)	45 (96%)	2 (4%)	26	48
All	All	2913/3585 (81%)	2846 (98%)	67 (2%)	44	64

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	93	CYS
1	A	124	ILE
1	A	158	SER
1	A	178	VAL
1	A	205	THR
1	A	253	ARG
1	A	314	TYR
1	A	337	ILE
1	A	371	PHE
1	A	384	ASP
1	A	486	PHE
1	A	508	MET
1	A	601	SER
1	A	657	GLU
1	A	742	TYR
1	A	751	MET
1	A	752	LEU
1	A	771	TYR
1	A	799	ASN
1	A	866	GLU
1	A	875	GLU
1	A	919	SER
1	A	929	LEU

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Mol	Chain	Res	Type
1	A	969	ILE
1	A	1014	ASP
1	A	1022	PHE
1	A	1050	SER
1	A	1134	PHE
1	A	1149	ASP
1	A	1173	PHE
1	A	1282	ASN
1	A	1418	LEU
1	A	1434	HIS
1	A	1499	PHE
1	A	1546	VAL
1	A	1630	THR
2	B	102	VAL
2	B	213	MET
2	B	273	THR
2	B	308	CYS
2	B	319	LEU
2	B	321	TYR
2	B	587	TYR
2	B	730	ASP
2	B	732	TRP
2	B	769	ILE
2	B	778	ASN
2	B	813	LEU
2	C	55	SER
2	C	67	VAL
2	C	134	HIS
2	C	210	LEU
2	C	257	GLN
2	C	271	GLU
2	C	321	TYR
2	C	326	CYS
2	C	460	THR
2	C	482	GLU
2	C	529	CYS
2	C	535	CYS
2	C	541	CYS
2	C	552	CYS
2	C	556	ILE
2	C	728	GLU
3	D	65	ARG

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Mol	Chain	Res	Type
3	D	83	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	245	ASN
1	A	307	ASN
1	A	332	HIS
1	A	497	HIS
1	A	703	HIS
1	A	1061	HIS
2	B	580	HIS
2	B	767	ASN
2	C	52	HIS
2	C	364	HIS
2	C	703	GLN
2	C	721	GLN
3	D	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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
4	NAG	E	1	1,4	14,14,15	0.75	0	17,19,21	0.94	2 (11%)
4	NAG	E	2	4	14,14,15	0.69	0	17,19,21	0.77	0
4	NAG	F	1	1,4	14,14,15	0.83	0	17,19,21	0.89	0
4	NAG	F	2	4	14,14,15	0.73	0	17,19,21	0.81	0
5	NAG	G	1	1,5	14,14,15	0.72	0	17,19,21	1.19	2 (11%)
5	NAG	G	2	5	14,14,15	0.69	0	17,19,21	1.12	2 (11%)
5	BMA	G	3	5	11,11,12	0.84	0	15,15,17	2.71	7 (46%)
4	NAG	H	1	4,2	14,14,15	0.70	0	17,19,21	1.53	2 (11%)
4	NAG	H	2	4	14,14,15	0.69	0	17,19,21	1.06	1 (5%)

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

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C1-O5-C5	7.61	122.39	112.19
4	H	1	NAG	C1-O5-C5	5.01	118.90	112.19
5	G	3	BMA	C3-C4-C5	3.60	116.75	110.23
5	G	3	BMA	C2-C3-C4	3.36	116.77	110.86
4	H	2	NAG	C1-O5-C5	2.98	116.18	112.19
5	G	2	NAG	O5-C1-C2	-2.90	106.80	111.29
5	G	3	BMA	C1-C2-C3	2.63	113.48	109.64
5	G	1	NAG	C3-C4-C5	-2.59	105.53	110.23
5	G	3	BMA	O4-C4-C3	-2.52	104.44	110.38
5	G	3	BMA	O3-C3-C2	-2.44	105.07	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O4-C4-C5	2.34	115.09	109.32
5	G	2	NAG	O4-C4-C3	-2.23	105.11	110.38
5	G	3	BMA	O5-C5-C4	2.23	116.25	110.83
5	G	1	NAG	C1-O5-C5	2.18	115.10	112.19
4	E	1	NAG	C4-C3-C2	-2.14	107.88	111.02
4	E	1	NAG	O5-C1-C2	-2.09	108.06	111.29

There are no chirality outliers.

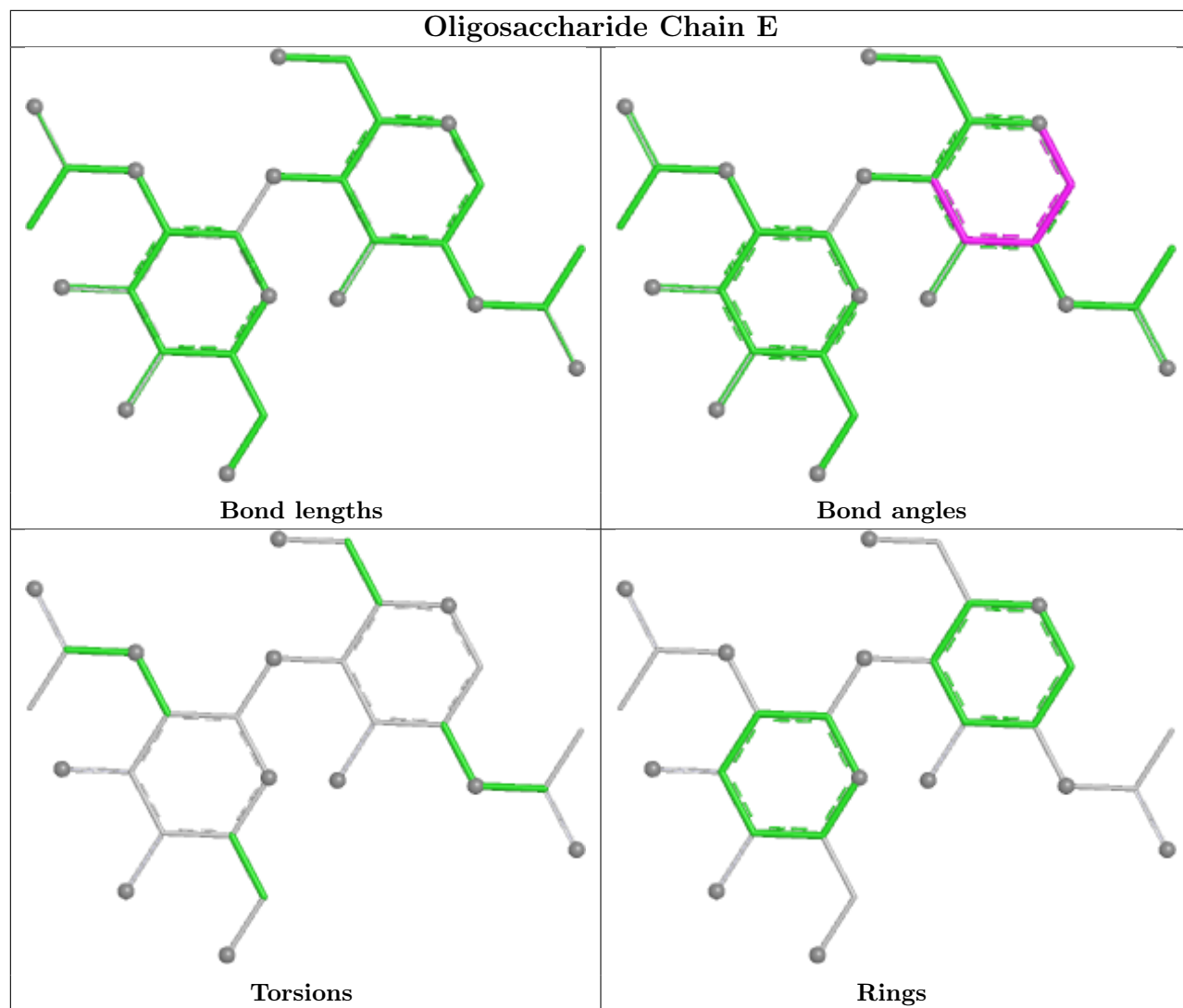
All (2) torsion outliers are listed below:

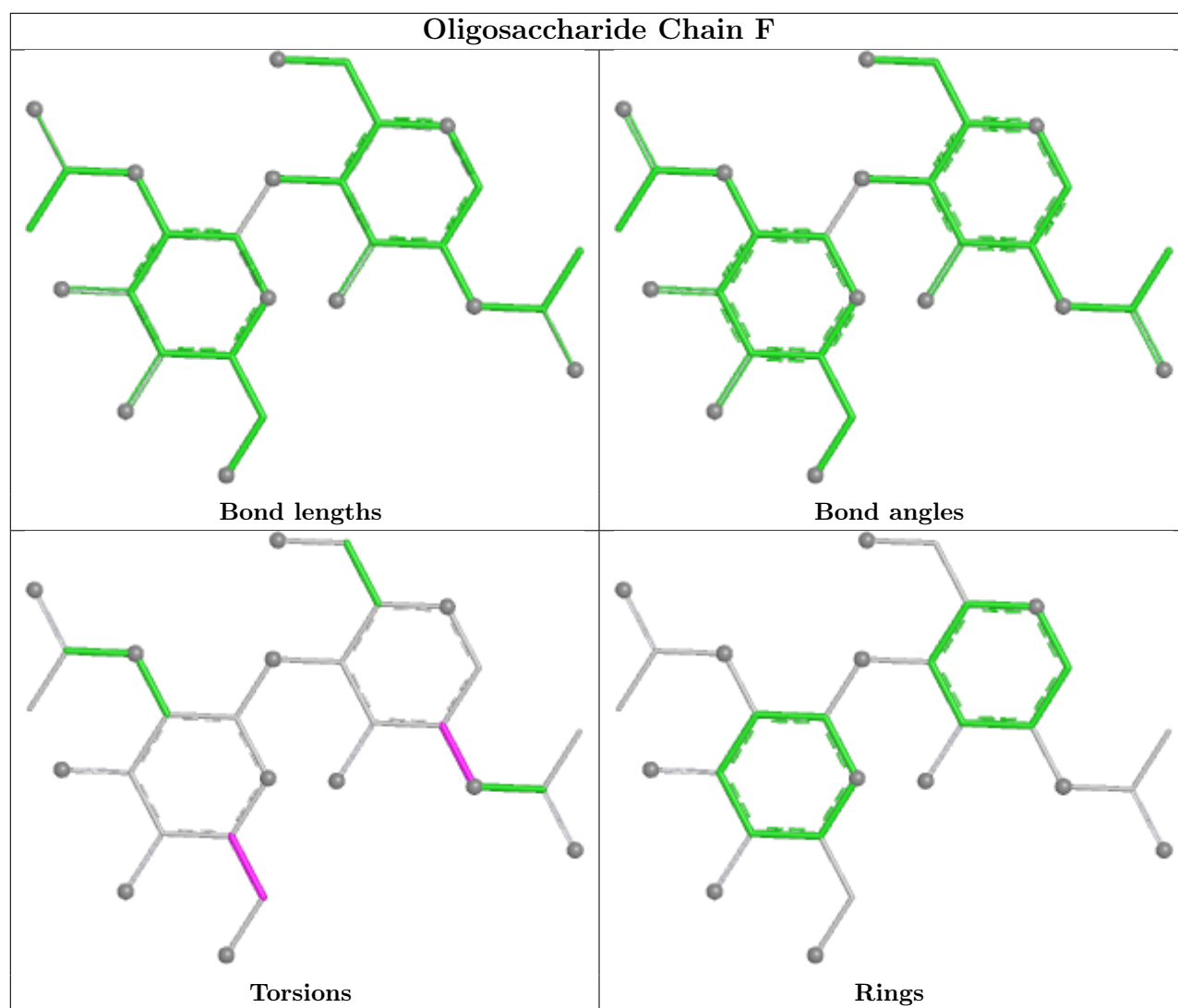
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7

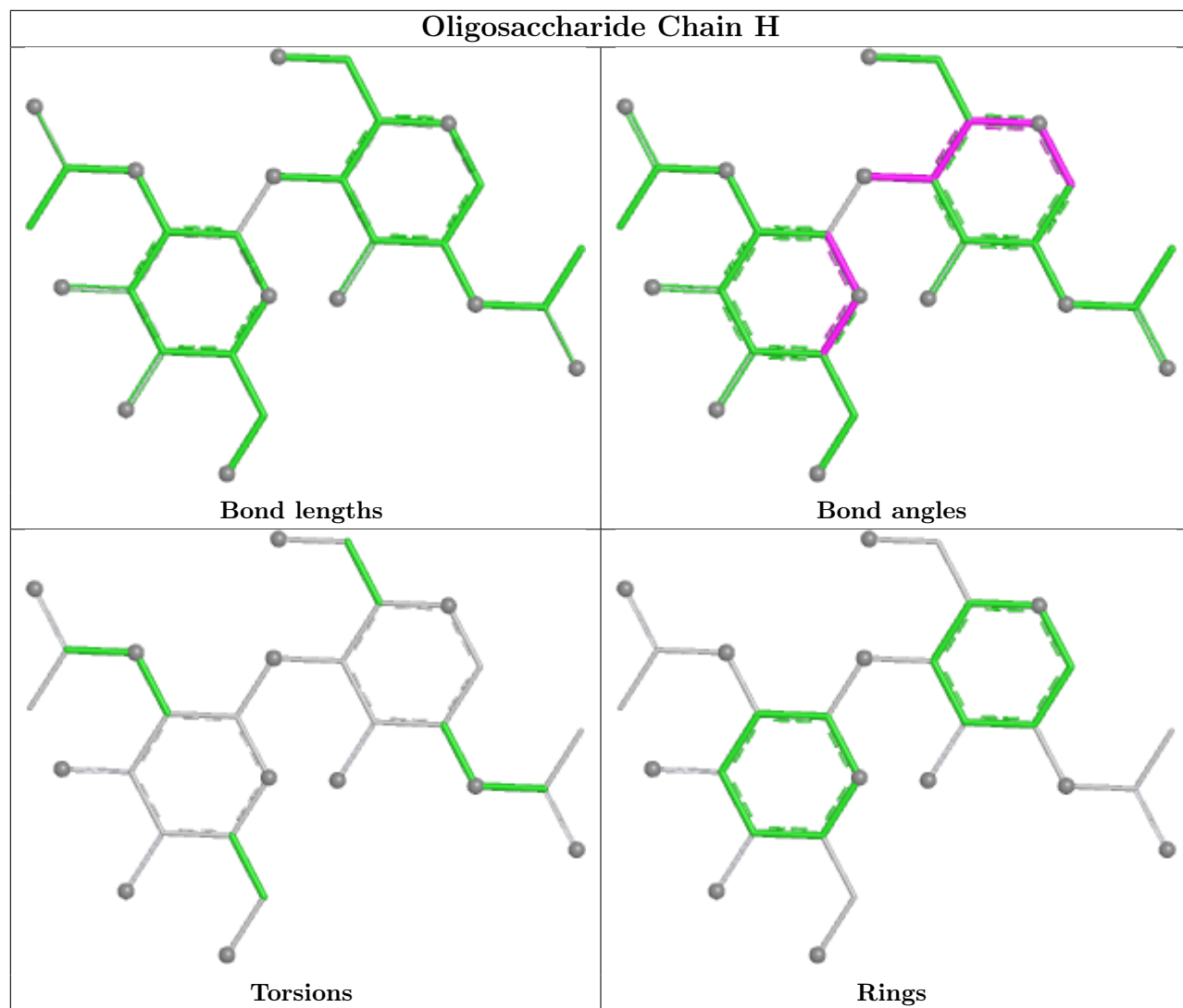
There are no ring outliers.

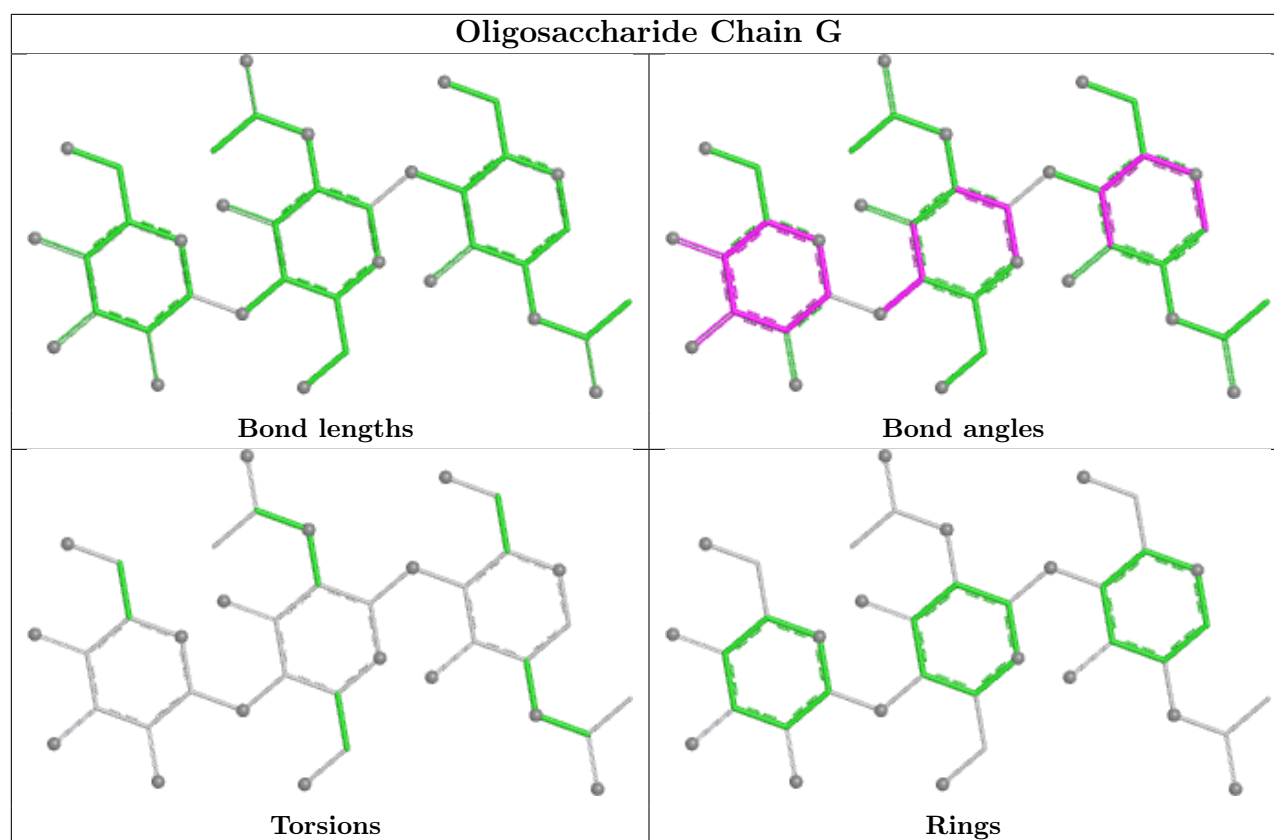
No monomer is involved in short contacts.

