



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:36 PM UTC

PDB ID : 7DX3 / pdb_00007dx3
EMDB ID : EMD-30894
Title : S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 1 (1 up RBD and no PD bound)
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on : 2021-01-18
Resolution : 3.50 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

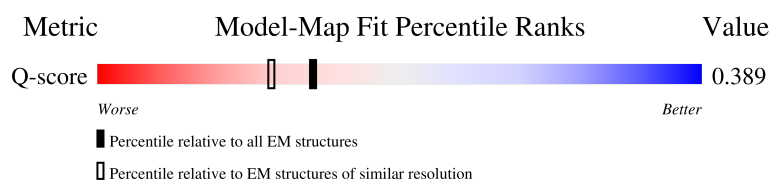
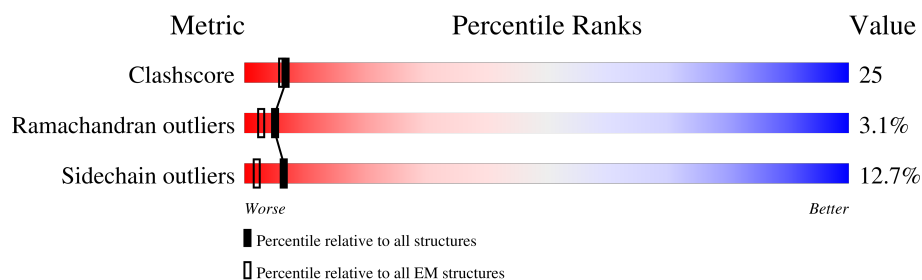
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



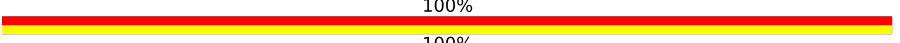
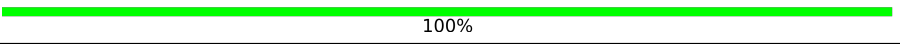
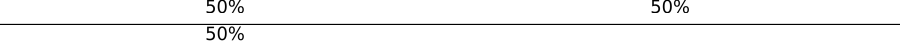
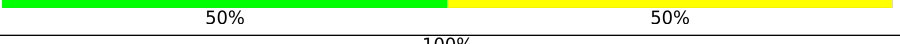
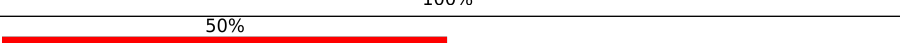
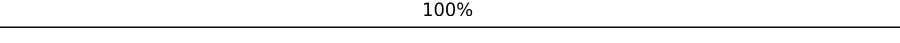
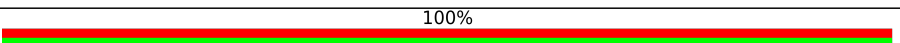
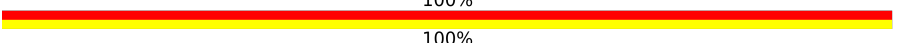
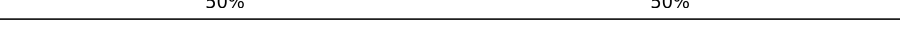
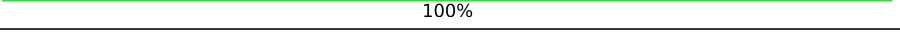
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1283	
1	B	1283	
1	C	1283	
2	D	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	100% 
2	F	2	100% 
2	G	2	50% 
2	H	2	50% 
2	I	2	50% 
2	J	2	50% 
2	K	2	100% 
2	L	2	100% 
2	M	2	50% 
2	N	2	50% 
2	O	2	50% 
2	P	2	100% 
2	Q	2	100% 
2	R	2	100% 
2	S	2	100% 
2	T	2	50% 
2	U	2	50% 
2	V	2	100% 
2	W	2	50% 
2	X	2	50% 
2	Y	2	100% 

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23752 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	972	Total	C	N	O	S	0	0
			7590	4846	1263	1447	34		
1	B	971	Total	C	N	O	S	0	0
			7584	4843	1262	1445	34		
1	C	971	Total	C	N	O	S	0	0
			7584	4843	1262	1445	34		

There are 36 discrepancies between the modelled and reference sequences:

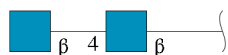
Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

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



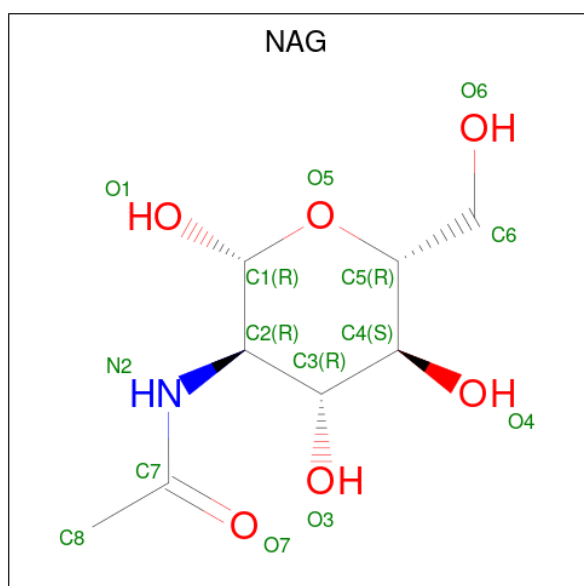
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