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](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	2410	1	14,14,15	0.77	0	17,19,21	0.73	0
6	NAG	A	2405	1	14,14,15	0.77	0	17,19,21	0.81	0
6	NAG	A	2412	1	14,14,15	0.83	0	17,19,21	0.78	0
6	NAG	A	2421	1	14,14,15	0.76	0	17,19,21	1.28	1 (5%)
6	NAG	A	2415	1	14,14,15	0.71	0	17,19,21	2.36	4 (23%)
6	NAG	A	2403	1	14,14,15	0.76	0	17,19,21	0.93	1 (5%)
6	NAG	B	2001	2	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
6	NAG	A	2404	1	14,14,15	0.82	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	2411	1	14,14,15	0.74	0	17,19,21	0.81	0
6	NAG	C	902	2	14,14,15	0.74	0	17,19,21	0.87	0
6	NAG	A	2409	1	14,14,15	0.76	0	17,19,21	1.34	1 (5%)
6	NAG	A	2419	1	14,14,15	0.78	0	17,19,21	0.97	0
6	NAG	A	2413	1	14,14,15	0.76	0	17,19,21	0.77	0
6	NAG	C	901	2	14,14,15	0.74	0	17,19,21	1.25	1 (5%)
6	NAG	A	2418	1	14,14,15	0.71	0	17,19,21	0.76	0
6	NAG	A	2407	1	14,14,15	0.73	0	17,19,21	0.86	0
6	NAG	A	2414	1	14,14,15	0.78	0	17,19,21	0.82	0
6	NAG	A	2402	1	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
6	NAG	A	2416	1	14,14,15	0.91	1 (7%)	17,19,21	1.46	2 (11%)
6	NAG	A	2420	1	14,14,15	0.76	0	17,19,21	0.69	0
6	NAG	A	2406	1	14,14,15	0.80	0	17,19,21	0.81	1 (5%)
6	NAG	C	904	2	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
6	NAG	A	2417	1	14,14,15	0.73	0	17,19,21	1.20	2 (11%)
6	NAG	C	905	2	14,14,15	0.72	0	17,19,21	0.82	1 (5%)
6	NAG	A	2408	1	14,14,15	0.74	0	17,19,21	0.81	0
6	NAG	A	2401	1	14,14,15	0.68	0	17,19,21	0.96	2 (11%)
6	NAG	B	2000	2	14,14,15	0.71	0	17,19,21	0.93	0
6	NAG	C	903	2	14,14,15	0.76	0	17,19,21	1.24	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	2410	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2412	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2421	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2415	1	-	2/6/23/26	0/1/1/1
6	NAG	A	2403	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2001	2	-	1/6/23/26	0/1/1/1
6	NAG	A	2404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2411	1	-	0/6/23/26	0/1/1/1
6	NAG	C	902	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2409	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2419	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2413	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	901	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2418	1	-	1/6/23/26	0/1/1/1
6	NAG	A	2407	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2414	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2402	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2416	1	-	1/6/23/26	0/1/1/1
6	NAG	A	2420	1	-	1/6/23/26	0/1/1/1
6	NAG	A	2406	1	-	0/6/23/26	0/1/1/1
6	NAG	C	904	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2417	1	-	2/6/23/26	0/1/1/1
6	NAG	C	905	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2408	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2401	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2000	2	-	0/6/23/26	0/1/1/1
6	NAG	C	903	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2416	NAG	C1-C2	2.13	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2415	NAG	C1-O5-C5	8.31	123.32	112.19
6	A	2421	NAG	C1-O5-C5	4.48	118.19	112.19
6	A	2409	NAG	C1-O5-C5	4.33	117.99	112.19
6	C	901	NAG	C1-O5-C5	4.27	117.91	112.19
6	C	903	NAG	C1-O5-C5	3.82	117.31	112.19
6	A	2415	NAG	O5-C1-C2	3.53	116.75	111.29
6	A	2416	NAG	C1-O5-C5	3.47	116.83	112.19
6	B	2001	NAG	C1-O5-C5	3.33	116.65	112.19
6	A	2402	NAG	C1-O5-C5	2.83	115.98	112.19
6	A	2417	NAG	C1-O5-C5	2.79	115.93	112.19
6	A	2416	NAG	C4-C3-C2	2.59	114.82	111.02
6	A	2401	NAG	C4-C3-C2	-2.33	107.60	111.02
6	A	2417	NAG	C1-C2-N2	2.29	114.04	110.43
6	A	2401	NAG	O5-C1-C2	-2.25	107.82	111.29
6	C	904	NAG	C4-C3-C2	-2.17	107.83	111.02
6	A	2403	NAG	C1-O5-C5	2.13	115.03	112.19
6	C	905	NAG	O5-C1-C2	-2.10	108.04	111.29
6	A	2415	NAG	C2-N2-C7	2.07	125.67	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2415	NAG	C3-C4-C5	-2.04	106.54	110.23
6	A	2404	NAG	C2-N2-C7	2.04	125.63	122.90
6	A	2406	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2417	NAG	C4-C5-C6-O6
6	A	2417	NAG	O5-C5-C6-O6
6	C	903	NAG	O5-C5-C6-O6
6	B	2001	NAG	O5-C5-C6-O6
6	A	2418	NAG	O5-C5-C6-O6
6	A	2420	NAG	C1-C2-N2-C7
6	A	2415	NAG	C3-C2-N2-C7
6	A	2416	NAG	C3-C2-N2-C7
6	A	2415	NAG	O5-C5-C6-O6

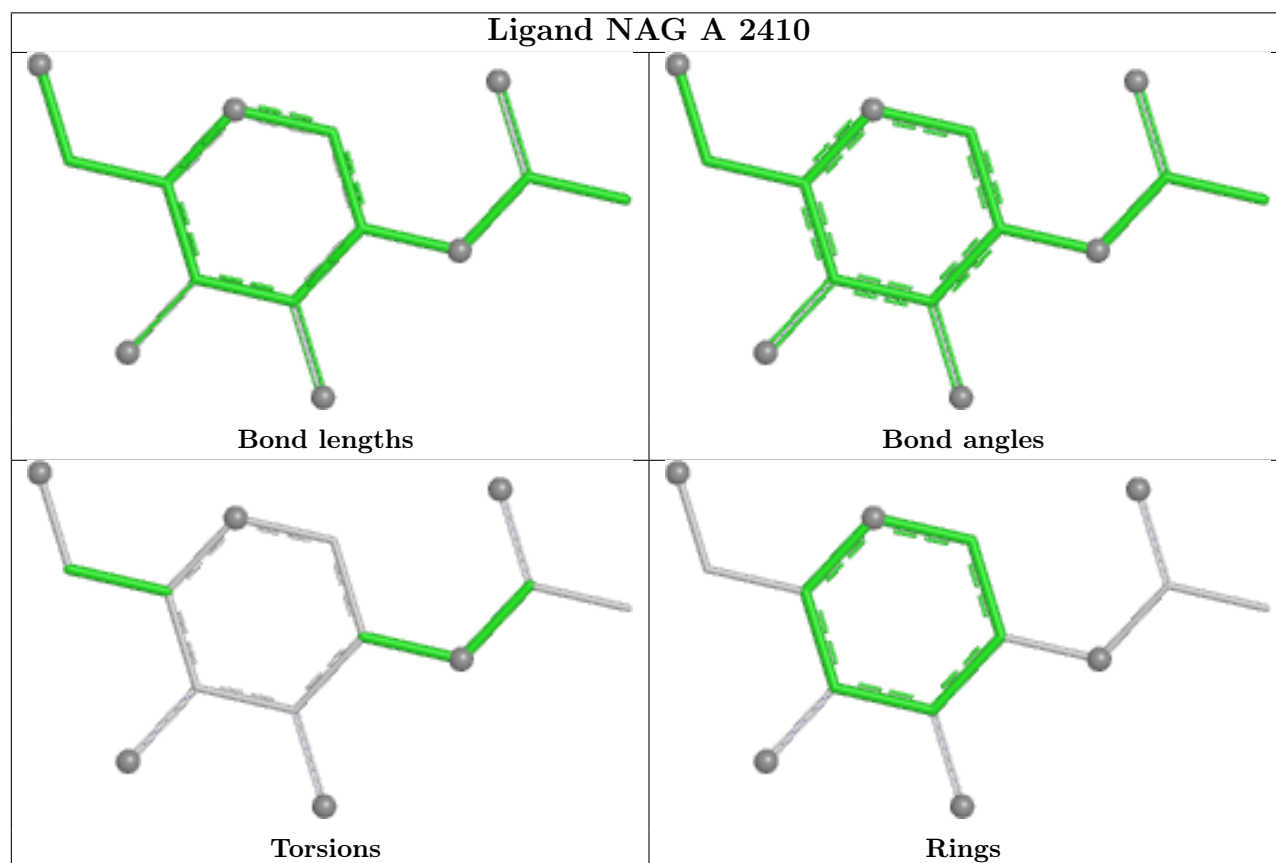
There are no ring outliers.

9 monomers are involved in 11 short contacts:

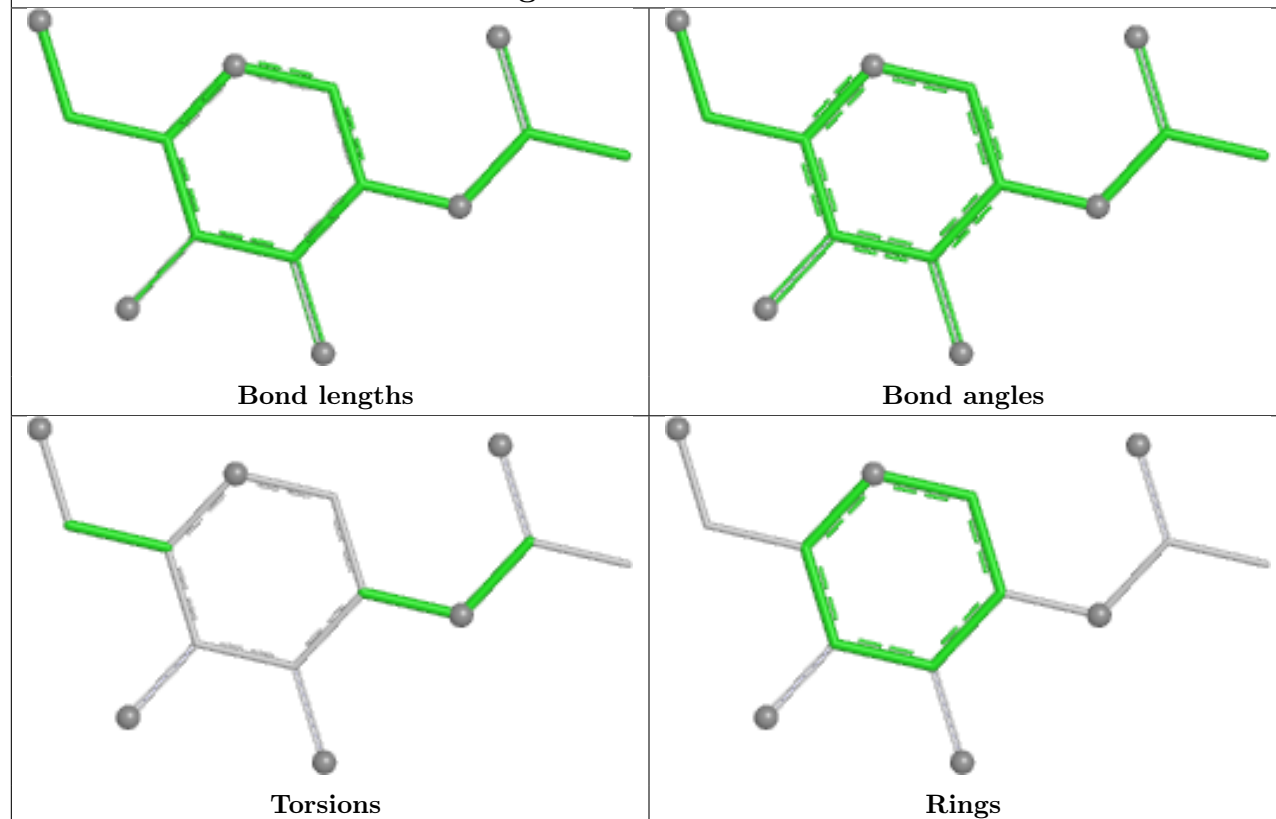
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2412	NAG	1	0
6	A	2415	NAG	1	0
6	A	2403	NAG	2	0
6	B	2001	NAG	1	0
6	A	2407	NAG	1	0
6	A	2414	NAG	1	0
6	A	2416	NAG	2	0
6	A	2406	NAG	1	0
6	A	2417	NAG	1	0

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.

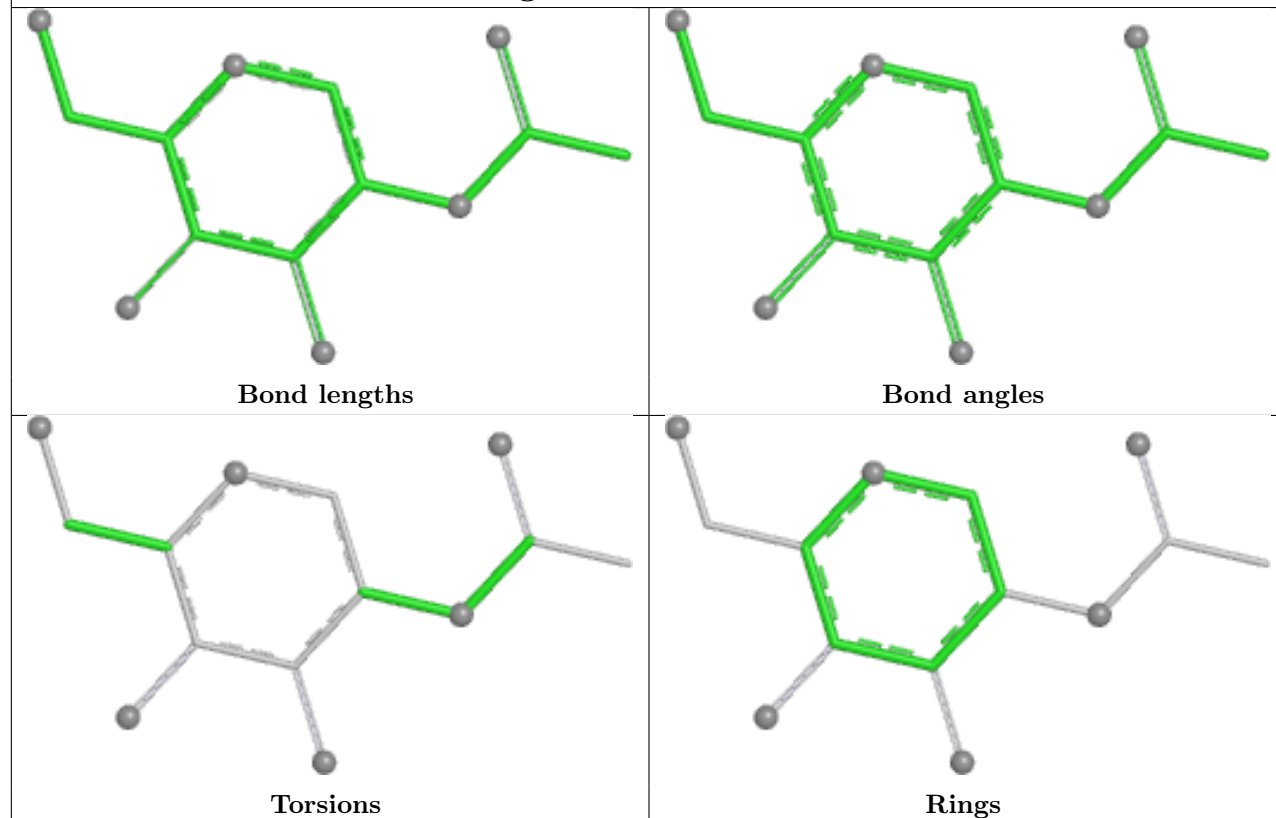
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

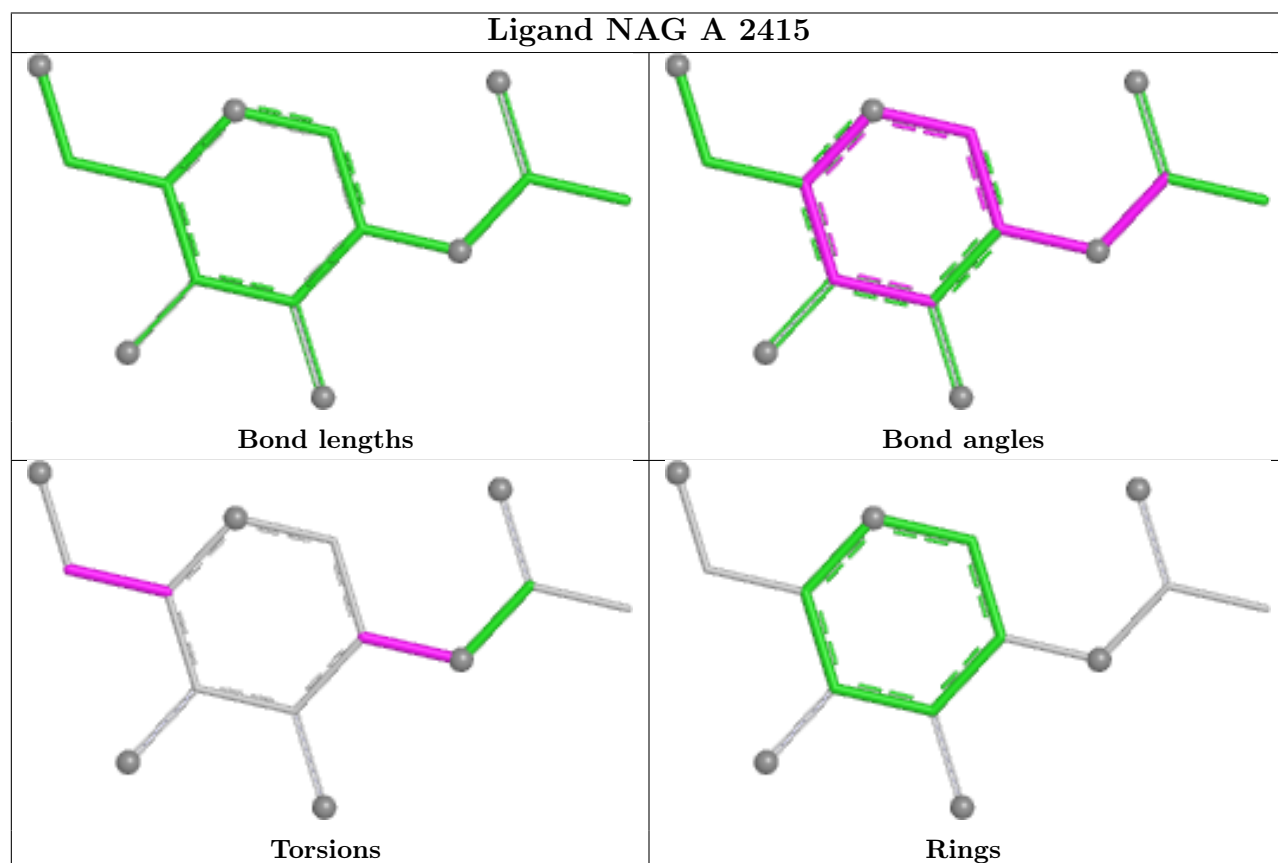
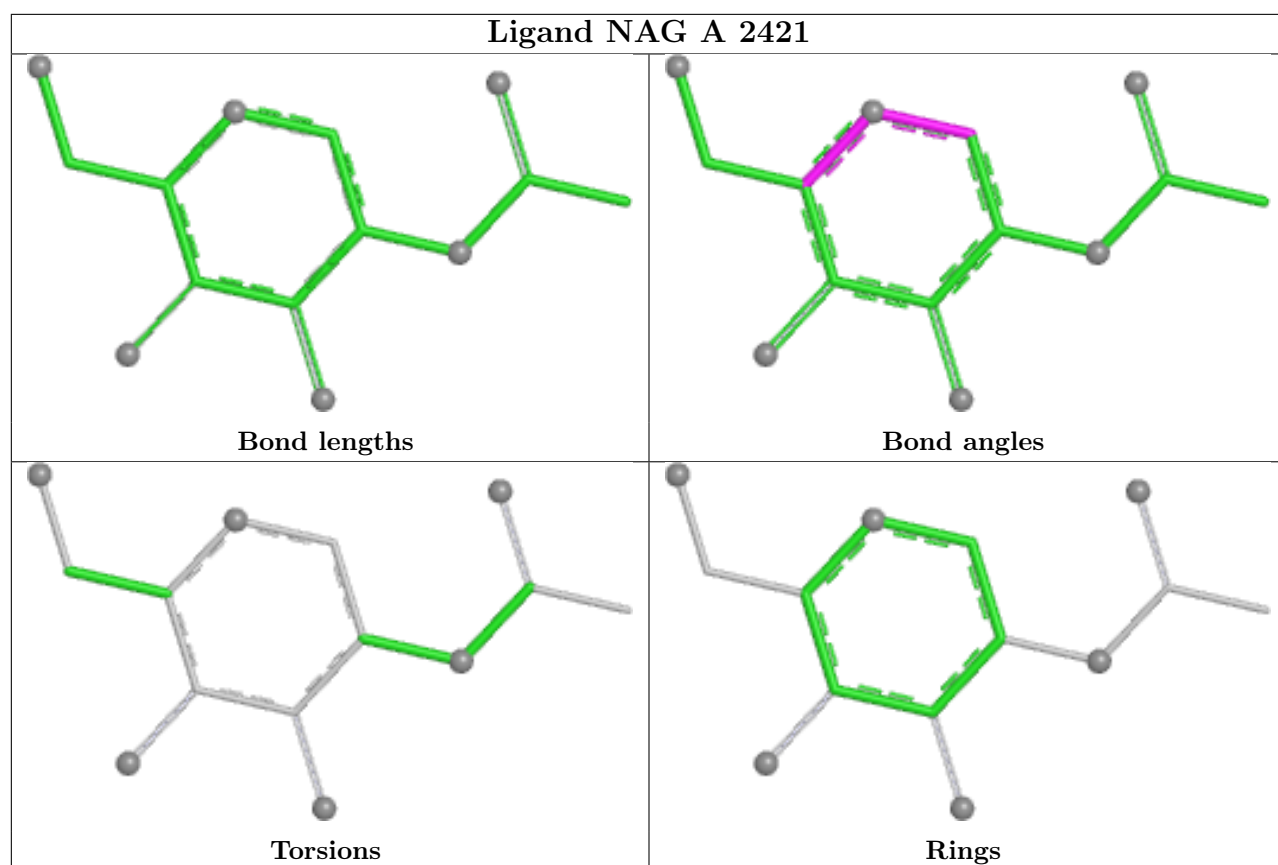


Ligand NAG A 2405

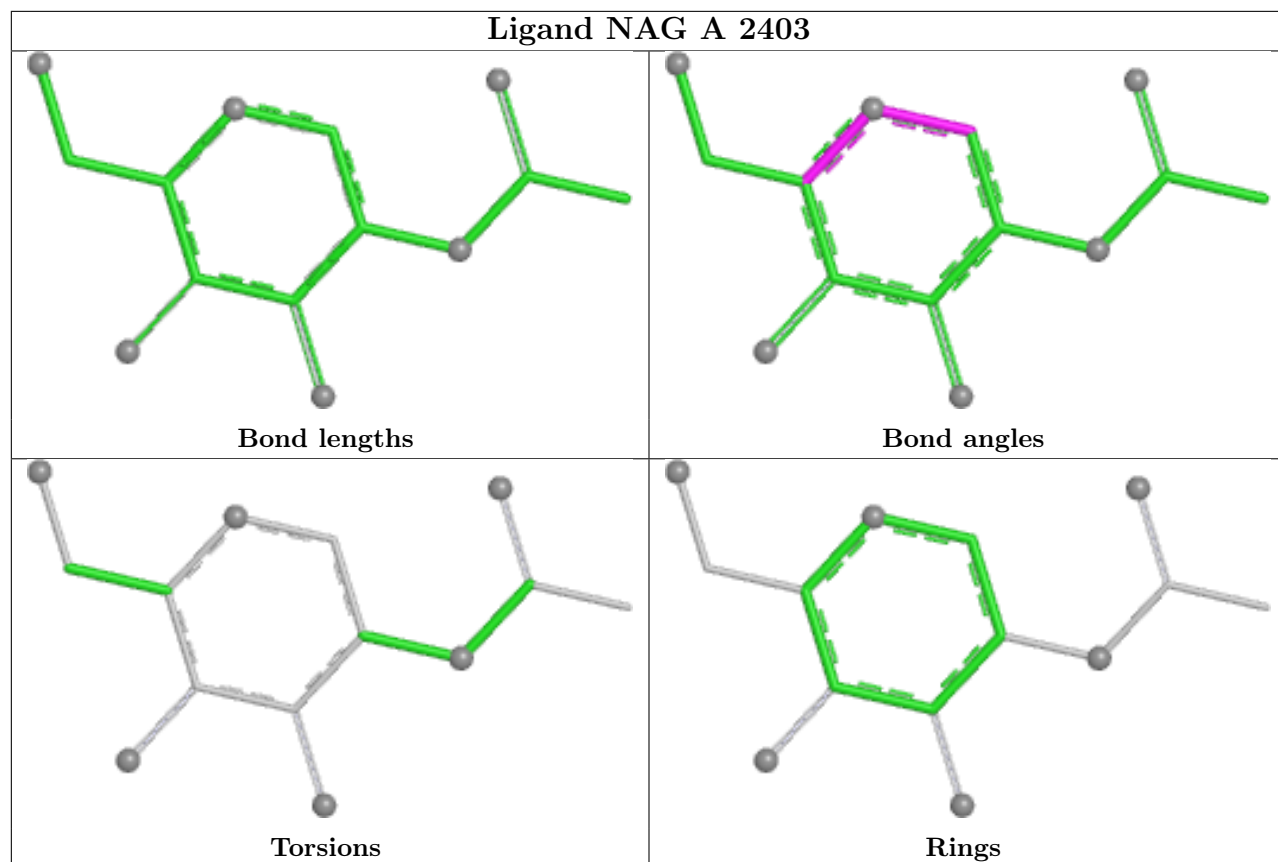


Ligand NAG A 2412

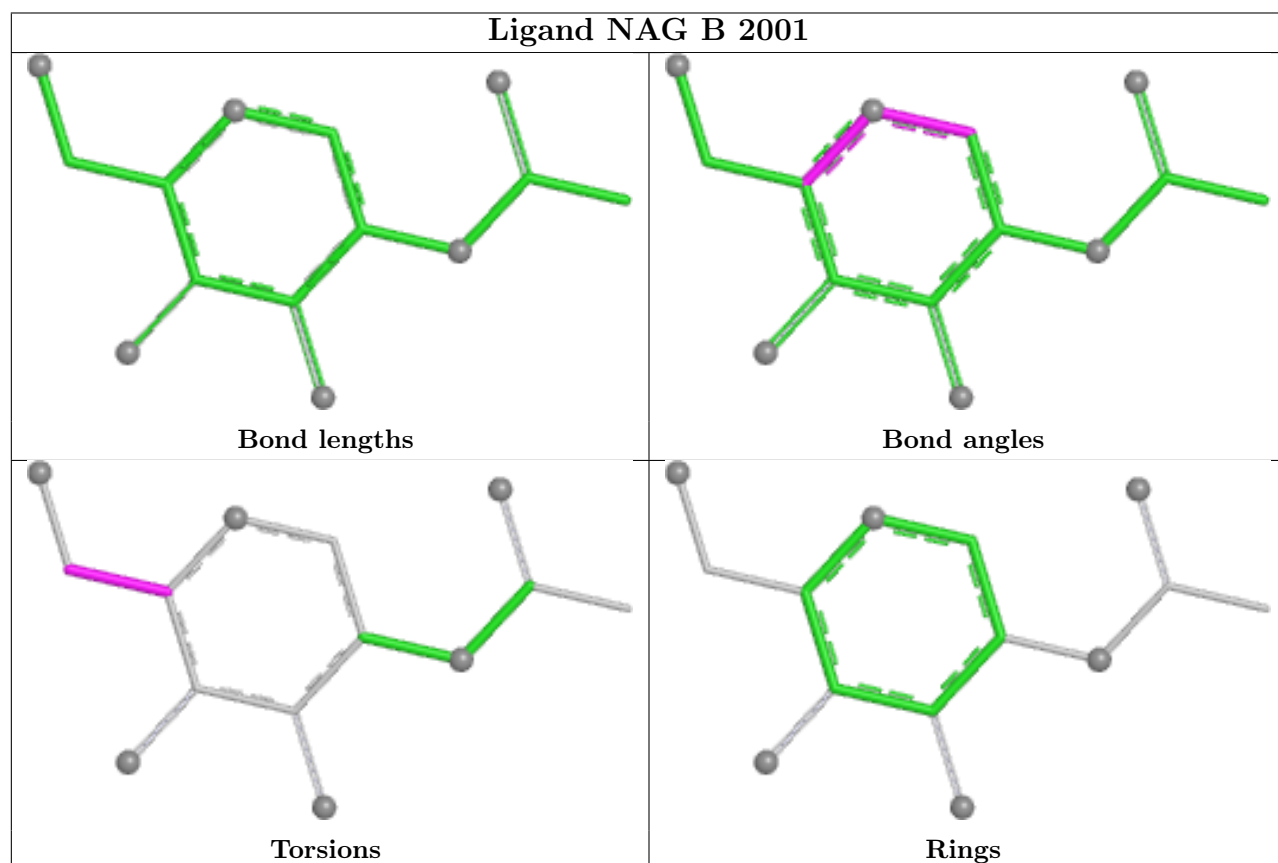




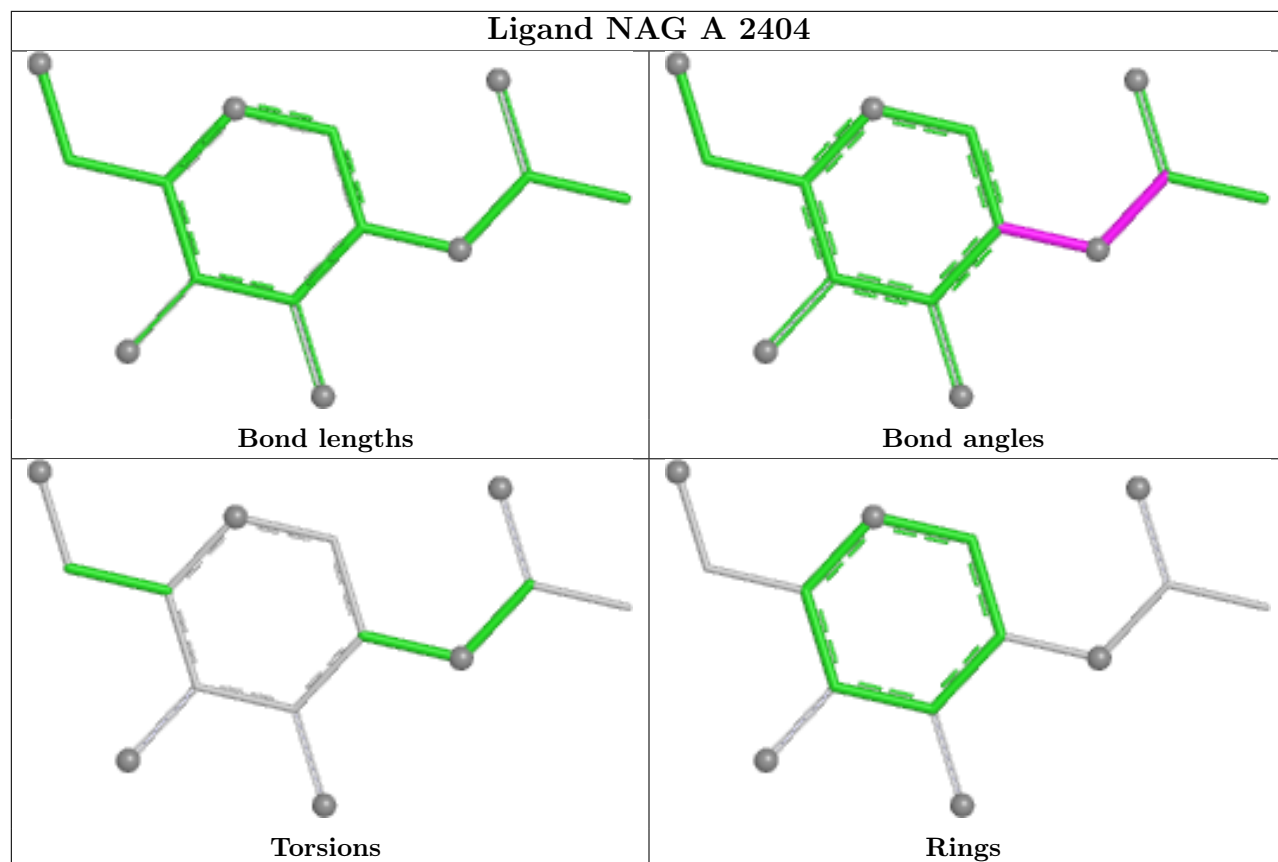
Ligand NAG A 2403



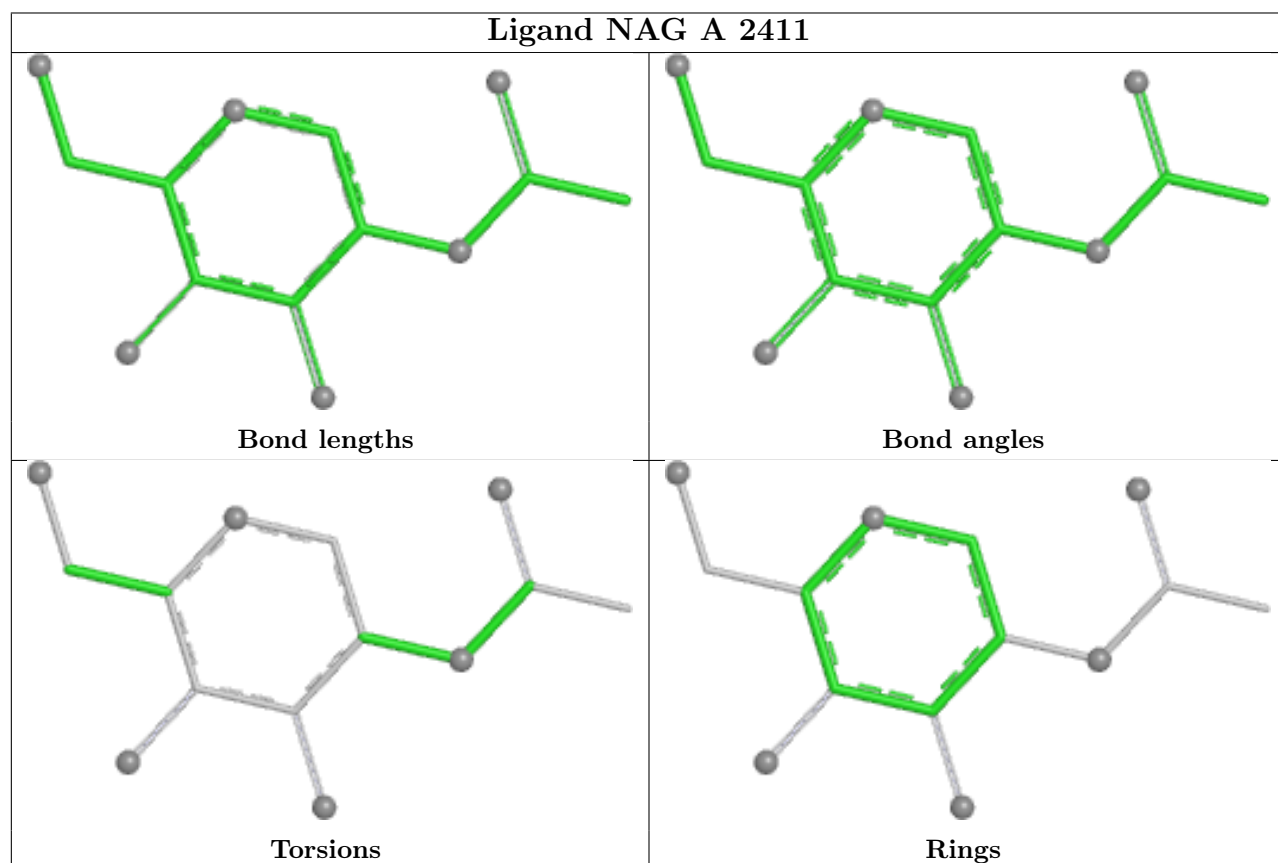
Ligand NAG B 2001

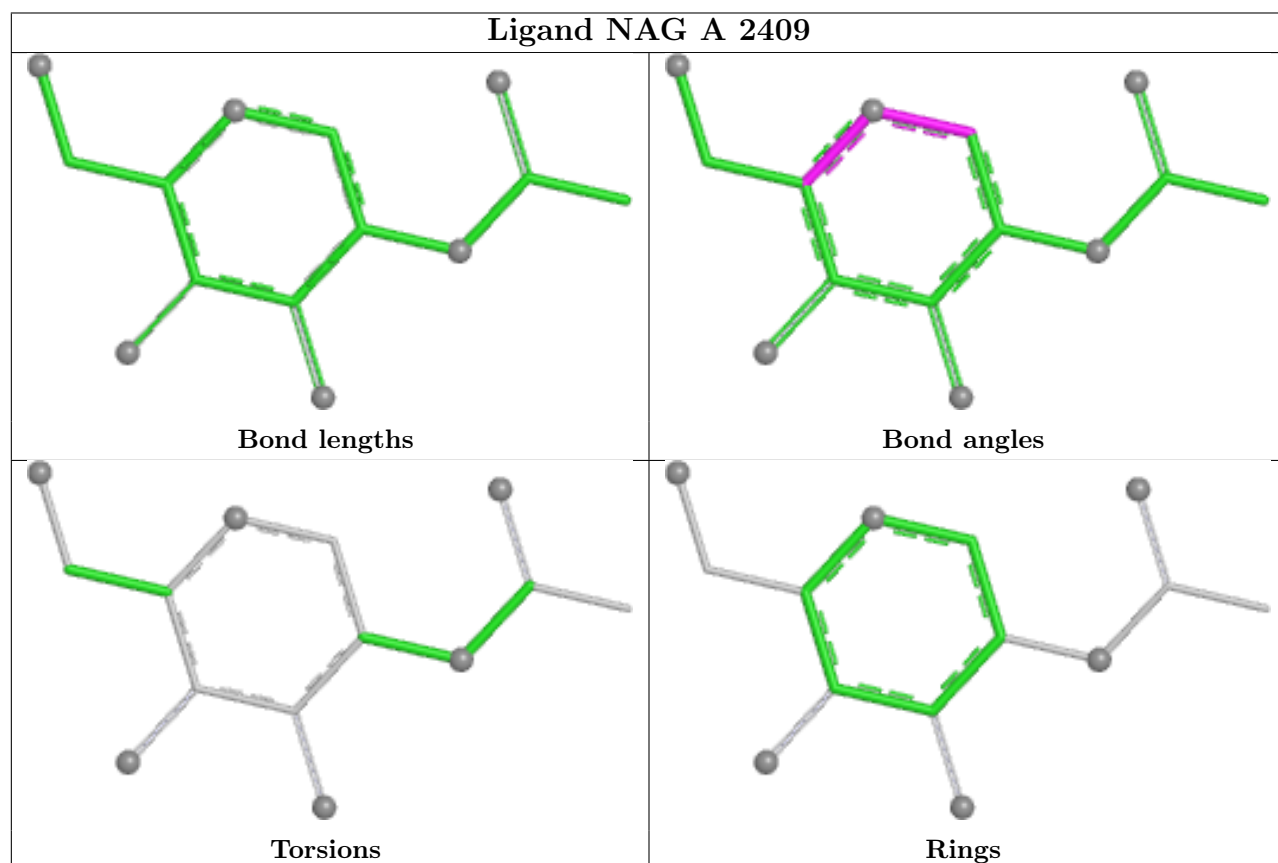
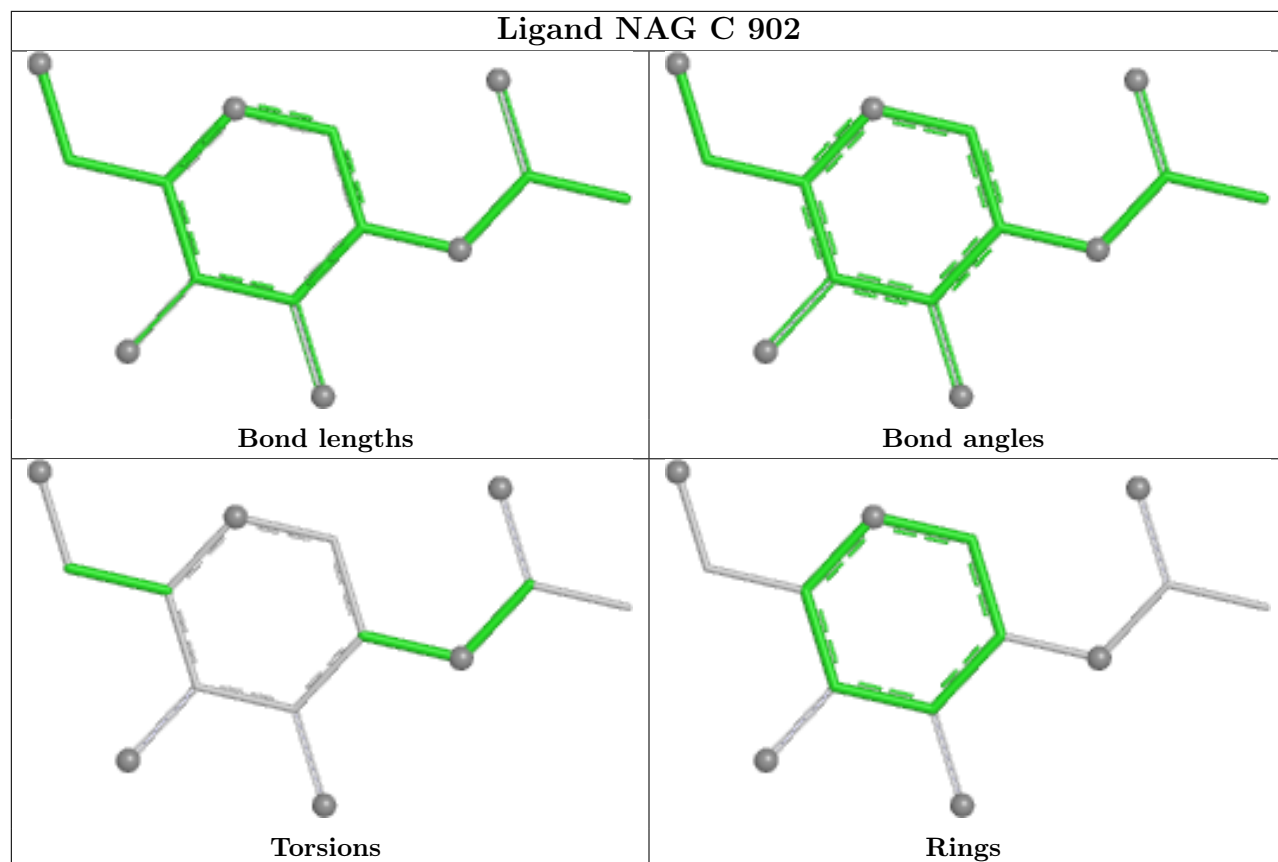