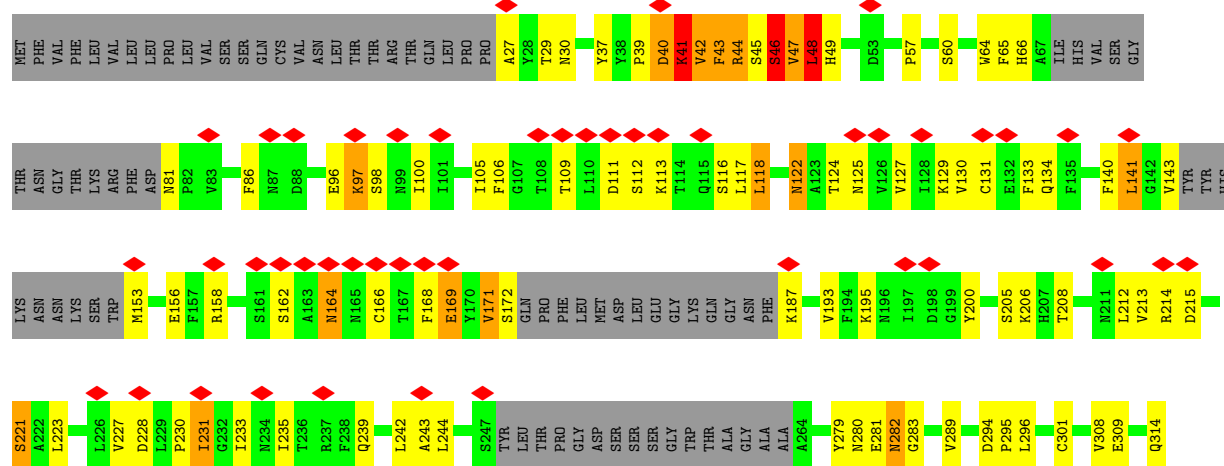
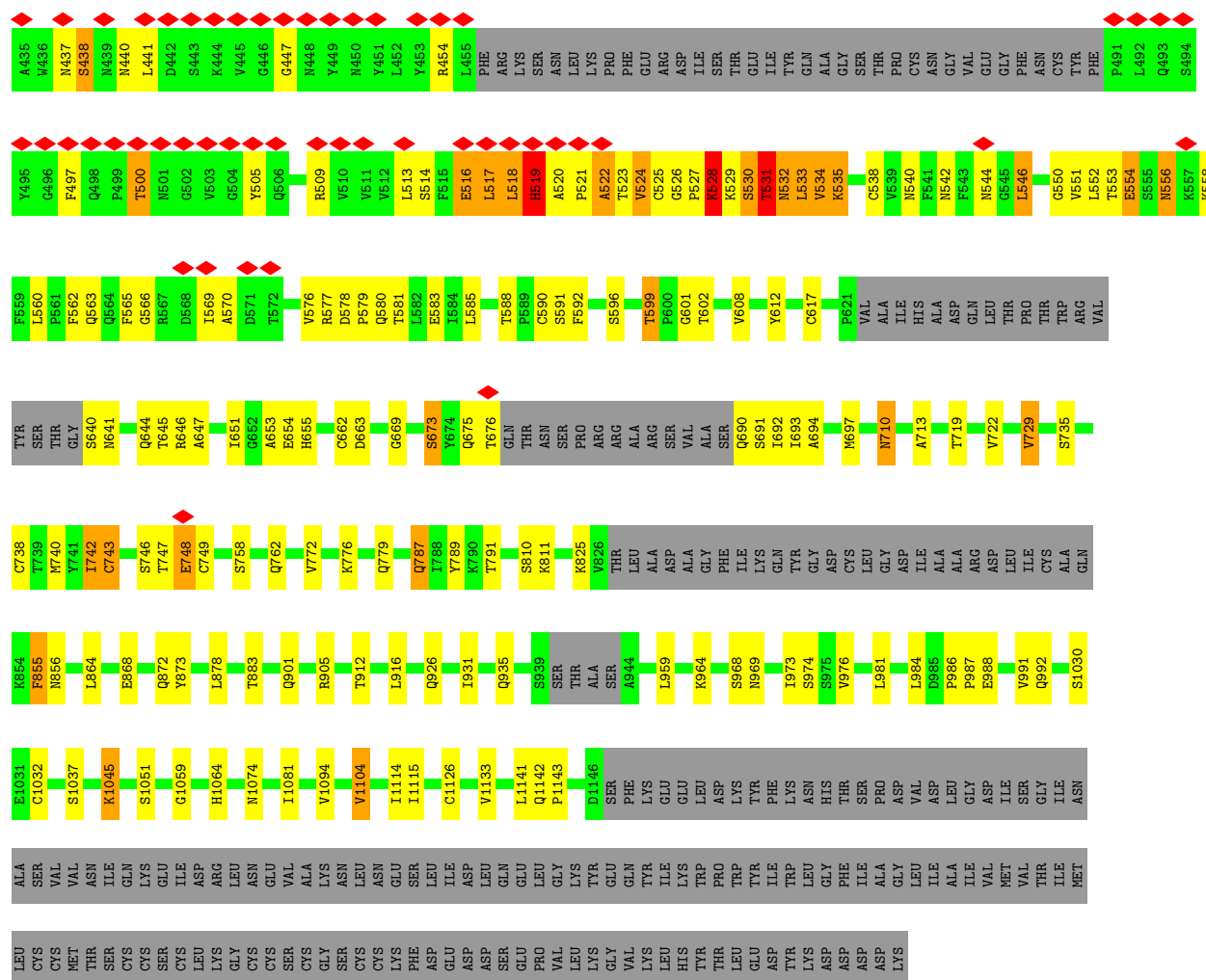


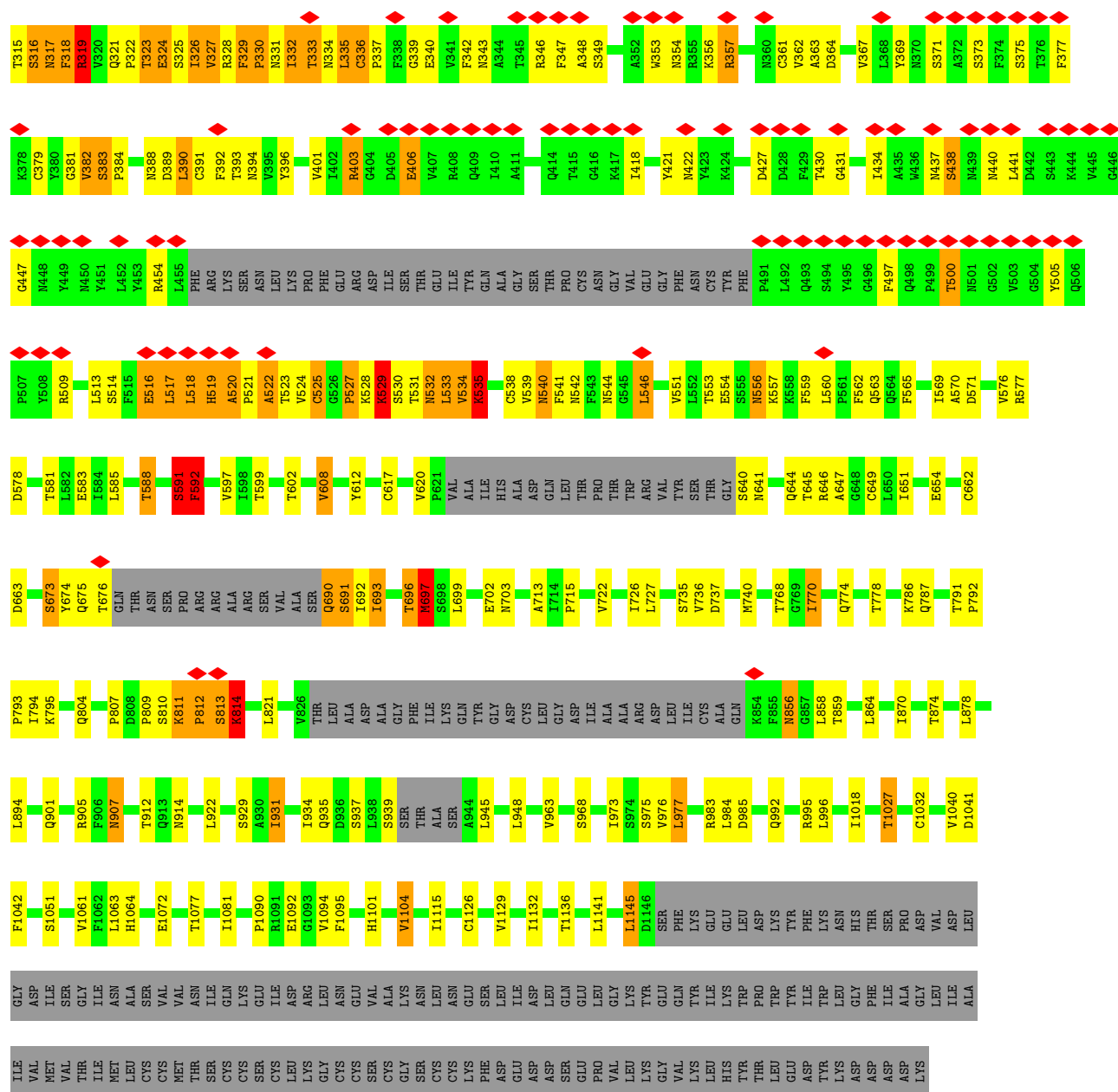
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3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

Continued on next page...

Continued from previous page...