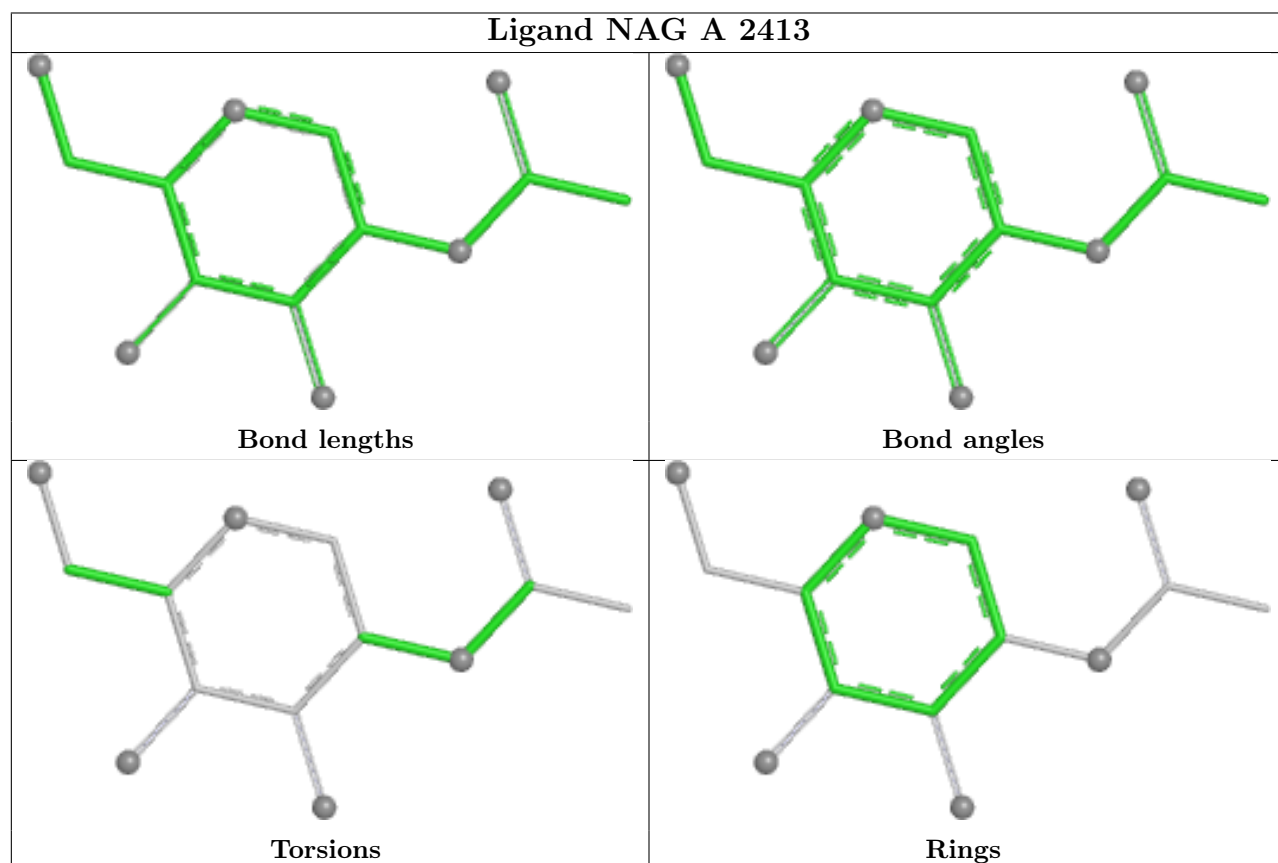
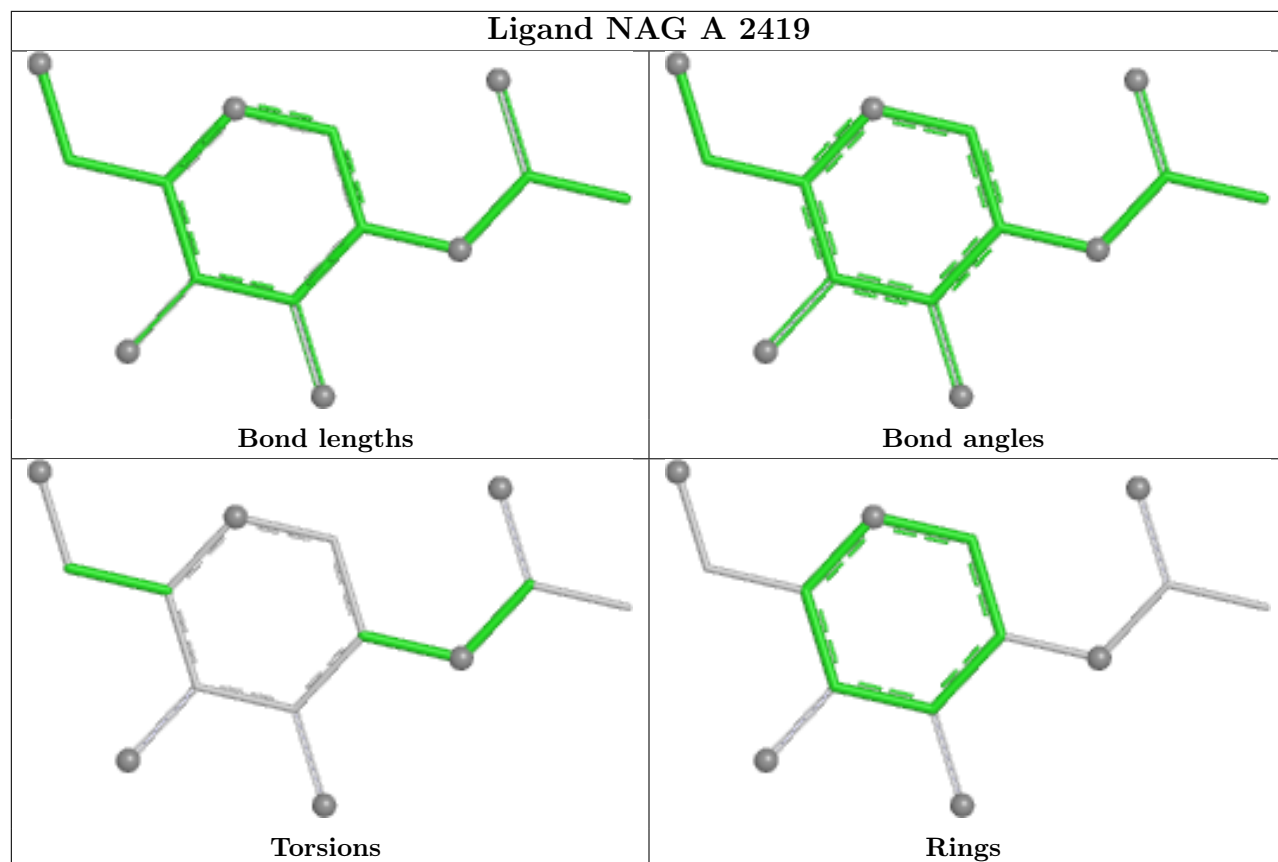
Ligand NAG A 2404

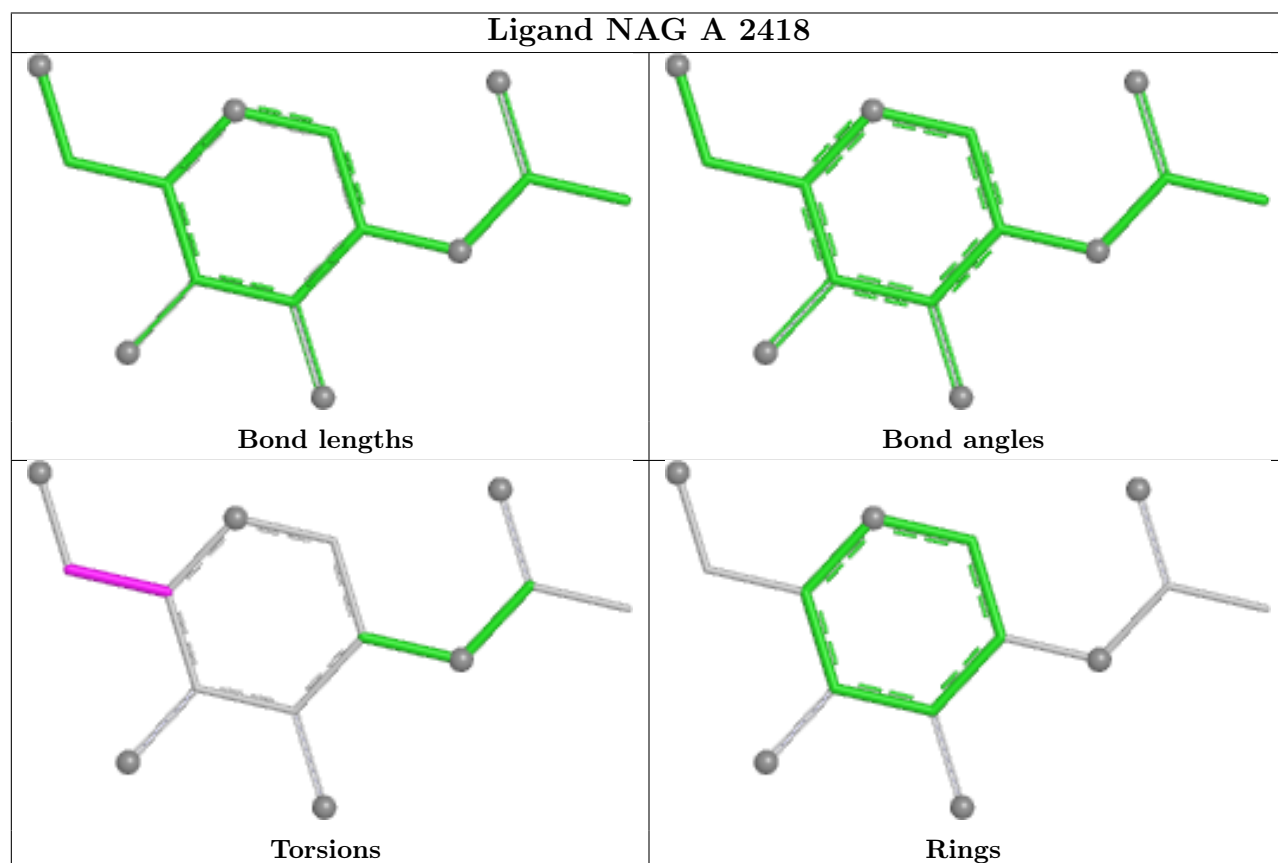
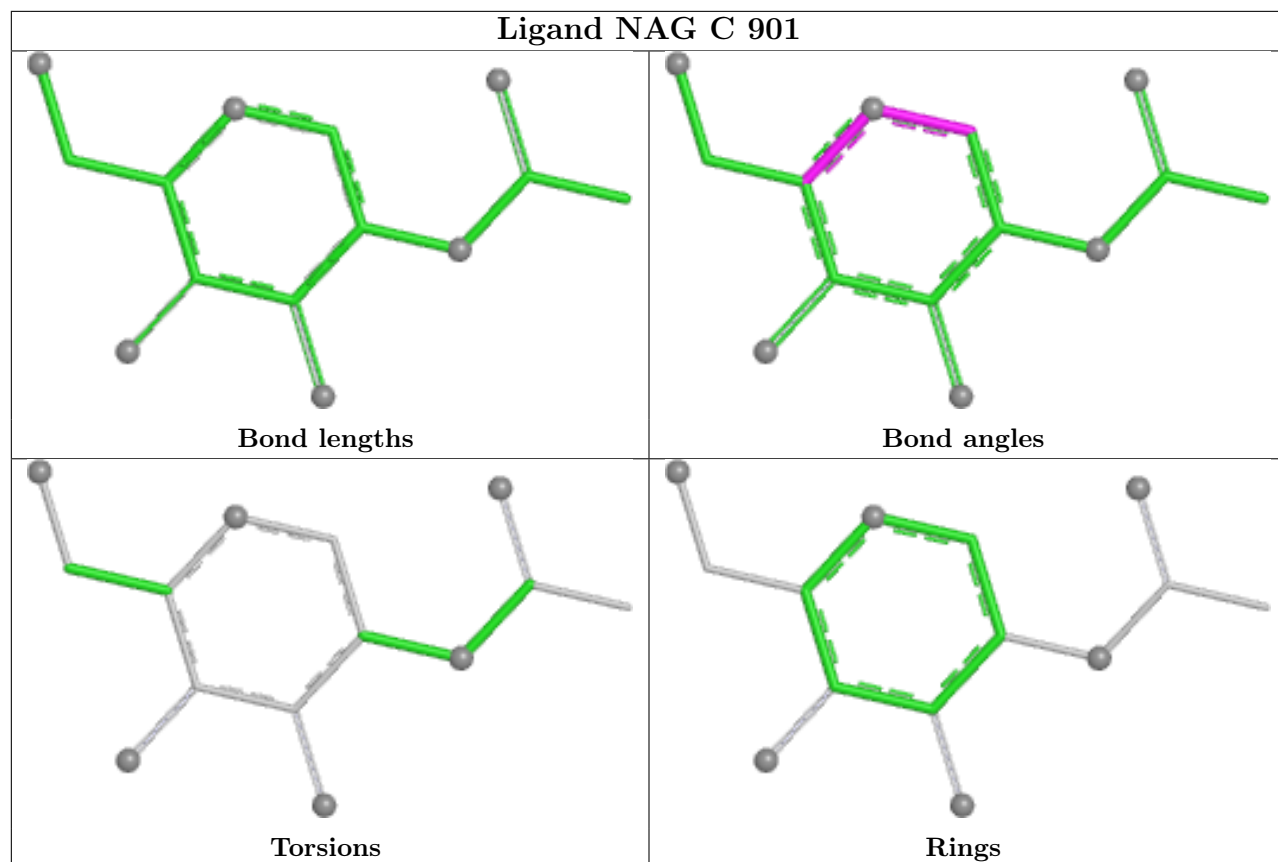