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





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



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





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

Chain F:  100%



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

Chain G:  50% 50%



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

Chain H:  50% 50%



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

Chain I:  50% 50%

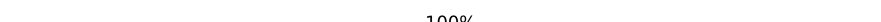


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



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

Chain K:  100% 50% 50%



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



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



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



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



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



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





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



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



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



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



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



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



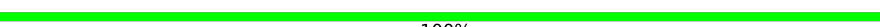


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%



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

Chain Y:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31585	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	1/7757 (0.0%)	0.62	3/10552 (0.0%)
1	B	0.51	0/7751	0.62	3/10544 (0.0%)
1	C	0.51	0/7751	0.61	2/10544 (0.0%)
All	All	0.52	1/23259 (0.0%)	0.62	8/31640 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	SER	CA-C	-6.55	1.44	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	GLN	N-CA-C	-9.05	97.74	110.50
1	A	538	CYS	N-CA-C	-6.20	100.87	110.10
1	B	86	PHE	CA-C-N	5.90	132.81	121.54
1	B	86	PHE	C-N-CA	5.90	132.81	121.54
1	C	86	PHE	CA-C-N	5.86	132.73	121.54
1	C	86	PHE	C-N-CA	5.86	132.73	121.54
1	A	86	PHE	CA-C-N	5.85	132.72	121.54
1	A	86	PHE	C-N-CA	5.85	132.72	121.54

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	7590	0	7409	411	0
1	B	7584	0	7404	376	0
1	C	7584	0	7402	461	0
2	D	28	0	25	0	0
2	E	28	0	25	3	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	3	0
2	L	28	0	25	3	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	3	0
2	T	28	0	25	1	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	1	0
2	X	28	0	25	2	0
2	Y	28	0	25	0	0
3	A	126	0	117	4	0
3	B	140	0	129	8	0
3	C	112	0	104	6	0
All	All	23752	0	23115	1146	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 25.