Ligand NAG A 2411

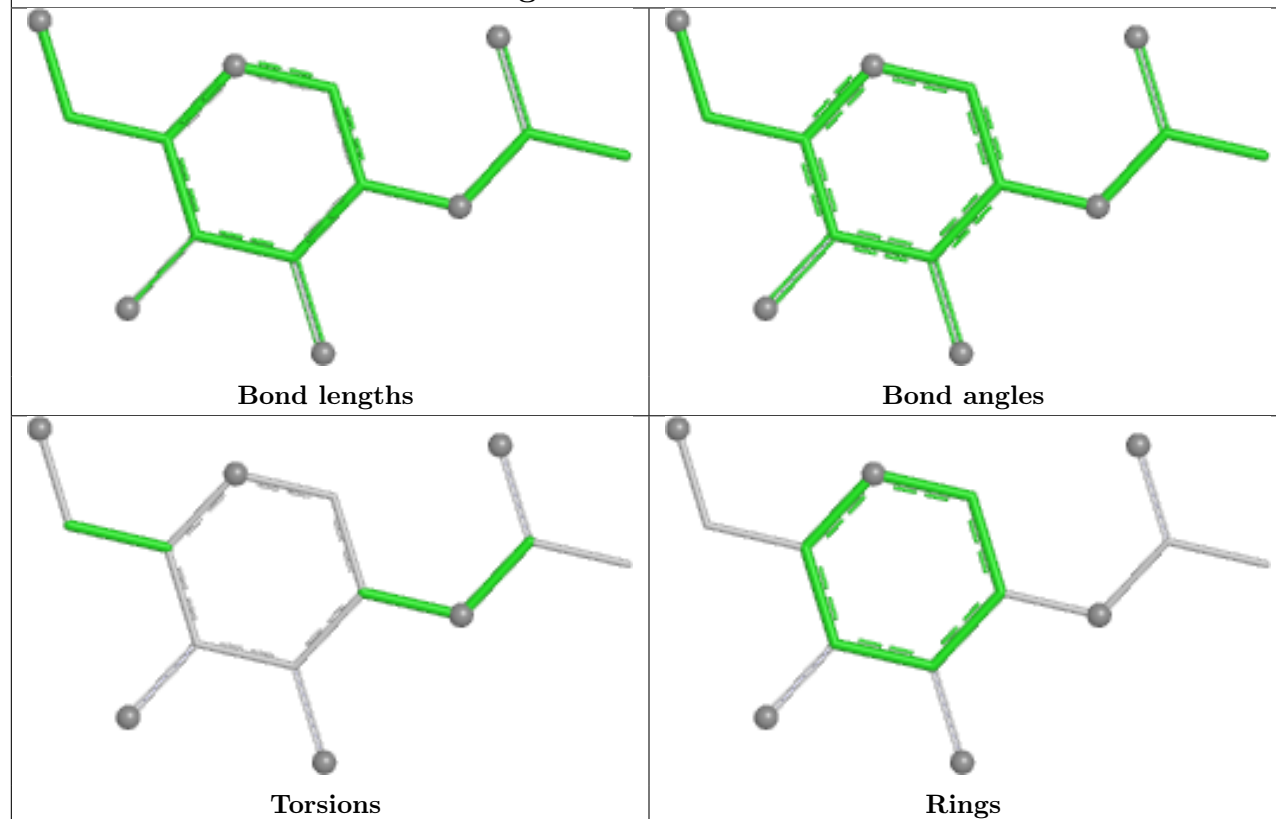




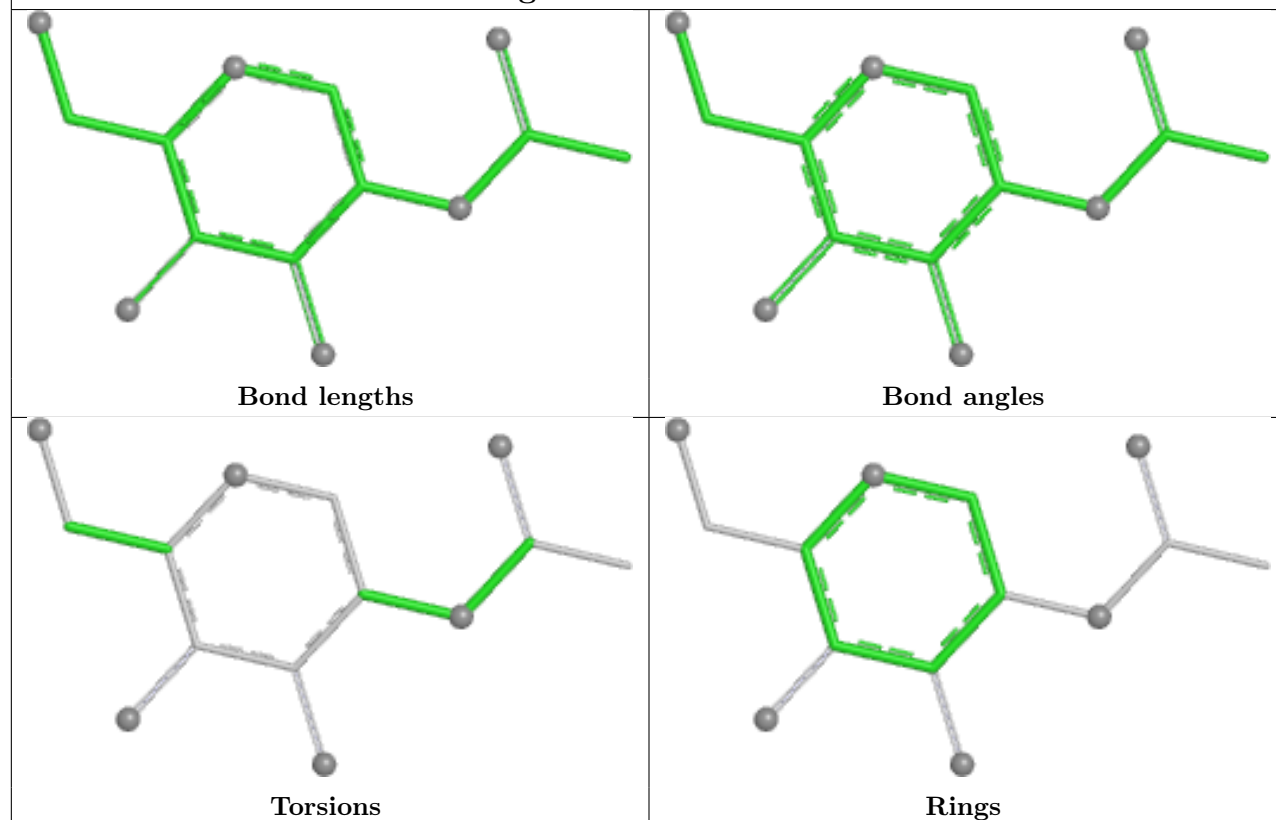


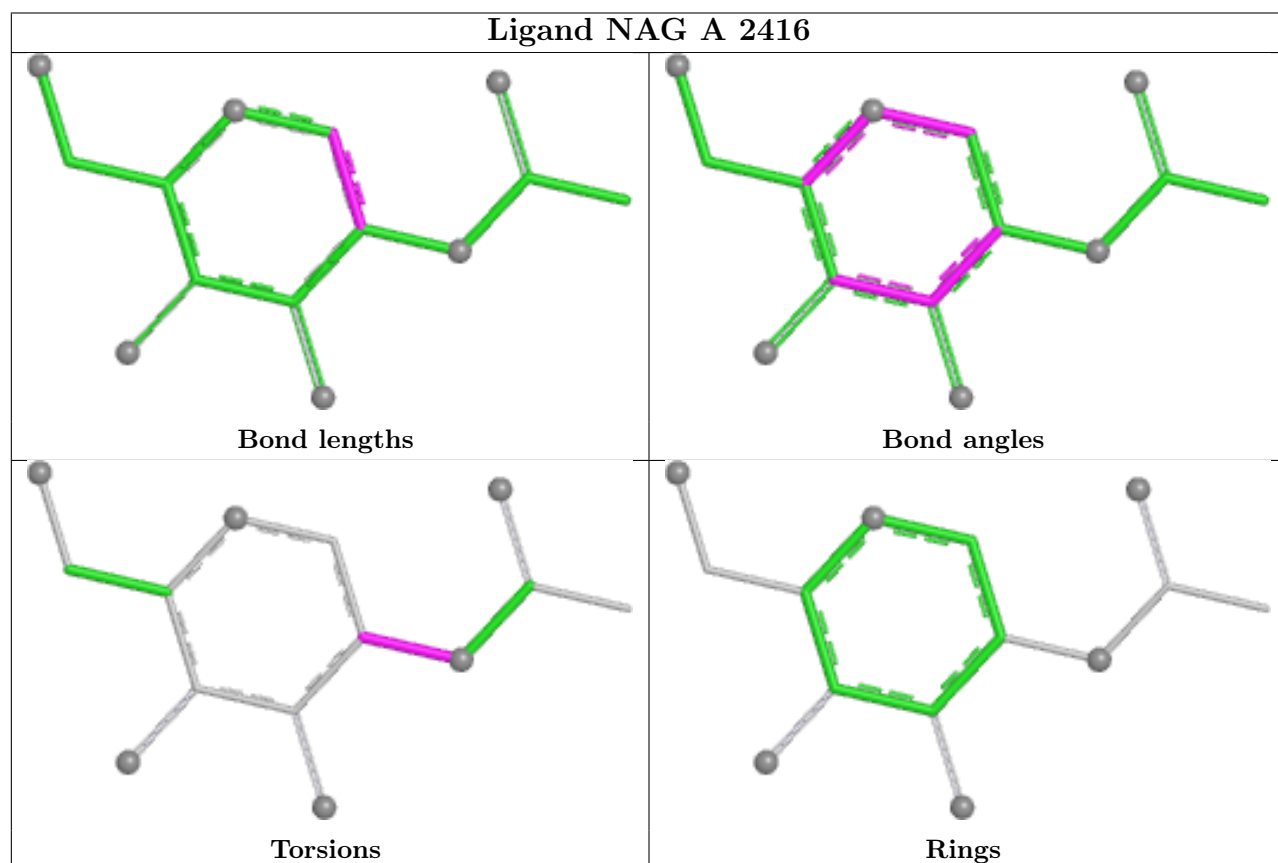
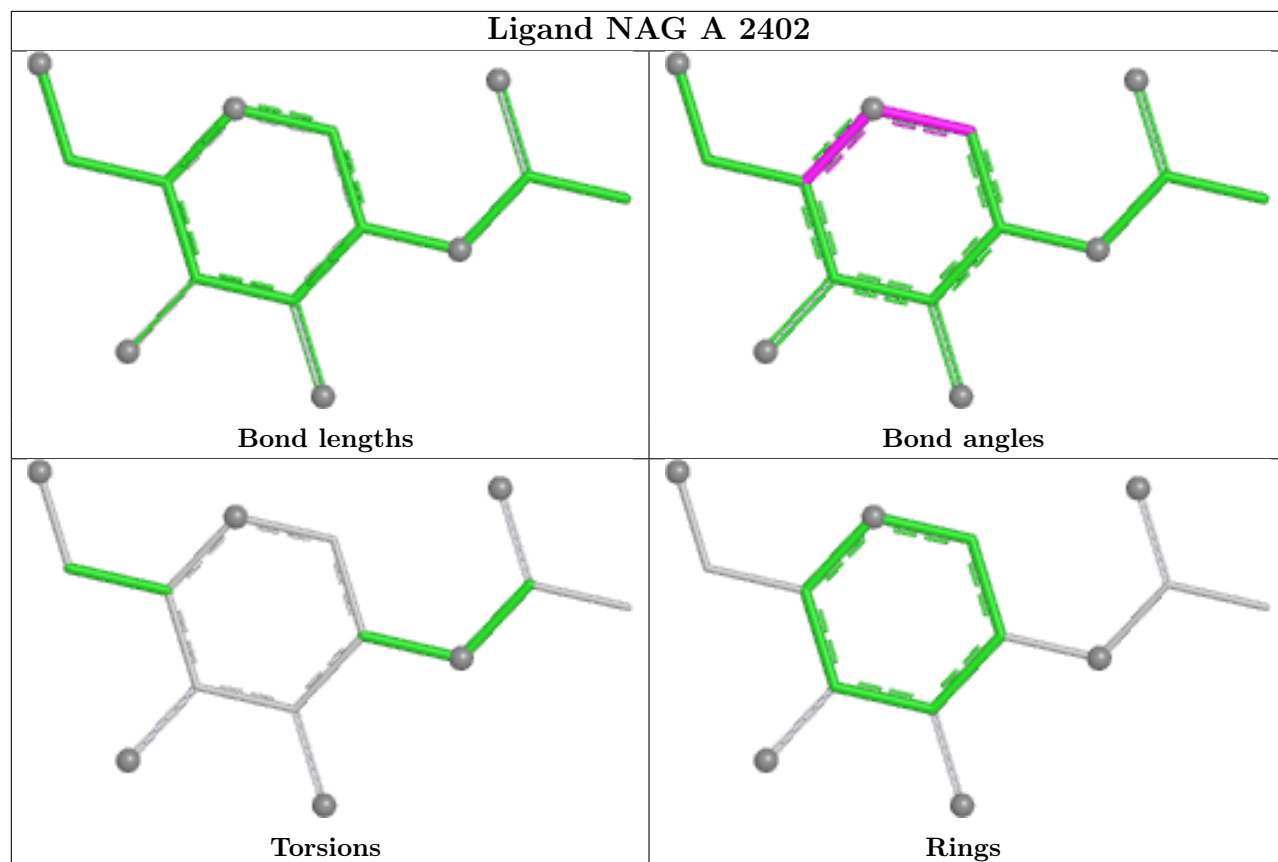