All (1146) 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)
3:B:1409:NAG:O4	3:B:1410:NAG:C1	1.63	1.45
1:A:41:LYS:HG3	1:C:562:PHE:CD2	1.64	1.31
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.29	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:O	1:B:517:LEU:HD22	1.31	1.26
1:A:329:PHE:CD2	1:A:528:LYS:HB3	1.72	1.23
1:C:392:PHE:CD2	1:C:517:LEU:HD21	1.73	1.23
1:A:328:ARG:NH1	1:A:533:LEU:HG	1.58	1.19
1:A:329:PHE:CE2	1:A:528:LYS:HB3	1.77	1.18
1:C:326:ILE:HD11	1:C:539:VAL:HG11	1.26	1.18
1:C:523:THR:HG22	1:C:524:VAL:H	1.00	1.17
1:C:333:THR:HA	1:C:362:VAL:HG21	1.19	1.15
1:B:328:ARG:HD2	1:B:578:ASP:OD1	1.47	1.14
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.22	1.13
1:A:319:ARG:HG2	1:A:592:PHE:HB2	1.27	1.13
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.13
1:B:392:PHE:HB3	1:B:517:LEU:CD2	1.78	1.12
1:B:392:PHE:CA	1:B:517:LEU:HD11	1.78	1.12
1:B:569:ILE:HG13	1:C:47:VAL:HG11	1.31	1.12
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.19	1.12
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.12
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.27	1.12
1:B:392:PHE:CB	1:B:517:LEU:HD21	1.80	1.10
1:A:523:THR:HG22	1:A:524:VAL:H	1.17	1.10
1:B:748:GLU:HG3	1:B:981:LEU:HD21	1.32	1.08
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.34	1.08
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.37	1.07
1:B:523:THR:HG22	1:B:524:VAL:H	0.96	1.07
1:A:42:VAL:HG23	1:C:519:HIS:HE1	1.19	1.07
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.36	1.07
1:C:529:LYS:H	1:C:529:LYS:HD3	1.18	1.07
1:B:393:THR:CG2	1:B:520:ALA:CB	2.33	1.07
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.36	1.07
1:B:393:THR:HG23	1:B:520:ALA:CB	1.85	1.06
1:B:393:THR:HG21	1:B:520:ALA:HB2	1.35	1.05
1:B:396:TYR:OH	1:C:230:PRO:HB3	1.56	1.05
1:A:391:CYS:SG	1:A:525:CYS:CB	2.44	1.05
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.04
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.87	1.04
1:B:569:ILE:HG12	1:C:47:VAL:HG12	1.39	1.03
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.34	1.03
1:A:391:CYS:SG	1:A:525:CYS:HB3	1.98	1.02
1:C:676:THR:O	1:C:690:GLN:HB3	1.59	1.02
1:B:339:GLY:O	1:B:343:ASN:HB2	1.57	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
1:B:523:THR:HG22	1:B:524:VAL:N	1.71	1.01
1:B:329:PHE:HB3	1:B:330:PRO:CD	1.89	1.01
1:C:333:THR:CA	1:C:362:VAL:HG21	1.88	1.01
1:C:403:ARG:NH1	1:C:505:TYR:HE1	1.58	1.01
1:C:335:LEU:H	1:C:362:VAL:HB	1.21	1.01
3:B:1409:NAG:C4	3:B:1410:NAG:C1	2.38	1.00
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.00
1:C:332:ILE:HD13	1:C:361:CYS:HA	1.39	1.00
1:A:329:PHE:CE2	1:A:528:LYS:HE2	1.96	1.00
1:A:403:ARG:NH1	1:A:505:TYR:HE1	1.58	1.00
1:A:523:THR:HG22	1:A:524:VAL:N	1.75	1.00
1:B:748:GLU:CG	1:B:981:LEU:HD21	1.91	1.00
1:C:44:ARG:O	1:C:283:GLY:HA2	1.61	0.99
1:B:523:THR:CG2	1:B:524:VAL:H	1.74	0.99
1:B:320:VAL:HG23	1:B:591:SER:O	1.61	0.99
1:C:533:LEU:HD12	1:C:534:VAL:H	1.25	0.99
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	0.99
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	0.98
1:B:516:GLU:C	1:B:517:LEU:HD22	1.87	0.98
1:B:392:PHE:HB3	1:B:517:LEU:HD21	0.99	0.98
1:C:329:PHE:CD2	1:C:330:PRO:HD2	1.97	0.98
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:C:319:ARG:HH21	1:C:319:ARG:HB2	1.28	0.98
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.93	0.98
1:B:569:ILE:HG13	1:C:47:VAL:CG1	1.93	0.98
1:C:531:THR:HG22	1:C:532:ASN:H	1.25	0.98
1:B:323:THR:O	1:B:324:GLU:HG2	1.62	0.98
1:B:533:LEU:HD12	1:B:533:LEU:H	1.27	0.98
1:B:392:PHE:HA	1:B:517:LEU:CD1	1.94	0.97
1:B:392:PHE:HA	1:B:517:LEU:HD11	0.98	0.97
1:C:322:PRO:HB3	1:C:538:CYS:SG	2.05	0.97
1:B:569:ILE:CG1	1:C:47:VAL:CG1	2.43	0.97
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.96
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.96
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.96
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.19	0.96
1:A:328:ARG:HH12	1:A:533:LEU:HG	1.25	0.96
1:C:329:PHE:HD2	1:C:330:PRO:HD2	1.29	0.96
1:C:403:ARG:NH1	1:C:505:TYR:CE1	2.33	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:SER:O	1:B:531:THR:O	1.83	0.95
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.47	0.95
1:B:393:THR:CG2	1:B:520:ALA:HB2	1.95	0.95
1:C:357:ARG:HB3	1:C:396:TYR:HE1	1.29	0.95
1:A:41:LYS:CA	1:C:563:GLN:HG2	1.96	0.95
1:C:523:THR:HG22	1:C:524:VAL:N	1.74	0.95
1:B:532:ASN:ND2	1:B:533:LEU:HD12	1.80	0.95
1:A:403:ARG:NH1	1:A:505:TYR:CE1	2.33	0.94
1:C:523:THR:CG2	1:C:524:VAL:H	1.78	0.94
1:B:675:GLN:O	1:B:690:GLN:HG3	1.66	0.94
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.49	0.94
1:B:569:ILE:CG1	1:C:47:VAL:HG12	1.97	0.94
1:C:392:PHE:HD2	1:C:517:LEU:CD2	1.80	0.94
1:C:332:ILE:CD1	1:C:361:CYS:HA	1.98	0.94
1:B:322:PRO:HB3	1:B:538:CYS:SG	2.07	0.94
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.03	0.94
1:A:703:ASN:OD1	1:B:789:TYR:HE1	1.50	0.93
1:B:580:GLN:O	2:K:1:NAG:H83	1.67	0.93
1:A:520:ALA:HB1	1:A:521:PRO:CD	1.97	0.93
1:C:393:THR:O	1:C:523:THR:HG21	1.66	0.93
1:B:519:HIS:O	1:C:41:LYS:HG2	1.69	0.93
1:C:326:ILE:HD11	1:C:539:VAL:CG1	2.00	0.92
1:C:690:GLN:HE21	1:C:690:GLN:HA	1.34	0.92
1:B:328:ARG:HE	1:B:533:LEU:HG	1.32	0.92
1:A:41:LYS:HG3	1:C:562:PHE:HD2	1.16	0.92
1:A:523:THR:CG2	1:A:524:VAL:H	1.82	0.92
1:B:333:THR:HG22	1:B:334:ASN:H	1.35	0.92
1:B:333:THR:HG22	1:B:334:ASN:N	1.83	0.92
1:C:332:ILE:HG23	1:C:333:THR:H	1.34	0.91
1:B:516:GLU:C	1:B:517:LEU:CD2	2.43	0.91
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.53	0.91
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.91
1:A:41:LYS:HG3	1:C:562:PHE:CE2	2.05	0.91
1:C:339:GLY:O	1:C:343:ASN:HB2	1.70	0.90
1:B:319:ARG:NH2	1:C:740:MET:HE2	1.87	0.90
1:C:392:PHE:HA	1:C:517:LEU:CD1	2.01	0.90
1:C:326:ILE:CD1	1:C:539:VAL:HG11	2.02	0.90
1:B:316:SER:O	1:B:317:ASN:ND2	2.03	0.90
1:A:42:VAL:CG2	1:C:519:HIS:HE1	1.84	0.89
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.02	0.89
1:B:393:THR:HG23	1:B:520:ALA:HB3	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PHE:O	1:C:523:THR:HB	1.71	0.89
1:A:319:ARG:CG	1:A:592:PHE:HB2	2.03	0.89
1:A:521:PRO:HB3	1:B:198:ASP:O	1.71	0.89
1:A:42:VAL:HG23	1:C:519:HIS:CE1	2.08	0.88
1:A:329:PHE:HD2	1:A:528:LYS:HB3	1.35	0.88
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.55	0.88
1:A:328:ARG:CZ	1:A:578:ASP:OD2	2.21	0.88
1:B:396:TYR:HE2	1:C:200:TYR:OH	1.54	0.88
1:A:42:VAL:N	1:C:563:GLN:HG2	1.87	0.88
1:C:329:PHE:HD2	1:C:330:PRO:CD	1.87	0.88
1:A:41:LYS:C	1:C:563:GLN:HG2	1.99	0.88
1:A:565:PHE:O	1:B:42:VAL:HA	1.73	0.87
1:B:316:SER:C	1:B:317:ASN:HD22	1.81	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.86
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.57	0.86