Ligand NAG A 2407

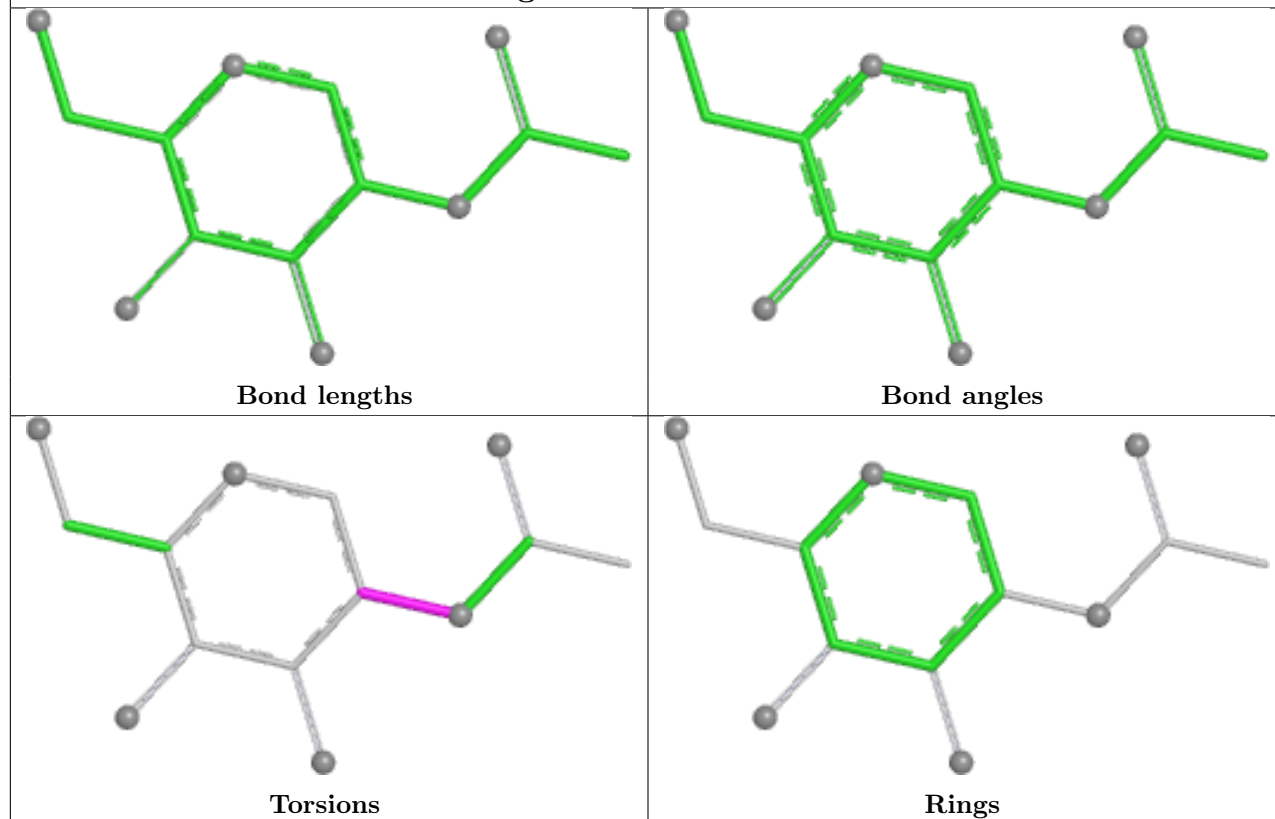


Ligand NAG A 2414

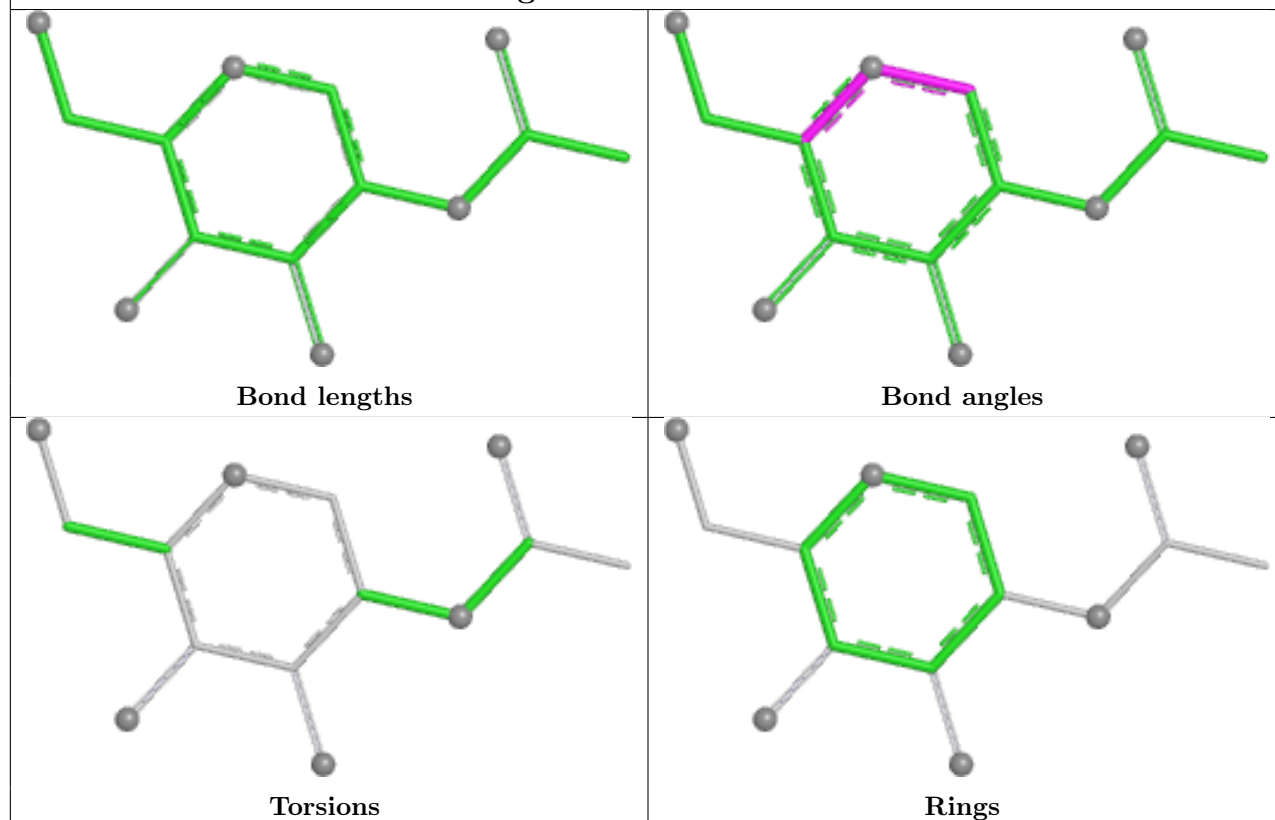


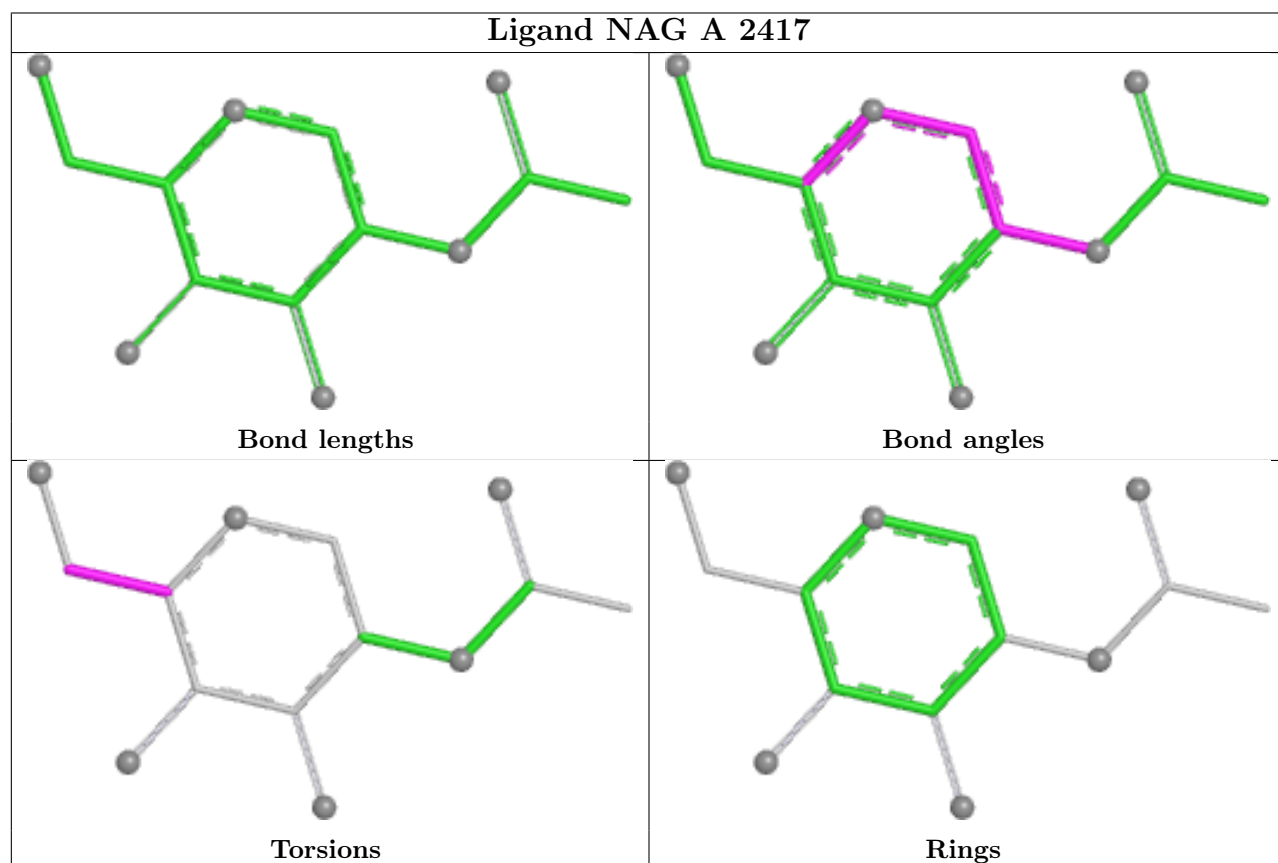
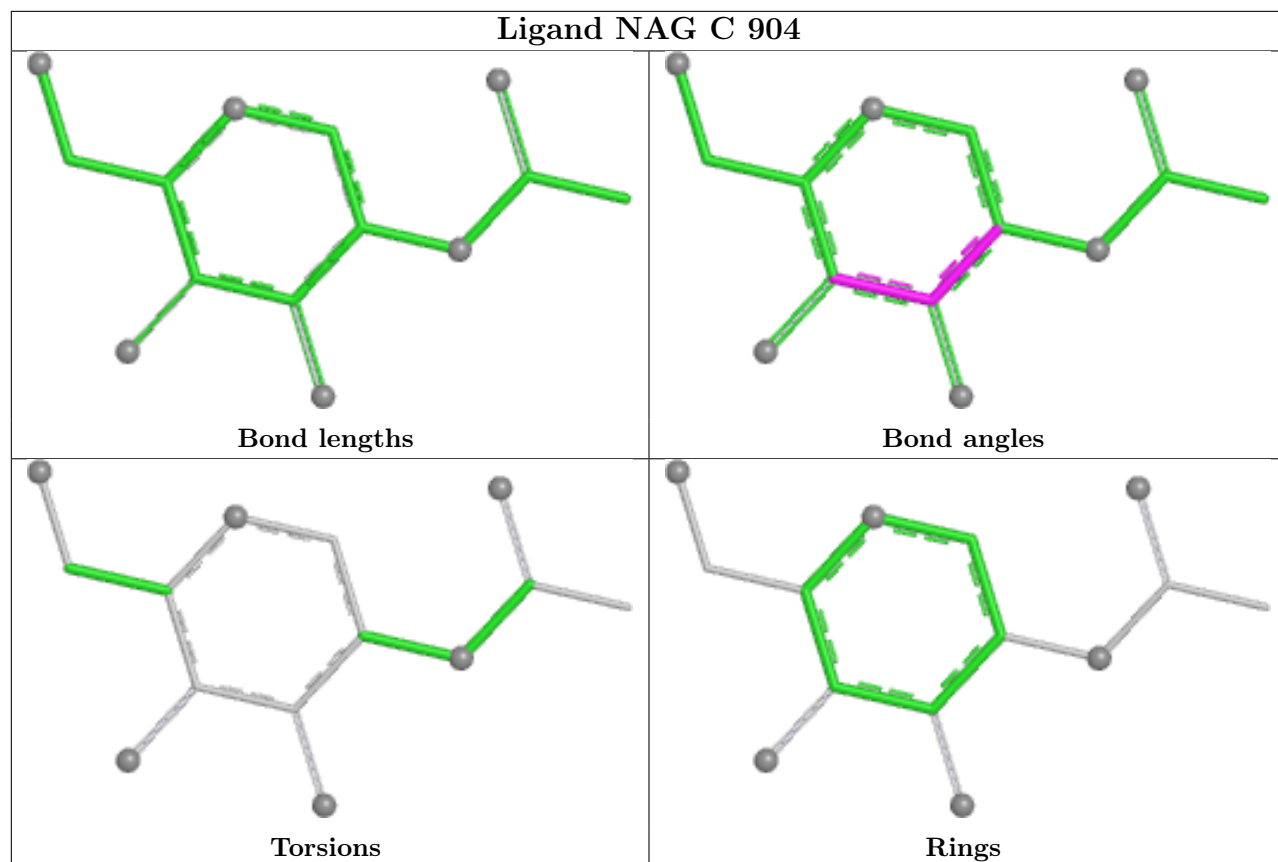


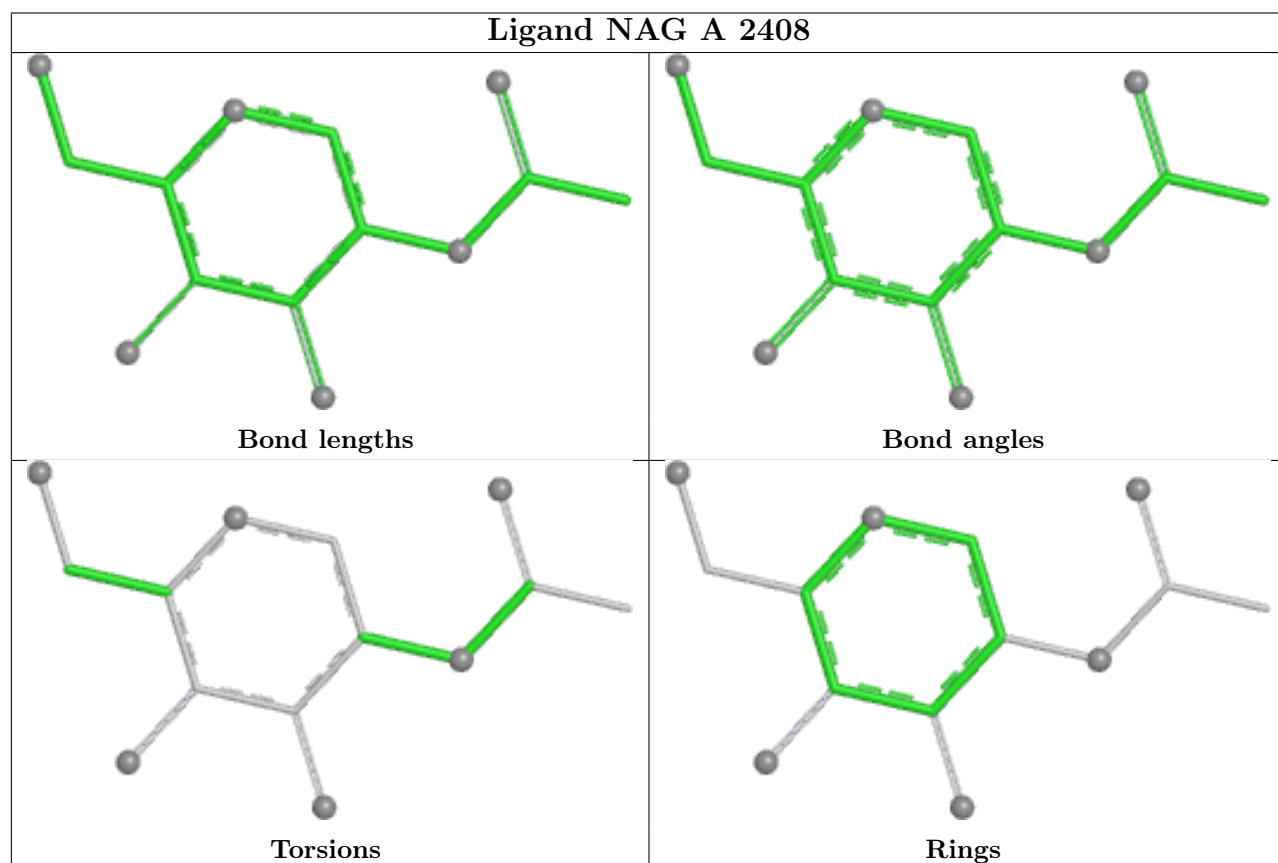
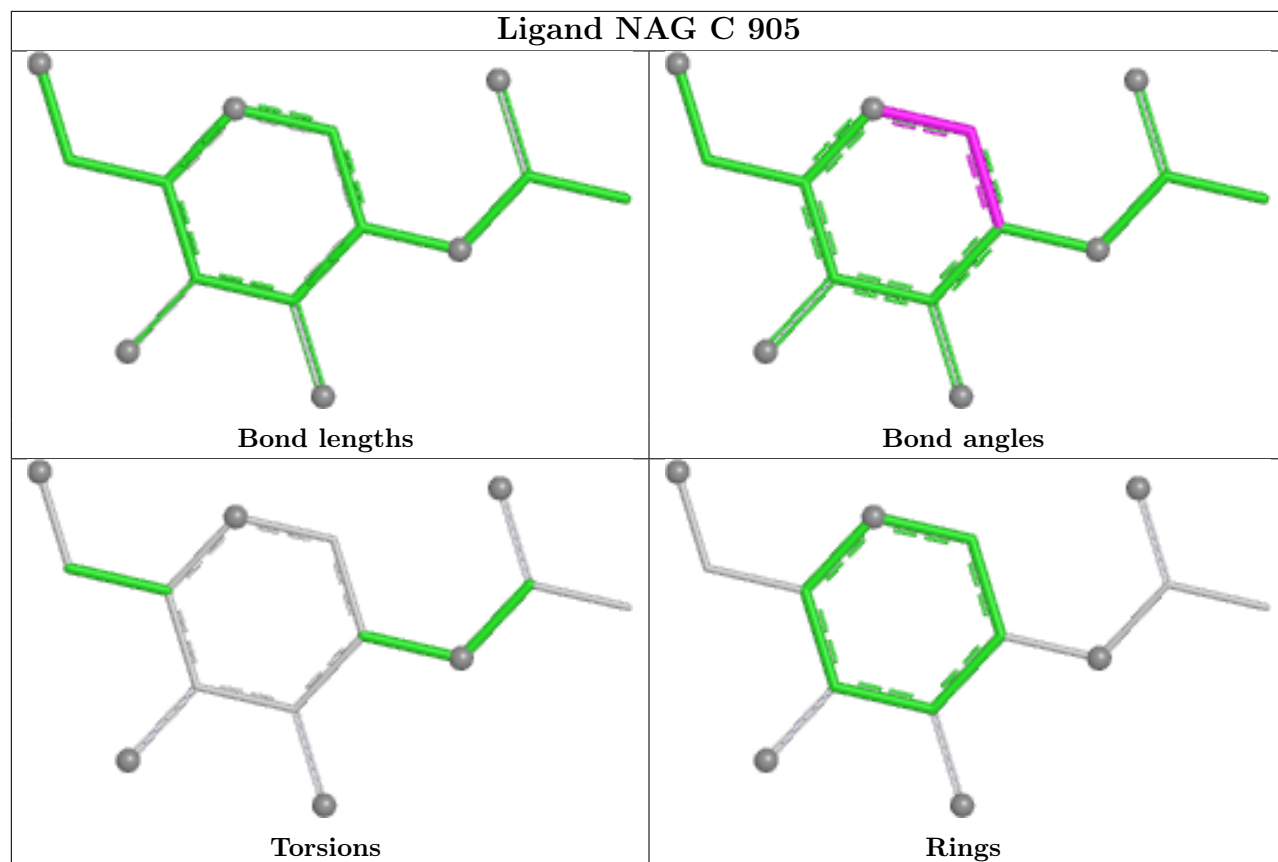
Ligand NAG A 2420

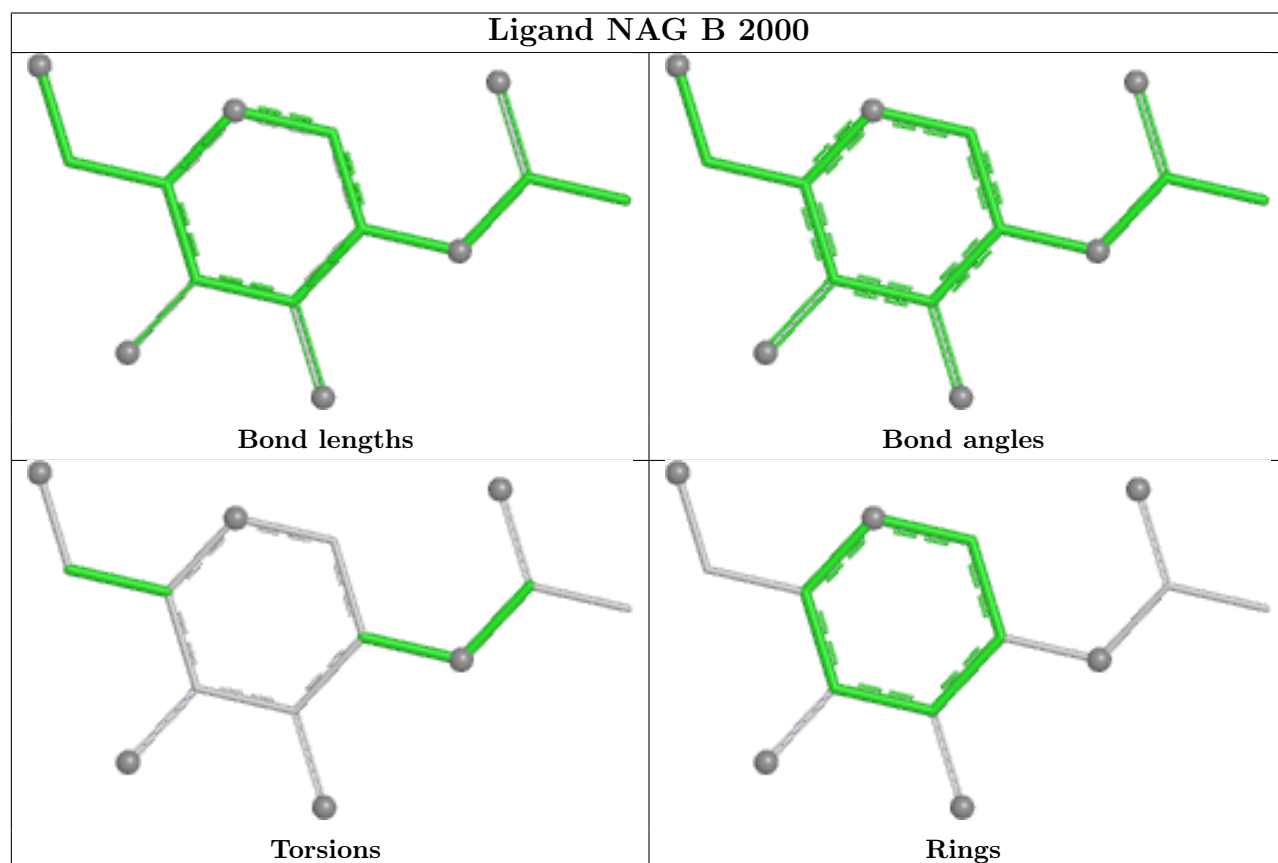
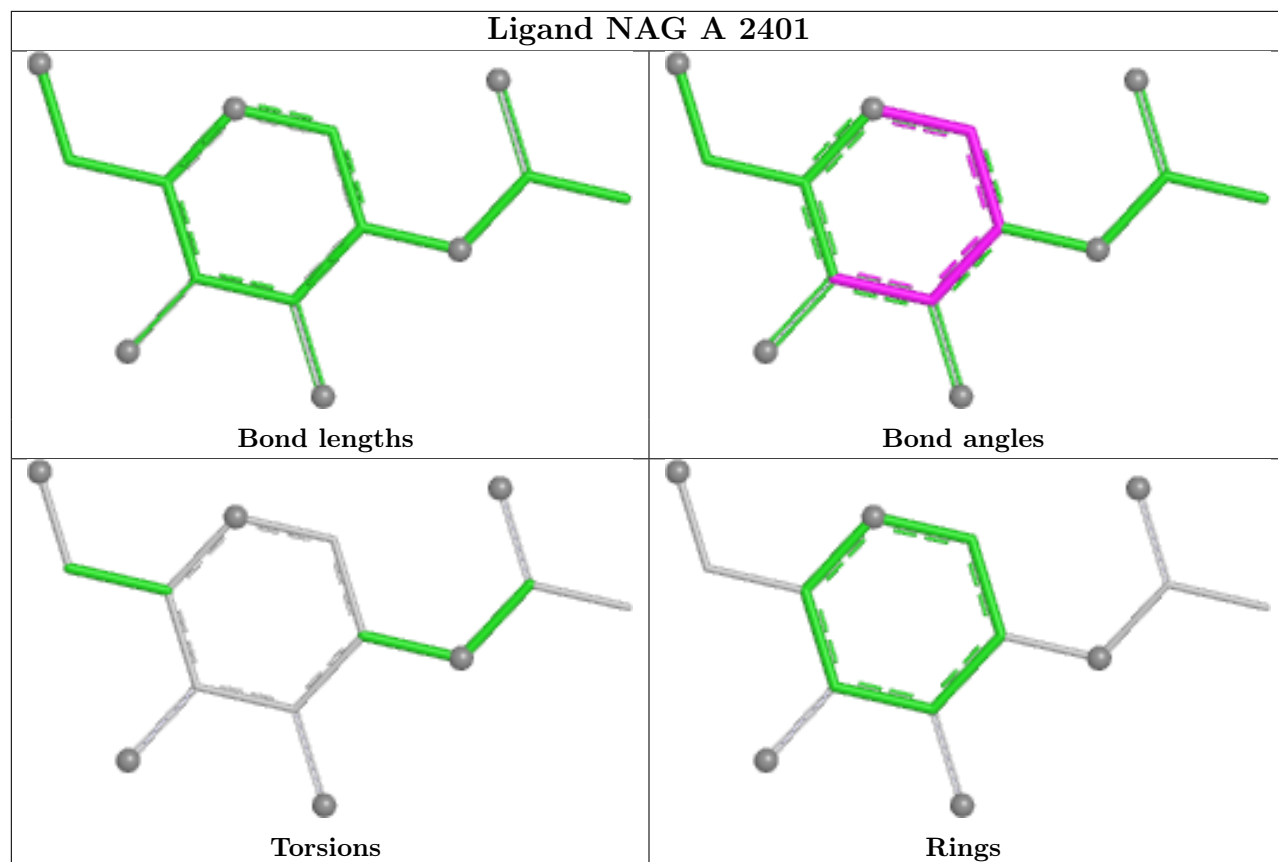


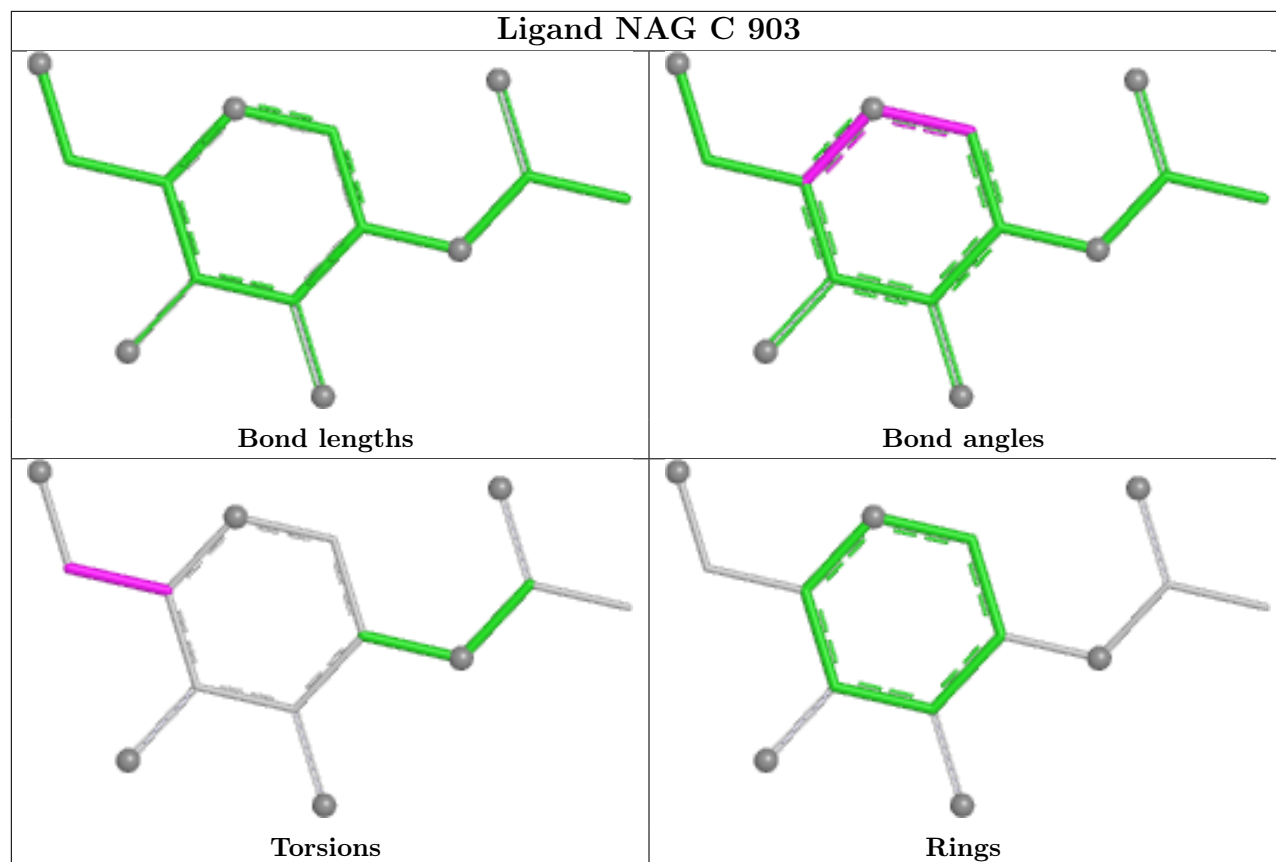
Ligand NAG A 2406











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.

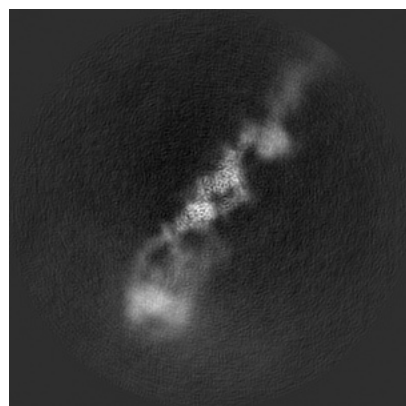
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71057. These allow visual inspection of the internal detail of the map and identification of artifacts.

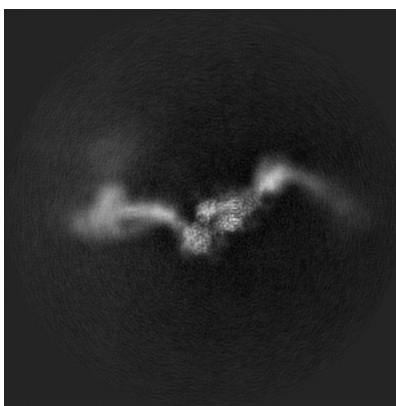
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

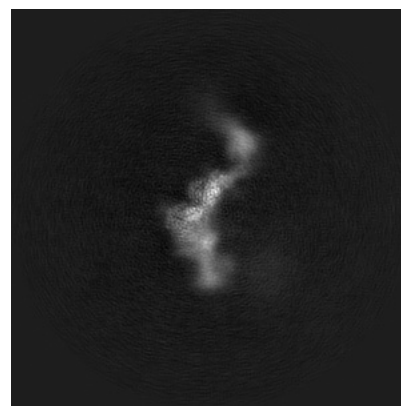
6.1.1 Primary map



X

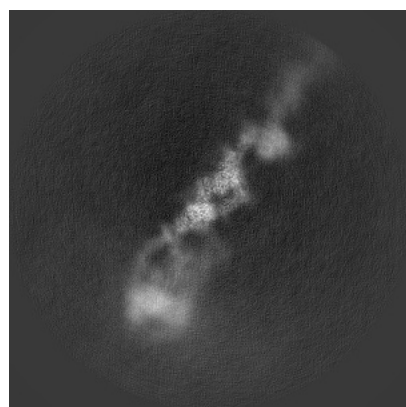


Y

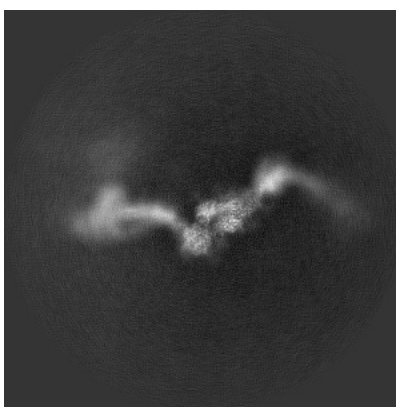


Z

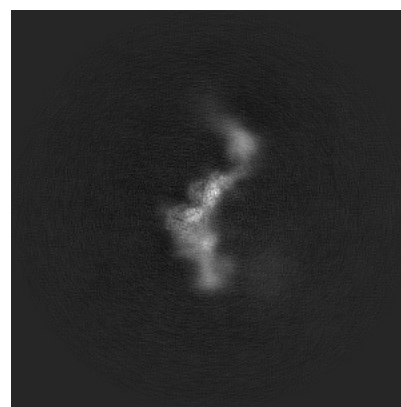
6.1.2 Raw map



X



Y

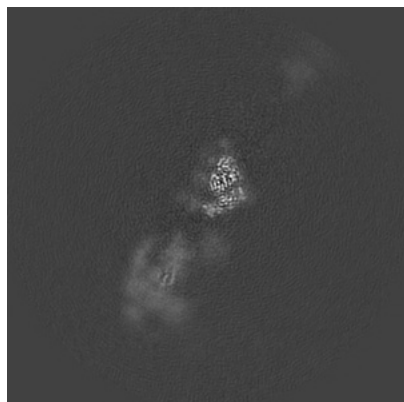


Z

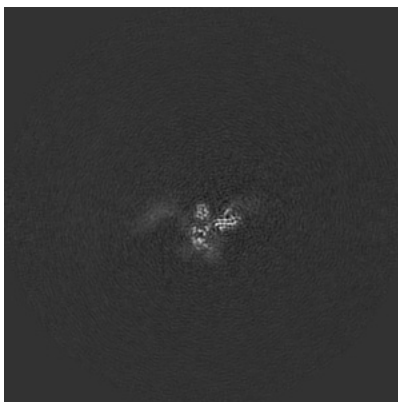
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

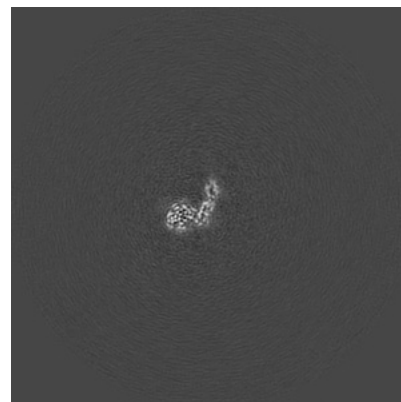
6.2.1 Primary map



X Index: 200

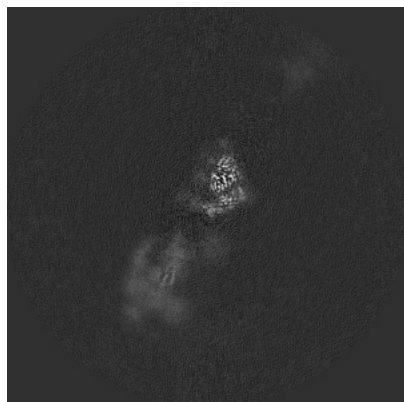


Y Index: 200



Z Index: 200

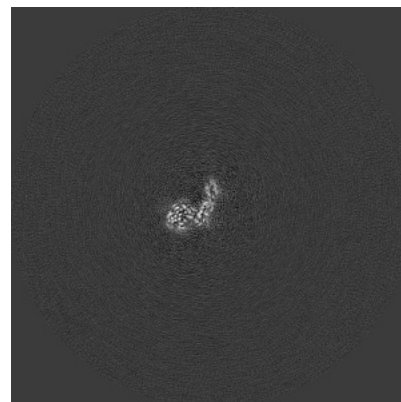
6.2.2 Raw map



X Index: 200



Y Index: 200

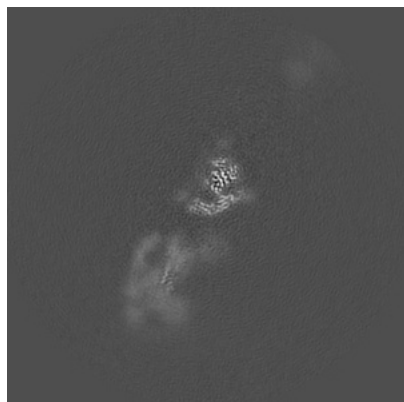


Z Index: 200

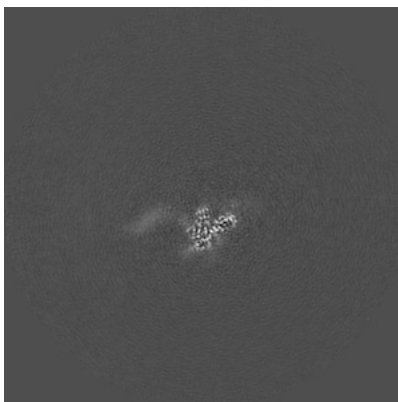
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

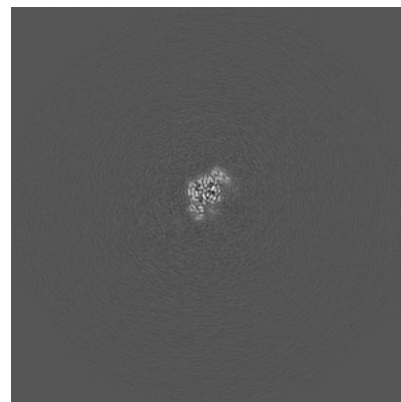
6.3.1 Primary map



X Index: 197



Y Index: 195

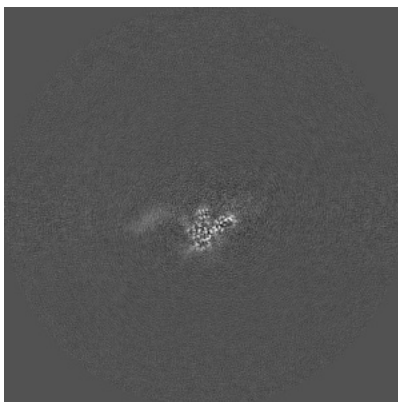


Z Index: 228

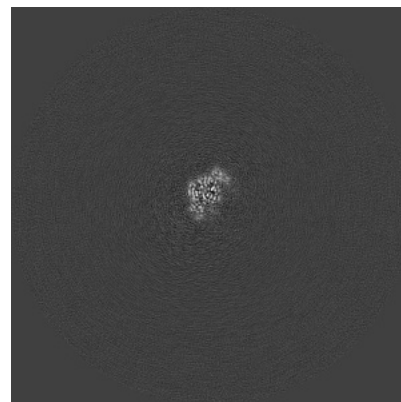
6.3.2 Raw map



X Index: 197



Y Index: 195

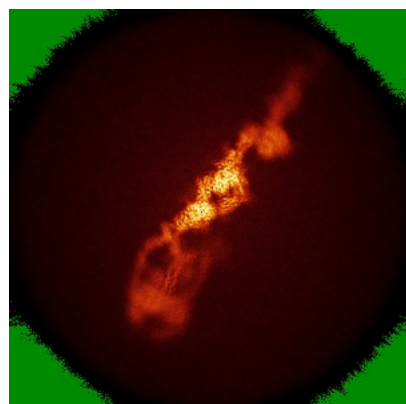


Z Index: 228

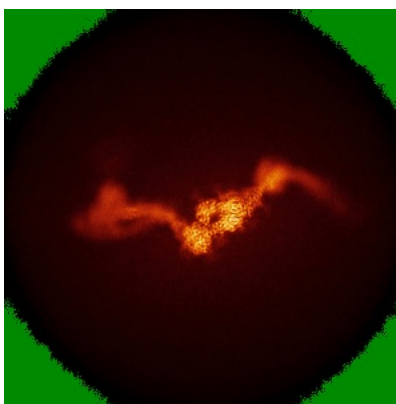
The images above show the largest variance slices of the map in three orthogonal directions.

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

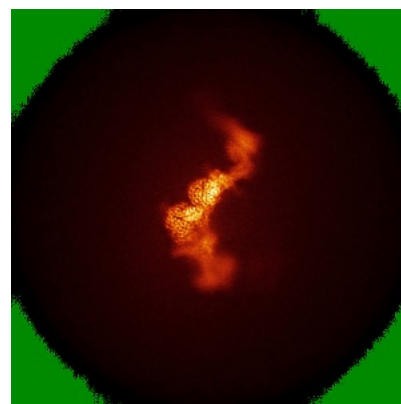
6.4.1 Primary map



X

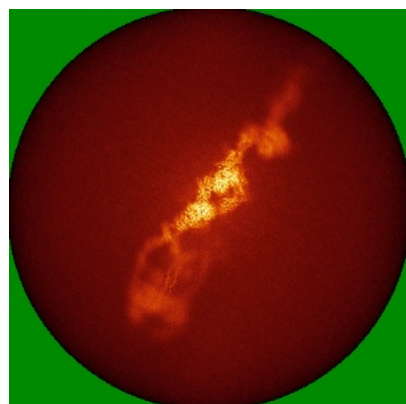


Y

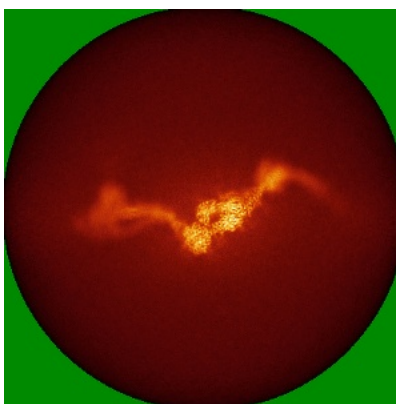


Z

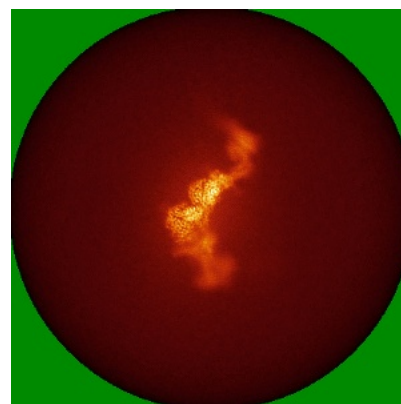
6.4.2 Raw map



X



Y

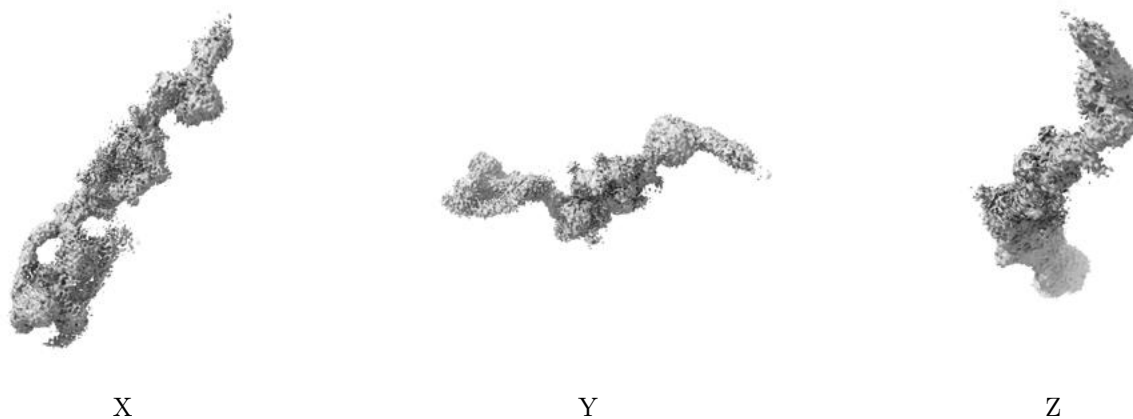


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

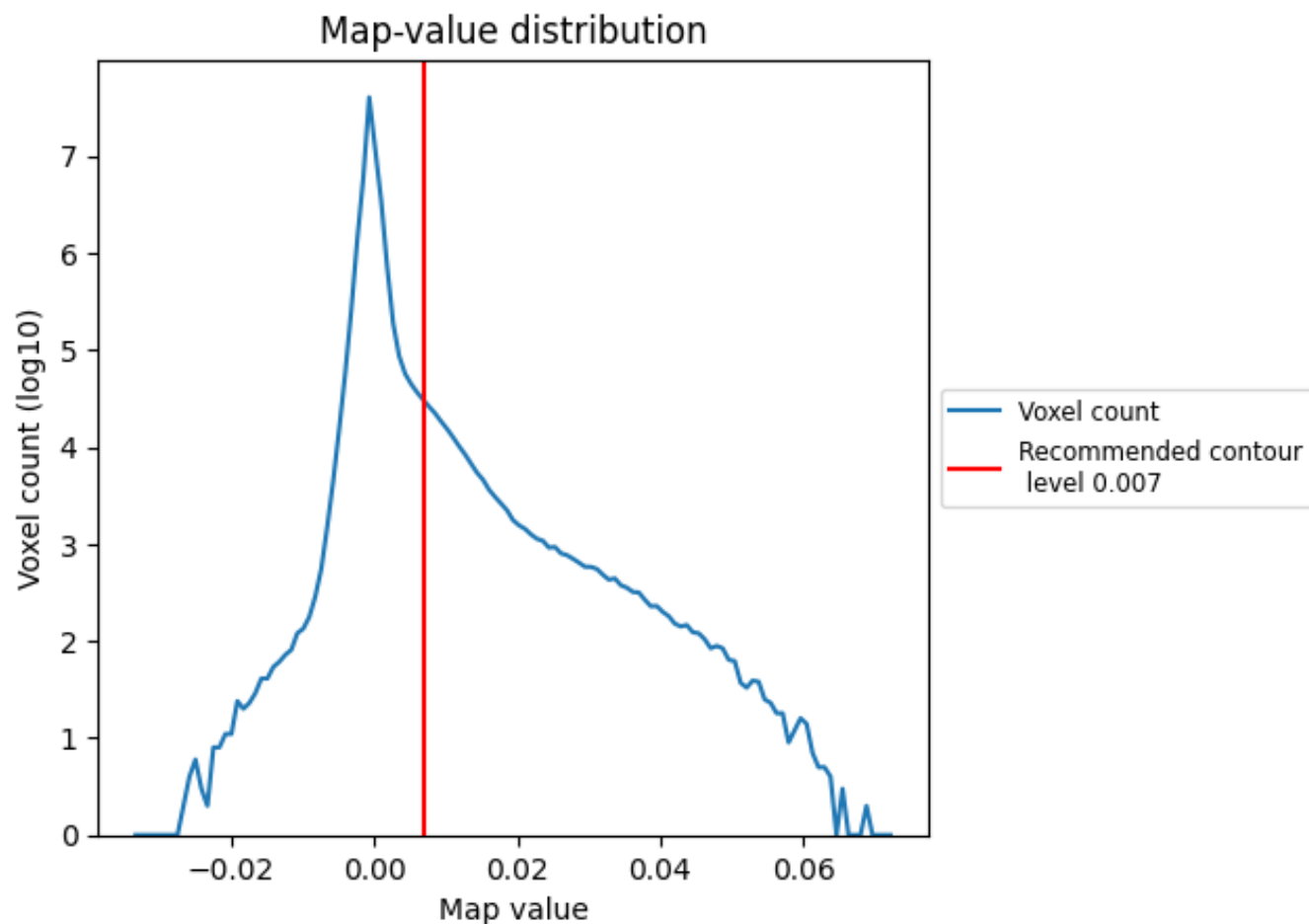
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