1:B:391:CYS:SG	1:B:524:VAL:O	2.33	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:C:388:ASN:OD1	1:C:527:PRO:HD2	1.75	0.85
1:B:328:ARG:CD	1:B:578:ASP:OD1	2.24	0.85
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.85
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.85
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.85
1:C:46:SER:HA	1:C:279:TYR:O	1.76	0.85
1:C:357:ARG:HB3	1:C:396:TYR:CE1	2.11	0.85
1:B:393:THR:O	1:B:523:THR:HG21	1.75	0.85
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.85
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.57	0.85
1:A:327:VAL:O	1:A:531:THR:HB	1.76	0.84
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.57	0.84
1:C:319:ARG:HH21	1:C:319:ARG:CB	1.88	0.84
1:A:319:ARG:HG2	1:A:592:PHE:CB	2.06	0.84
1:C:551:VAL:HB	1:C:588:THR:HG23	1.58	0.84
1:B:393:THR:CG2	1:B:520:ALA:HB3	2.05	0.84
1:B:516:GLU:O	1:B:517:LEU:CD2	2.19	0.83
1:A:335:LEU:HD12	1:A:335:LEU:H	1.41	0.83
1:A:703:ASN:OD1	1:B:789:TYR:CE1	2.32	0.83
1:A:654:GLU:O	1:A:693:ILE:HA	1.79	0.83
1:B:328:ARG:O	1:B:579:PRO:CG	2.27	0.83
1:C:393:THR:HG23	1:C:520:ALA:HB3	1.60	0.83
1:A:41:LYS:CG	1:C:562:PHE:CD2	2.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLY:O	1:B:343:ASN:CB	2.26	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.82
1:C:329:PHE:CD2	1:C:330:PRO:CD	2.62	0.82
1:C:335:LEU:N	1:C:362:VAL:HB	1.94	0.82
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:B:335:LEU:HA	1:B:362:VAL:HB	1.61	0.81
1:B:396:TYR:OH	1:C:230:PRO:CB	2.28	0.81
1:C:318:PHE:CZ	1:C:620:VAL:O	2.33	0.81
1:B:393:THR:HG21	1:B:520:ALA:CB	2.03	0.81
1:A:328:ARG:HG3	1:A:531:THR:O	1.80	0.81
1:C:332:ILE:HG12	1:C:334:ASN:H	1.46	0.81
1:A:41:LYS:HE2	1:C:562:PHE:CE2	2.16	0.80
1:A:328:ARG:NH1	1:A:533:LEU:CG	2.43	0.80
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.80
1:A:329:PHE:HD2	1:A:528:LYS:CB	1.93	0.80
1:B:748:GLU:N	1:B:748:GLU:OE2	2.14	0.80
1:C:654:GLU:HG3	1:C:693:ILE:CG2	2.11	0.80
1:A:326:ILE:HG21	1:A:534:VAL:HG13	1.63	0.80
1:A:336:CYS:HB2	1:A:362:VAL:O	1.82	0.80
1:A:41:LYS:CG	1:C:562:PHE:HD2	1.92	0.79
1:A:41:LYS:HB3	1:C:563:GLN:HA	1.63	0.79
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.65	0.79
1:B:328:ARG:HD2	1:B:578:ASP:CG	2.08	0.79
1:A:390:LEU:HD23	1:A:391:CYS:H	1.48	0.78
1:B:743:CYS:SG	1:B:749:CYS:C	2.66	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.48	0.78
1:A:329:PHE:HE2	1:A:528:LYS:HB3	1.47	0.78
1:B:519:HIS:CE1	1:C:42:VAL:HG23	2.18	0.78
1:B:392:PHE:O	1:B:523:THR:HB	1.83	0.78
1:C:325:SER:C	1:C:326:ILE:HG13	2.09	0.78
1:C:332:ILE:HD11	1:C:334:ASN:HB2	1.63	0.78
1:C:551:VAL:HB	1:C:588:THR:CG2	2.14	0.78
1:B:329:PHE:CB	1:B:330:PRO:HD2	2.09	0.77
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.77
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.77
1:B:319:ARG:NH2	1:C:740:MET:CE	2.47	0.77
1:B:357:ARG:O	1:B:357:ARG:HD3	1.85	0.77
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:C:533:LEU:HD12	1:C:534:VAL:N	1.98	0.76
1:A:363:ALA:O	1:A:527:PRO:HD3	1.86	0.76
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HD3	1:C:532:ASN:O	1.86	0.76
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.76
1:B:390:LEU:HD23	1:B:391:CYS:H	1.49	0.76
1:C:676:THR:HA	1:C:690:GLN:HG3	1.68	0.76
1:C:403:ARG:HH11	1:C:505:TYR:HE1	1.32	0.76
1:B:357:ARG:HH21	1:B:357:ARG:HG2	1.51	0.76
1:C:318:PHE:HZ	1:C:620:VAL:O	1.69	0.76
1:C:735:SER:OG	1:C:859:THR:CG2	2.34	0.76
1:A:41:LYS:CD	1:C:519:HIS:O	2.35	0.75
1:A:538:CYS:SG	1:A:590:CYS:CB	2.75	0.75
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.15	0.75
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.75
1:A:703:ASN:CB	1:B:787:GLN:OE1	2.23	0.75
1:B:519:HIS:HE1	1:C:42:VAL:HG23	1.50	0.75
1:A:854:LYS:C	1:A:855:PHE:HD1	1.95	0.75
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.75
1:A:403:ARG:HH11	1:A:505:TYR:HE1	1.32	0.75
1:A:329:PHE:O	1:A:579:PRO:HG2	1.87	0.74
1:C:47:VAL:O	1:C:49:HIS:N	2.20	0.74
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.74
1:A:43:PHE:CE2	1:C:557:LYS:HD2	2.22	0.74
1:A:391:CYS:HB3	1:A:525:CYS:SG	2.26	0.74
1:B:47:VAL:O	1:B:49:HIS:N	2.20	0.74
1:B:328:ARG:O	1:B:579:PRO:HG3	1.87	0.74
1:A:330:PRO:CA	1:A:579:PRO:HB2	2.18	0.74
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.33	0.74
1:A:654:GLU:HG3	1:A:693:ILE:CG2	2.17	0.74
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.16	0.74
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.74
1:B:528:LYS:HG2	1:B:529:LYS:N	2.02	0.74
1:C:324:GLU:OE2	1:C:325:SER:N	2.21	0.74
1:C:339:GLY:O	1:C:343:ASN:CB	2.36	0.74
1:A:225:PRO:HG2	1:C:562:PHE:CE1	2.23	0.73
1:A:335:LEU:HD12	1:A:335:LEU:N	2.03	0.73
1:B:327:VAL:O	1:B:328:ARG:HG2	1.89	0.73
1:B:532:ASN:ND2	1:B:533:LEU:H	1.85	0.73
1:B:328:ARG:O	1:B:579:PRO:HG2	1.88	0.73
1:C:529:LYS:HD3	1:C:529:LYS:N	1.99	0.73
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.70	0.72
1:B:392:PHE:CD2	1:B:517:LEU:HD21	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
1:C:676:THR:C	1:C:690:GLN:HB3	2.14	0.72
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.72
1:C:322:PRO:CB	1:C:538:CYS:SG	2.77	0.72
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.72
1:C:332:ILE:HG23	1:C:333:THR:N	2.05	0.72
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.72
1:A:592:PHE:CE2	1:B:740:MET:HE1	2.25	0.71
1:A:964:LYS:HE3	1:C:569:ILE:HG22	1.72	0.71
3:B:1409:NAG:H4	3:B:1410:NAG:C1	2.21	0.71
1:B:519:HIS:HE1	1:C:42:VAL:CG2	2.02	0.71
1:A:391:CYS:CB	1:A:525:CYS:SG	2.78	0.71
1:B:357:ARG:HG2	1:B:357:ARG:NH2	2.03	0.71
1:B:532:ASN:ND2	1:B:533:LEU:CD1	2.53	0.71
1:A:983:ARG:O	1:C:382:VAL:HA	1.91	0.71
1:B:319:ARG:HH22	1:C:740:MET:HE2	1.54	0.71
1:A:535:LYS:HG2	1:A:536:ASN:OD1	1.91	0.71
1:A:41:LYS:CB	1:C:563:GLN:HG2	2.20	0.70
1:A:124:THR:HG21	3:A:1402:NAG:HN2	1.56	0.70
1:C:323:THR:C	1:C:324:GLU:HG3	2.16	0.70
1:B:335:LEU:HD22	1:B:335:LEU:C	2.17	0.70
1:C:124:THR:HG21	3:C:1402:NAG:HN2	1.56	0.70
1:C:531:THR:HG22	1:C:532:ASN:N	2.03	0.70
1:B:124:THR:HG21	3:B:1402:NAG:HN2	1.56	0.70
1:A:963:VAL:HG12	1:C:570:ALA:CB	2.21	0.70
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.70
1:A:327:VAL:O	1:A:531:THR:N	2.24	0.70
1:B:326:ILE:O	1:B:326:ILE:HG13	1.92	0.69
1:B:533:LEU:HD12	1:B:533:LEU:N	2.03	0.69
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69
1:A:41:LYS:HB3	1:C:563:GLN:HG2	1.73	0.69
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.69
1:C:332:ILE:HD13	1:C:361:CYS:CA	2.20	0.69
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.69
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.69
1:A:41:LYS:HD3	1:C:519:HIS:O	1.93	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
1:A:328:ARG:C	1:A:329:PHE:HD1	2.01	0.69
1:B:392:PHE:CG	1:B:517:LEU:HD21	2.27	0.69
1:A:592:PHE:CD2	1:B:740:MET:HE1	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.69
1:C:393:THR:HG23	1:C:520:ALA:CB	2.22	0.68
1:C:674:TYR:HA	1:C:691:SER:O	1.93	0.68
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.74	0.68
1:C:662:CYS:HB2	1:C:697:MET:CE	2.23	0.68
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.68
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.29	0.68
1:C:44:ARG:O	1:C:283:GLY:CA	2.40	0.68
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.68
1:A:533:LEU:HD13	1:A:533:LEU:O	1.93	0.67
1:A:327:VAL:O	1:A:531:THR:CB	2.41	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:B:396:TYR:HE2	1:C:200:TYR:HH	0.74	0.67
1:C:532:ASN:C	1:C:532:ASN:HD22	2.02	0.67
1:A:675:GLN:O	1:A:690:GLN:HG3	1.94	0.67
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.10	0.67
1:C:522:ALA:O	1:C:523:THR:OG1	2.13	0.67
1:B:551:VAL:HB	1:B:588:THR:CG2	2.25	0.67
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.67
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.67
1:C:335:LEU:HA	1:C:362:VAL:O	1.95	0.67
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.66
1:B:388:ASN:OD1	1:B:527:PRO:HD3	1.95	0.66
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.76	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:C:529:LYS:H	1:C:529:LYS:CD	2.03	0.66
1:A:329:PHE:HE2	1:A:528:LYS:HE2	1.59	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.61	0.66
1:B:570:ALA:CB	1:C:963:VAL:CG1	2.74	0.66
1:B:570:ALA:CB	1:C:963:VAL:HG12	2.26	0.66
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.66
1:C:675:GLN:O	1:C:690:GLN:CG	2.43	0.66
1:A:535:LYS:HE3	1:A:554:GLU:OE2	1.96	0.66
1:C:329:PHE:CB	1:C:330:PRO:CD	2.70	0.66
1:C:569:ILE:H	1:C:569:ILE:HD12	1.60	0.66
1:C:363:ALA:O	1:C:527:PRO:HD3	1.96	0.66
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.66
1:A:569:ILE:HD12	1:A:569:ILE:H	1.61	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:A:669:GLY:N	1:B:864:LEU:O	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.66
1:B:516:GLU:C	1:B:517:LEU:HD23	2.21	0.66
1:B:538:CYS:HG	1:B:590:CYS:HG	0.70	0.66
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.68	0.65
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.65
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.65
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.65
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.65
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.65
1:B:580:GLN:O	2:K:1:NAG:C8	2.43	0.65
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.65
1:B:558:LYS:HZ2	3:C:1405:NAG:HN2	1.45	0.65
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.79	0.65
1:A:41:LYS:CA	1:C:563:GLN:CG	2.75	0.65
1:B:329:PHE:CD1	1:B:528:LYS:HB2	2.32	0.65
1:C:388:ASN:OD1	1:C:527:PRO:CD	2.44	0.65
1:A:41:LYS:HE3	1:A:41:LYS:H	1.61	0.65
1:A:43:PHE:HE2	1:C:557:LYS:HD2	1.61	0.65
1:C:333:THR:CA	1:C:362:VAL:CG2	2.70	0.65
1:C:690:GLN:HE21	1:C:690:GLN:CA	2.06	0.64
1:B:558:LYS:NZ	3:C:1405:NAG:HN2	1.95	0.64
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.19	0.64
1:C:393:THR:CG2	1:C:520:ALA:HB3	2.25	0.64
1:A:42:VAL:CG2	1:C:519:HIS:CE1	2.74	0.64
1:A:534:VAL:HG23	1:A:535:LYS:N	2.11	0.64
1:B:396:TYR:CE2	1:C:200:TYR:OH	2.37	0.64
1:B:396:TYR:HH	1:C:230:PRO:HB3	1.58	0.64
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.64
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.64
1:B:551:VAL:HB	1:B:588:THR:HG22	1.79	0.64
1:A:41:LYS:HA	1:C:563:GLN:CG	2.28	0.64
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.64
1:A:324:GLU:O	1:A:324:GLU:HG2	1.96	0.64
1:A:535:LYS:CE	1:A:554:GLU:OE2	2.46	0.63
1:C:332:ILE:HG23	1:C:362:VAL:HG23	1.79	0.63
1:A:43:PHE:CE1	1:A:282:ASN:O	2.51	0.63
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.63
1:C:676:THR:C	1:C:690:GLN:CB	2.71	0.63
1:A:319:ARG:HH21	1:A:319:ARG:HG3	1.63	0.63
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LYS:CE	1:C:569:ILE:HG22	2.28	0.63
1:C:392:PHE:CA	1:C:517:LEU:HD11	2.15	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:A:329:PHE:CE2	1:A:528:LYS:CE	2.78	0.63
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.63
1:C:393:THR:CG2	1:C:520:ALA:CB	2.77	0.63
1:A:41:LYS:HE2	1:C:562:PHE:HE2	1.64	0.63
1:A:41:LYS:HD2	1:C:519:HIS:O	1.96	0.63
1:A:533:LEU:H	1:A:533:LEU:CD1	2.11	0.63
1:A:43:PHE:HE1	1:A:282:ASN:O	1.82	0.62
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.62
1:C:43:PHE:CE1	1:C:282:ASN:O	2.52	0.62
1:A:700:GLY:O	1:A:701:ALA:O	2.17	0.62
1:B:570:ALA:HB1	1:C:963:VAL:CG1	2.29	0.62
1:A:41:LYS:HB3	1:C:563:GLN:CG	2.29	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:A:326:ILE:O	1:A:326:ILE:HG13	1.99	0.62
1:C:318:PHE:O	1:C:319:ARG:HB2	1.99	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:C:521:PRO:O	1:C:522:ALA:HB2	1.99	0.62
1:C:534:VAL:HG23	1:C:535:LYS:N	2.14	0.62
1:C:43:PHE:HE1	1:C:282:ASN:O	1.83	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.82	0.62
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.62
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.62
1:C:516:GLU:C	1:C:517:LEU:HD22	2.24	0.62
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.81	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.61
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.32	0.61
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.81	0.61
1:B:392:PHE:CA	1:B:517:LEU:CD1	2.68	0.61
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.61
1:A:854:LYS:NZ	1:A:855:PHE:CE1	2.60	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:B:570:ALA:HB1	1:C:963:VAL:HG12	1.83	0.61
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:CYS:HG	1:A:525:CYS:CB	2.05	0.61
1:C:528:LYS:C	1:C:530:SER:H	2.08	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:A:983:ARG:CB	1:C:382:VAL:HB	2.31	0.61
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.61
1:C:334:ASN:O	1:C:335:LEU:HB3	1.99	0.61
1:B:528:LYS:O	1:B:529:LYS:HD3	2.00	0.60
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.60
1:B:322:PRO:CB	1:B:538:CYS:SG	2.86	0.60
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.60
1:B:987:PRO:HG3	1:C:427:ASP:OD2	2.01	0.60
1:C:556:ASN:HD22	1:C:556:ASN:H	1.49	0.60
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:C:326:ILE:CD1	1:C:539:VAL:CG1	2.71	0.60
1:A:329:PHE:CZ	1:A:528:LYS:HE2	2.35	0.60
1:A:533:LEU:O	1:A:533:LEU:HD22	2.01	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:C:532:ASN:HD22	1:C:533:LEU:N	2.00	0.60
1:A:321:GLN:HB3	1:A:322:PRO:HD2	1.83	0.60
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.84	0.60
1:A:983:ARG:O	1:C:381:GLY:O	2.20	0.59
1:B:329:PHE:HD2	1:B:525:CYS:SG	2.25	0.59
1:B:556:ASN:H	1:B:556:ASN:HD22	1.49	0.59
1:A:225:PRO:CG	1:C:562:PHE:CZ	2.84	0.59