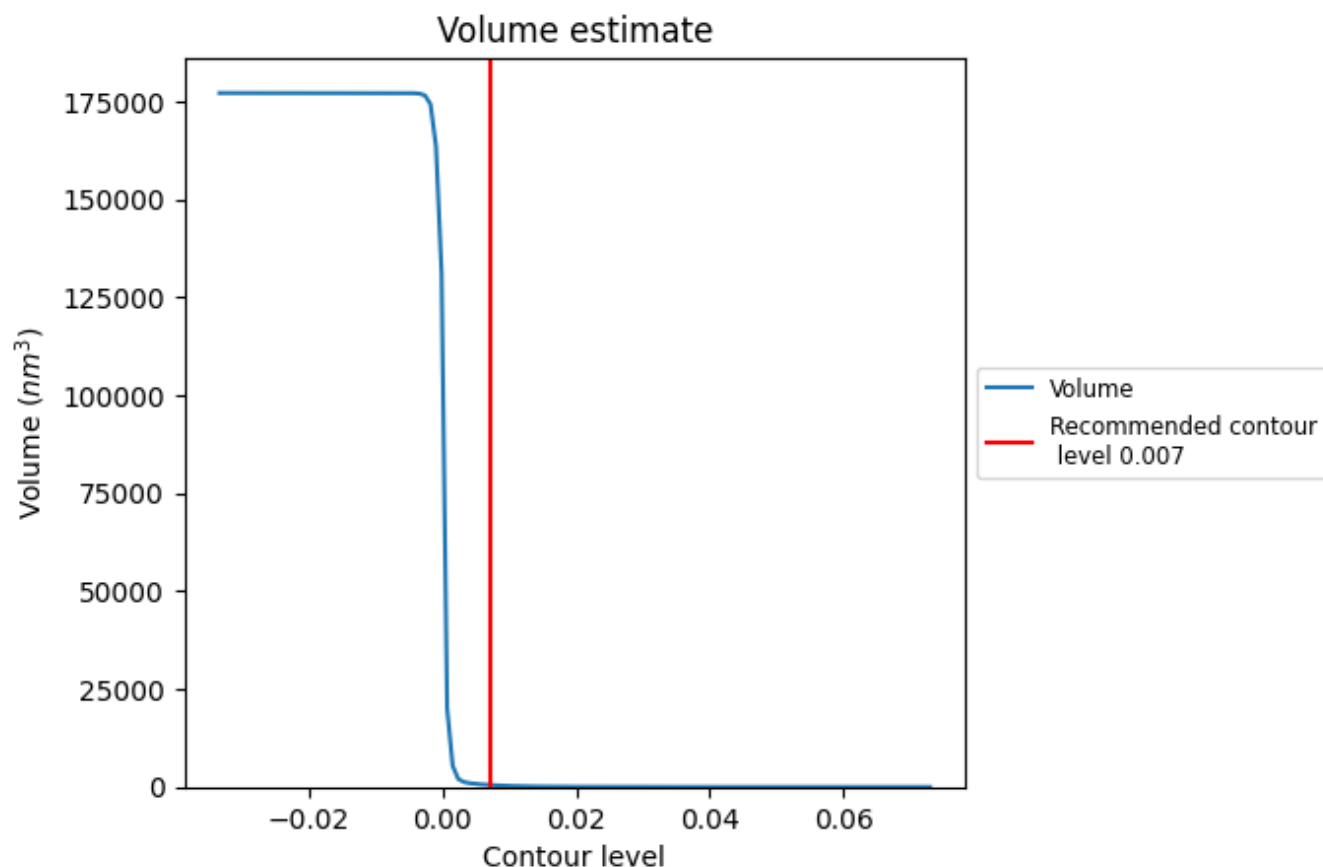
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

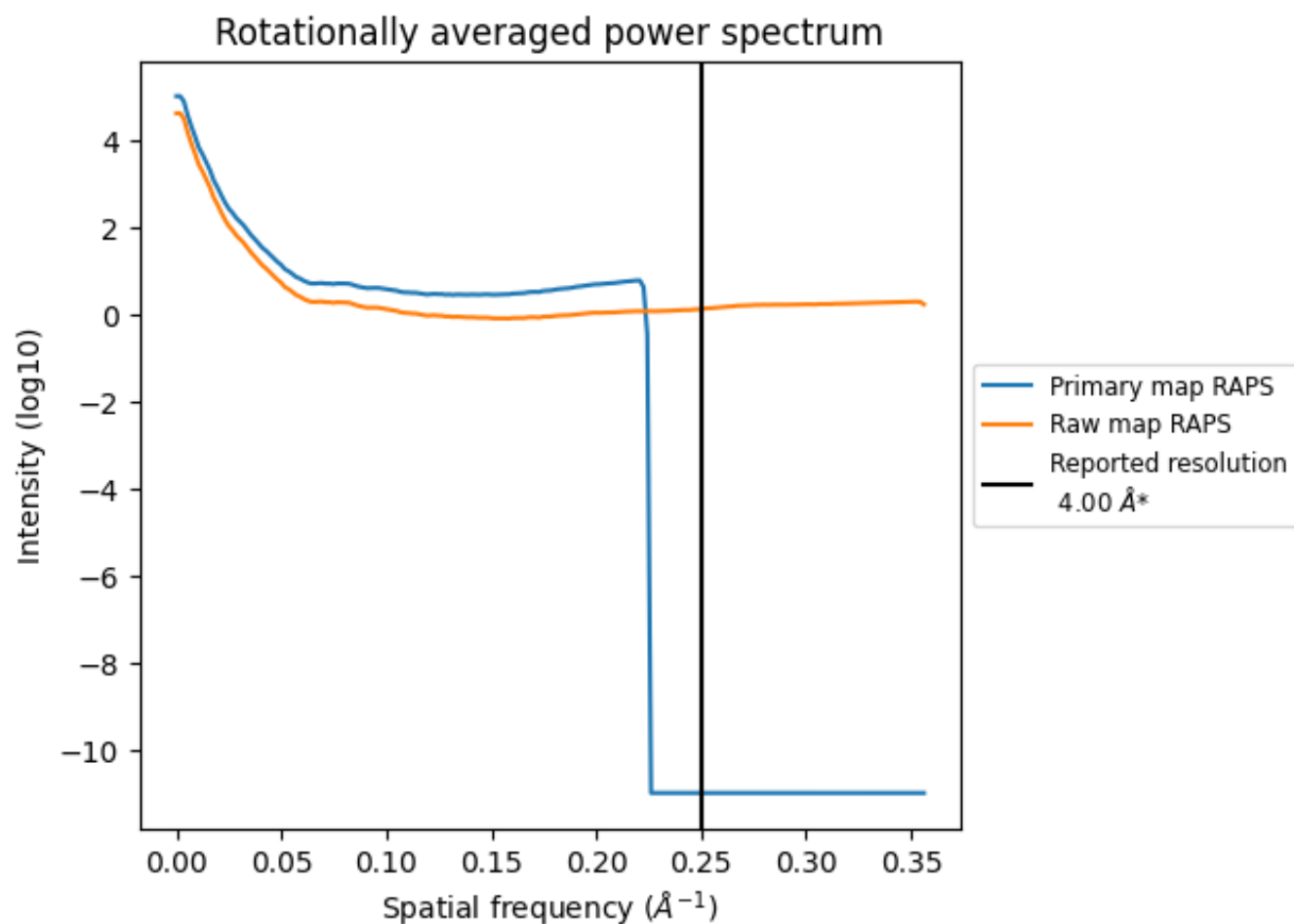
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm^3 ; this corresponds to an approximate mass of 463 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 ⓘ

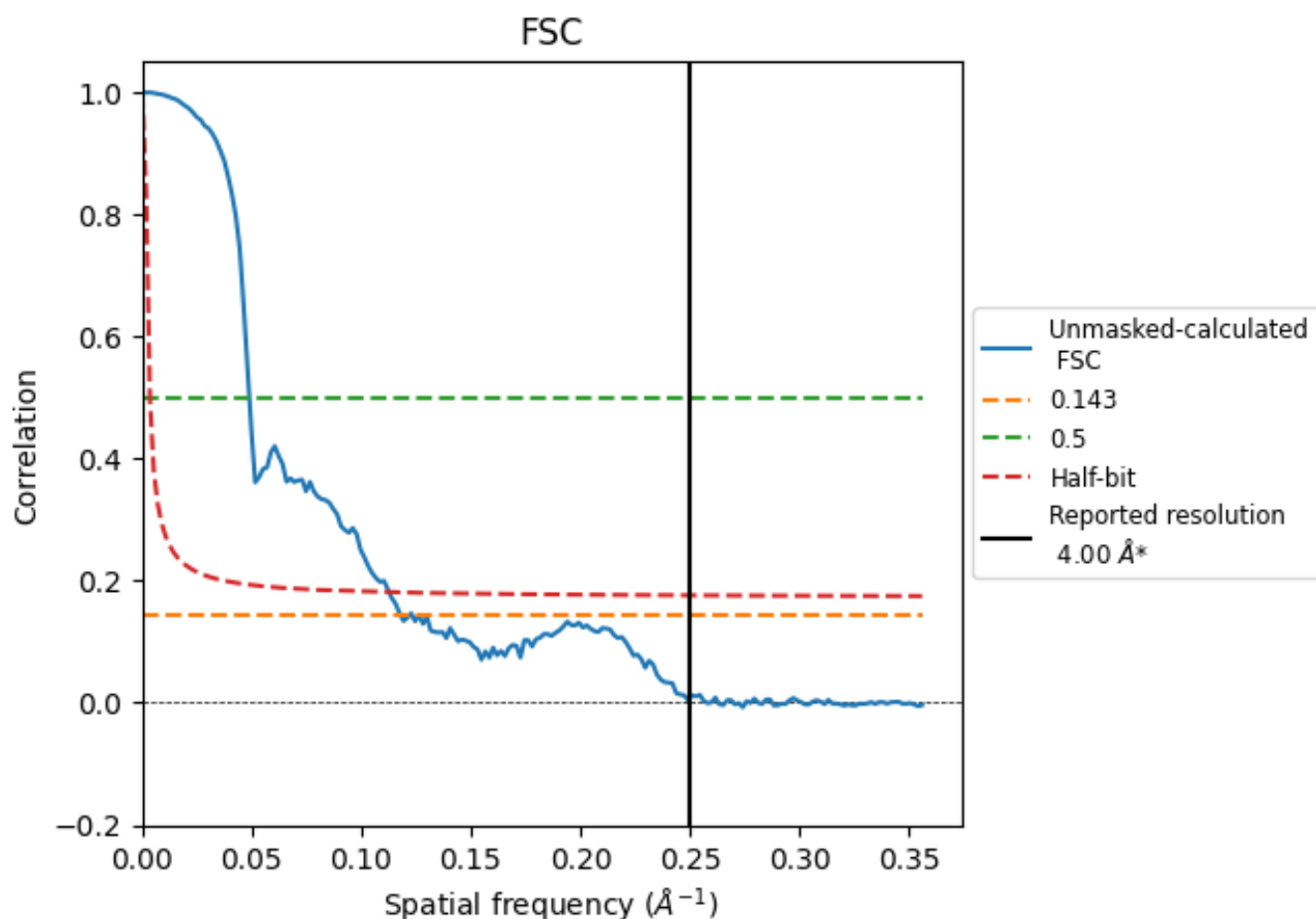


*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

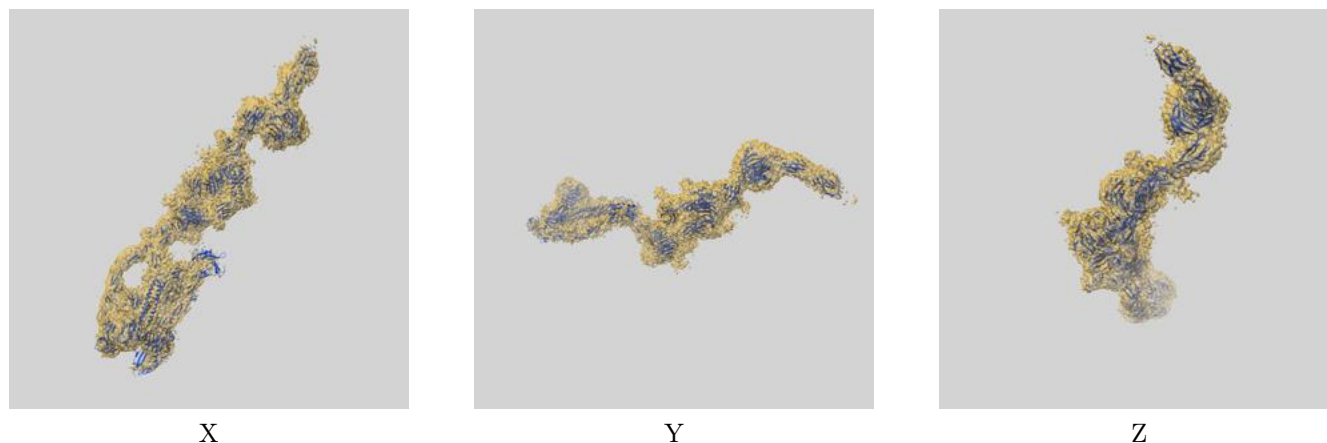
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.47	20.45	8.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.47 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

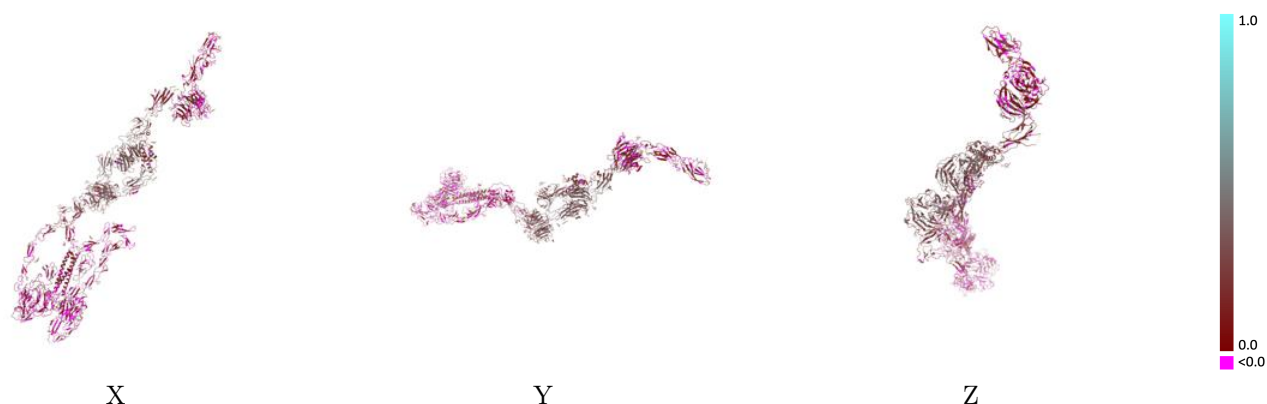
This section contains information regarding the fit between EMDB map EMD-71057 and PDB model 9OZC. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



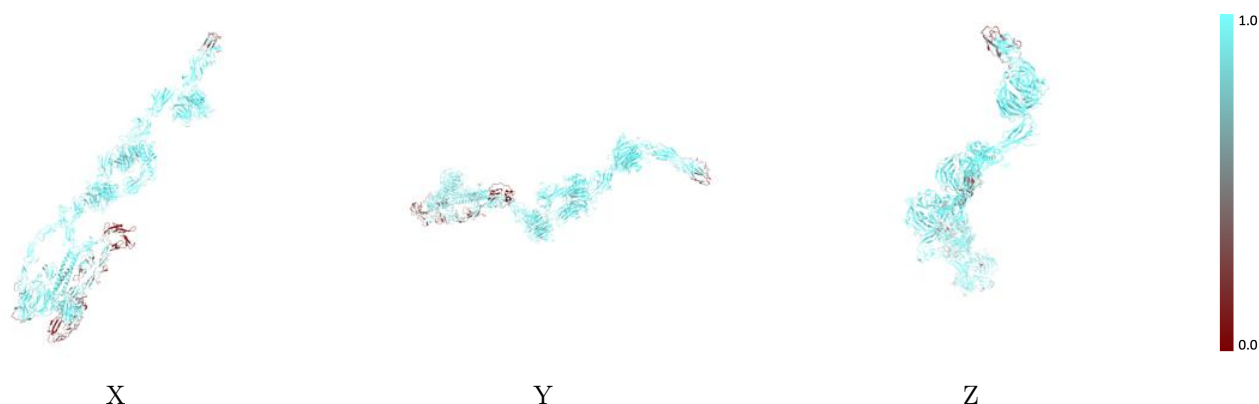
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



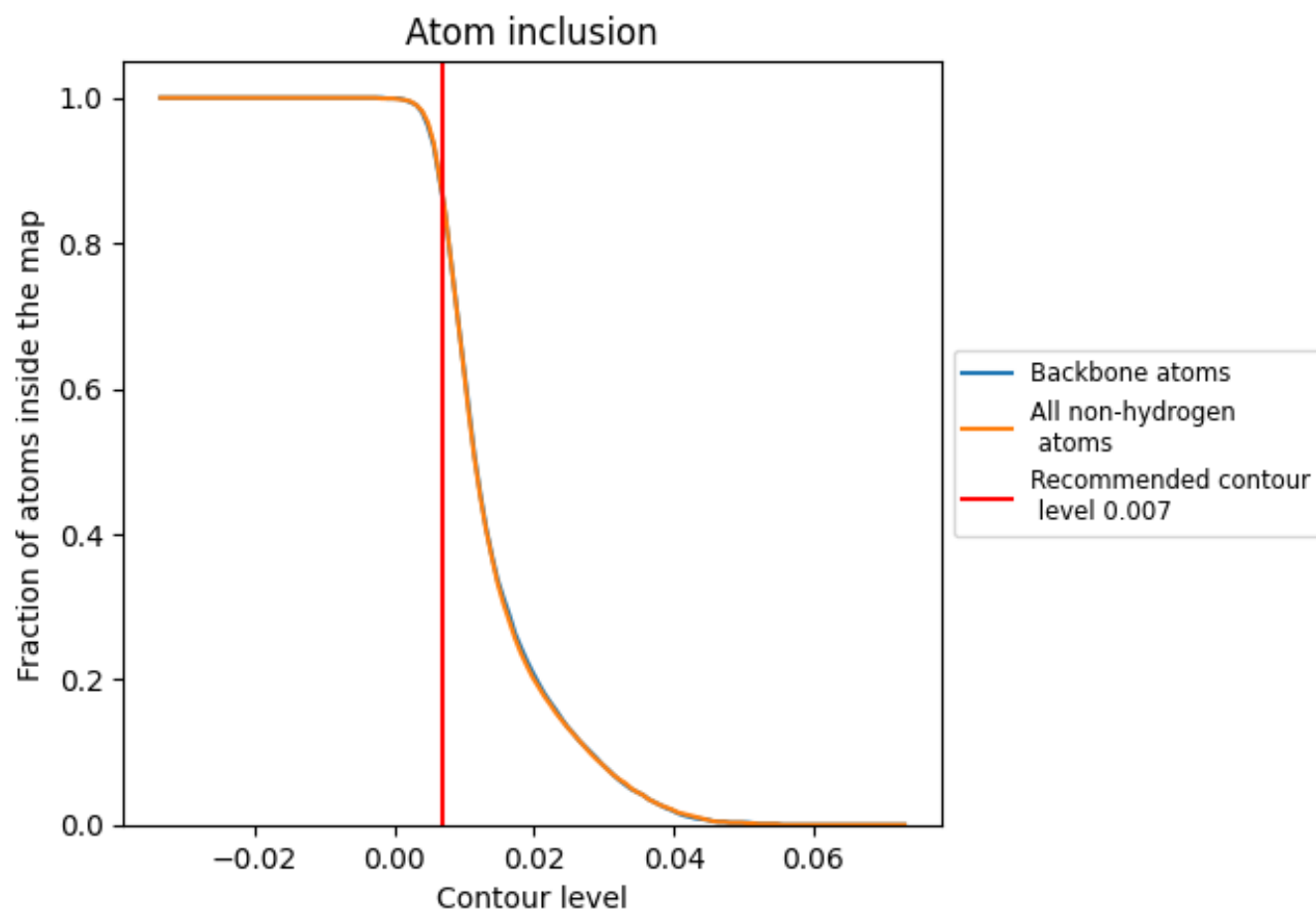
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8620	<div></div> 0.1610
A	<div></div> 0.9460	<div></div> 0.2390
B	<div></div> 0.6270	<div></div> 0.0580
C	<div></div> 0.8900	<div></div> 0.1010
D	<div></div> 0.9280	<div></div> 0.0920
E	<div></div> 1.0000	<div></div> 0.3090
F	<div></div> 1.0000	<div></div> 0.2260
G	<div></div> 0.8210	<div></div> 0.0480
H	<div></div> 0.8930	<div></div> 0.1030