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:A:319:ARG:CG	1:A:319:ARG:HH21	2.14	0.59
1:A:556:ASN:HD22	1:A:556:ASN:H	1.50	0.59
1:B:357:ARG:HH21	1:B:357:ARG:CG	2.15	0.59
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.59
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.59
1:C:516:GLU:O	1:C:517:LEU:HD22	2.03	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:B:327:VAL:HG12	1:B:328:ARG:N	2.16	0.59
1:B:329:PHE:CG	1:B:528:LYS:HE3	2.38	0.59
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.59
1:C:328:ARG:HE	1:C:533:LEU:HD22	1.67	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:A:41:LYS:HE3	1:A:41:LYS:N	2.18	0.59
1:C:319:ARG:HH21	1:C:319:ARG:CG	2.14	0.59
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.59
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:B:319:ARG:HH21	1:C:740:MET:CE	2.15	0.58
1:B:524:VAL:HG22	1:B:525:CYS:N	2.17	0.58
1:B:530:SER:O	1:B:531:THR:C	2.46	0.58
1:B:738:CYS:O	1:B:742:ILE:HG13	2.03	0.58
1:A:552:LEU:HD23	1:A:587:ILE:HG12	1.85	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.58
1:A:327:VAL:CG1	1:A:329:PHE:CE1	2.85	0.58
3:B:1405:NAG:H83	3:B:1405:NAG:H3	1.86	0.58
1:C:326:ILE:HD12	1:C:541:PHE:HB3	1.86	0.58
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.58
1:B:335:LEU:HD13	1:B:335:LEU:N	2.18	0.58
1:B:534:VAL:HG23	1:B:535:LYS:N	2.18	0.58
3:A:1405:NAG:H3	3:A:1405:NAG:H83	1.86	0.58
1:B:391:CYS:SG	1:B:523:THR:O	2.61	0.58
1:A:225:PRO:HG3	1:C:562:PHE:CZ	2.38	0.58
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.58
2:W:2:NAG:H3	2:W:2:NAG:H83	1.86	0.58
1:B:526:GLY:O	1:B:528:LYS:NZ	2.37	0.58
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.58
1:A:654:GLU:O	1:A:693:ILE:CA	2.51	0.58
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.58
1:A:533:LEU:H	1:A:533:LEU:HD12	1.69	0.57
1:B:521:PRO:O	1:B:522:ALA:HB2	2.03	0.57
1:B:655:HIS:HD2	1:B:694:ALA:O	1.86	0.57
1:C:322:PRO:CA	1:C:538:CYS:SG	2.92	0.57
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:C:332:ILE:HD11	1:C:334:ASN:CB	2.33	0.57
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.57
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.57
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
1:A:393:THR:HA	1:A:523:THR:HB	1.87	0.57
1:C:328:ARG:CZ	1:C:578:ASP:OD2	2.52	0.57
1:B:41:LYS:O	1:B:42:VAL:HB	2.05	0.57
1:C:324:GLU:OE2	1:C:539:VAL:HG23	2.05	0.57
1:C:516:GLU:O	1:C:516:GLU:HG3	2.02	0.57
1:C:528:LYS:O	1:C:530:SER:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.57
3:C:1405:NAG:H3	3:C:1405:NAG:H83	1.86	0.57
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.57
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.57
1:A:521:PRO:HG3	1:B:199:GLY:HA3	1.87	0.57
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.57
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.57
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
1:C:342:PHE:HB3	2:S:1:NAG:H82	1.87	0.57
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.57
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.57
1:B:396:TYR:OH	1:C:200:TYR:CE1	2.57	0.57
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.57
2:X:2:NAG:H83	2:X:2:NAG:H3	1.87	0.57
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.56
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.56
1:C:675:GLN:O	1:C:690:GLN:HG3	2.05	0.56
1:C:735:SER:OG	1:C:859:THR:HG23	2.04	0.56
1:A:41:LYS:HG2	1:C:562:PHE:O	2.05	0.56
1:A:42:VAL:H	1:C:563:GLN:HG2	1.68	0.56
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.56
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:538:CYS:SG	1:A:590:CYS:HB3	2.44	0.56
1:A:983:ARG:HB2	1:C:382:VAL:HB	1.87	0.56
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.56
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.86	0.56
1:C:321:GLN:HA	1:C:321:GLN:OE1	2.04	0.56
1:A:535:LYS:HB2	1:A:535:LYS:HZ2	1.68	0.56
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:A:854:LYS:NZ	1:A:855:PHE:CZ	2.72	0.56
1:B:532:ASN:HD21	1:B:533:LEU:HD12	1.69	0.56
1:B:563:GLN:O	1:B:577:ARG:NH1	2.38	0.56
1:A:334:ASN:HB3	1:A:362:VAL:HG23	1.86	0.56
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.56
1:A:328:ARG:C	1:A:329:PHE:CD1	2.83	0.56
1:A:342:PHE:HB3	2:E:1:NAG:H82	1.87	0.56
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:HG2	1:A:536:ASN:CG	2.31	0.56
1:A:963:VAL:HG12	1:C:570:ALA:HB1	1.88	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:535:LYS:HG2	1:B:552:LEU:O	2.06	0.56
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.86	0.56
1:C:592:PHE:N	1:C:592:PHE:CD1	2.73	0.56
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.40	0.56
1:A:854:LYS:O	1:A:855:PHE:HD1	1.88	0.56
1:C:45:SER:O	1:C:279:TYR:HB2	2.05	0.56
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.56
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.56
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.56
1:B:385:THR:HG1	1:B:386:LYS:HZ3	1.54	0.56
1:B:523:THR:O	1:B:524:VAL:O	2.24	0.56
1:C:45:SER:HA	1:C:280:ASN:O	2.06	0.56
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.55
1:A:329:PHE:CD1	1:A:329:PHE:N	2.73	0.55
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.55
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.55
1:A:326:ILE:CD1	1:A:533:LEU:HA	2.37	0.55
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.55
1:B:342:PHE:HB3	2:L:1:NAG:H82	1.87	0.55
1:B:353:TRP:H	1:B:353:TRP:CD1	2.23	0.55
1:C:326:ILE:HD11	1:C:539:VAL:HG21	1.88	0.55
1:C:332:ILE:CD1	1:C:334:ASN:HB2	2.32	0.55
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.55
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.70	0.55
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.55
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.55
1:A:366:SER:N	1:A:388:ASN:HD21	2.04	0.55
1:C:318:PHE:HB3	1:C:592:PHE:O	2.06	0.55
1:C:534:VAL:O	1:C:535:LYS:HD3	2.07	0.55
1:A:41:LYS:H	1:A:41:LYS:CE	2.20	0.55
1:C:29:THR:HG22	1:C:30:ASN:H	1.70	0.55
2:L:1:NAG:H61	2:L:2:NAG:HN2	1.71	0.55
1:A:521:PRO:O	1:A:522:ALA:HB2	2.07	0.55
1:A:675:GLN:O	1:A:690:GLN:CG	2.55	0.55
1:C:690:GLN:HA	1:C:690:GLN:NE2	2.15	0.55
2:H:2:NAG:H3	2:H:2:NAG:H83	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:CA	1:C:362:VAL:O	2.55	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
2:S:1:NAG:H61	2:S:2:NAG:HN2	1.72	0.55
1:B:676:THR:C	1:B:691:SER:H	2.15	0.55
1:C:332:ILE:CG2	1:C:333:THR:H	2.14	0.55
1:A:328:ARG:NE	1:A:578:ASP:OD1	2.40	0.54
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.54
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.54
1:B:748:GLU:HG3	1:B:981:LEU:CD2	2.23	0.54
1:A:324:GLU:O	1:A:539:VAL:CG2	2.56	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:B:388:ASN:OD1	1:B:527:PRO:CD	2.55	0.54
1:A:327:VAL:CG1	1:A:329:PHE:HE1	2.21	0.54
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.54
1:A:523:THR:O	1:A:524:VAL:O	2.25	0.54
1:B:329:PHE:CB	1:B:330:PRO:CD	2.66	0.54
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.54
1:A:520:ALA:CB	1:A:521:PRO:CD	2.71	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:B:519:HIS:HB3	1:C:41:LYS:HD3	1.90	0.54
1:C:534:VAL:C	1:C:535:LYS:HG2	2.30	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
2:E:1:NAG:H61	2:E:2:NAG:HN2	1.72	0.54
1:B:532:ASN:HD21	1:B:533:LEU:CD1	2.19	0.54
1:C:329:PHE:CD2	1:C:330:PRO:HD3	2.43	0.54
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54
1:B:748:GLU:HG2	1:B:981:LEU:HD21	1.83	0.54
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
1:A:329:PHE:CB	1:A:330:PRO:CD	2.70	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.42	0.54
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.54
1:C:337:PRO:C	1:C:339:GLY:H	2.16	0.54
1:B:328:ARG:HH21	1:B:532:ASN:HD22	1.54	0.53
1:B:528:LYS:CG	1:B:529:LYS:N	2.68	0.53
1:B:310:LYS:HA	1:B:599:THR:O	2.08	0.53
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.53
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HE2	1:C:562:PHE:CD2	2.42	0.53
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.53
1:A:576:VAL:HG22	1:A:587:ILE:HD11	1.90	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:B:535:LYS:HD2	1:B:554:GLU:OE2	2.08	0.53
1:B:556:ASN:HD22	1:B:556:ASN:N	2.05	0.53
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.53
1:A:225:PRO:CG	1:C:562:PHE:CE1	2.91	0.53
1:A:552:LEU:CD2	1:A:587:ILE:HG12	2.39	0.53
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.53
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.53
1:C:530:SER:OG	1:C:531:THR:N	2.42	0.53
1:C:532:ASN:O	1:C:533:LEU:CB	2.56	0.53
1:A:327:VAL:C	1:A:531:THR:HB	2.34	0.53
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.53
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:B:329:PHE:CD2	1:B:525:CYS:SG	3.02	0.53
1:C:41:LYS:O	1:C:42:VAL:HB	2.09	0.53
1:C:316:SER:OG	1:C:317:ASN:N	2.38	0.53
1:A:983:ARG:HA	1:C:382:VAL:HG23	1.90	0.53
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.53
1:C:331:ASN:O	1:C:332:ILE:HB	2.09	0.53
1:A:316:SER:OG	1:A:317:ASN:N	2.41	0.53
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.53
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.52
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.52
1:A:41:LYS:O	1:A:42:VAL:HB	2.08	0.52
1:B:334:ASN:O	1:B:335:LEU:HB3	2.09	0.52
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.52
1:C:332:ILE:HG12	1:C:334:ASN:N	2.22	0.52
2:G:2:NAG:H83	2:G:2:NAG:H3	1.90	0.52
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.44	0.52
1:A:43:PHE:HB2	1:C:559:PHE:CD1	2.45	0.52
1:A:327:VAL:HG12	1:A:329:PHE:CE1	2.44	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52
1:C:1101:HIS:CD2	2:X:1:NAG:H5	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.52
1:C:403:ARG:NH1	1:C:505:TYR:CD1	2.78	0.52
1:A:535:LYS:NZ	1:A:535:LYS:CB	2.73	0.52
1:A:694:ALA:O	1:A:695:TYR:HB3	2.10	0.52
1:A:319:ARG:HB3	1:A:319:ARG:CZ	2.40	0.51
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.51
1:A:521:PRO:HD3	1:B:199:GLY:HA3	1.93	0.51
1:B:393:THR:N	1:B:517:LEU:HD13	2.24	0.51
1:B:570:ALA:HB2	1:C:963:VAL:HG12	1.92	0.51
1:C:332:ILE:HG23	1:C:362:VAL:CG2	2.39	0.51
1:A:388:ASN:OD1	1:A:388:ASN:N	2.42	0.51
1:A:964:LYS:HE3	1:C:569:ILE:CG2	2.38	0.51
1:B:316:SER:C	1:B:317:ASN:ND2	2.62	0.51
1:C:591:SER:C	1:C:592:PHE:HD1	2.18	0.51
1:A:319:ARG:CZ	1:A:319:ARG:CB	2.88	0.51
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.51
1:A:963:VAL:HG12	1:C:570:ALA:HB2	1.93	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.51
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.51
1:A:533:LEU:CD1	1:A:533:LEU:N	2.73	0.51
1:B:524:VAL:CG2	1:B:525:CYS:N	2.73	0.51
1:C:324:GLU:OE2	1:C:539:VAL:CG2	2.59	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51
1:B:329:PHE:CD2	1:B:528:LYS:HE3	2.44	0.51
1:B:392:PHE:HD2	1:B:517:LEU:CD2	2.24	0.51
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.51
1:C:388:ASN:CG	1:C:527:PRO:HD2	2.36	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:A:705:VAL:HB	1:B:883:THR:HG21	1.93	0.51
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.51
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
1:B:335:LEU:N	1:B:335:LEU:CD1	2.74	0.51
1:B:528:LYS:C	1:B:529:LYS:HG2	2.36	0.51
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.51
1:B:392:PHE:CD2	1:B:517:LEU:CD2	2.94	0.50
1:C:516:GLU:C	1:C:517:LEU:CD2	2.84	0.50
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.50
2:P:1:NAG:H62	2:P:2:NAG:H2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.12	0.50
1:A:328:ARG:NH1	1:A:533:LEU:HB3	2.27	0.50
1:B:654:GLU:HG3	1:B:693:ILE:HG22	1.94	0.50
1:A:319:ARG:CG	1:A:319:ARG:NH2	2.73	0.50
1:A:676:THR:C	1:A:690:GLN:HB3	2.37	0.50
1:B:327:VAL:CG1	1:B:328:ARG:N	2.74	0.50
1:B:523:THR:CG2	1:B:524:VAL:N	2.44	0.50
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.50
1:C:393:THR:O	1:C:523:THR:CG2	2.51	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.77	0.50
1:A:327:VAL:HG13	1:A:329:PHE:HE1	1.77	0.50
1:A:523:THR:O	1:A:524:VAL:C	2.55	0.50
1:A:740:MET:HE1	1:C:592:PHE:CD2	2.46	0.50
1:B:319:ARG:HG3	1:B:592:PHE:HB2	1.94	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.50
1:C:335:LEU:C	1:C:362:VAL:O	2.55	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
1:A:403:ARG:NH1	1:A:505:TYR:CD1	2.78	0.49
1:B:396:TYR:OH	1:C:200:TYR:HE1	1.94	0.49
1:C:533:LEU:CD1	1:C:534:VAL:N	2.73	0.49
1:B:580:GLN:O	2:K:1:NAG:C7	2.60	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.49
1:B:396:TYR:HH	1:C:200:TYR:HE1	1.50	0.49
1:C:391:CYS:SG	1:C:523:THR:O	2.70	0.49
1:A:41:LYS:C	1:C:563:GLN:HE21	2.21	0.49
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.49
1:A:524:VAL:HG22	1:A:525:CYS:N	2.28	0.49
1:A:592:PHE:HZ	1:B:855:PHE:O	1.96	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:B:308:VAL:O	1:B:601:GLY:HA2	2.12	0.49
1:B:313:TYR:O	1:B:596:SER:HA	2.13	0.49
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.49
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.49
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.49
1:C:534:VAL:C	1:C:535:LYS:CG	2.85	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.49
1:C:122:ASN:OD1	1:C:122:ASN:N	2.46	0.49
1:C:319:ARG:HB2	1:C:319:ARG:NH2	2.11	0.49
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.49
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.49
1:C:326:ILE:HG21	1:C:533:LEU:HA	1.94	0.49
1:A:393:THR:CA	1:A:523:THR:HB	2.43	0.49
1:A:521:PRO:CG	1:B:199:GLY:HA3	2.42	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:B:335:LEU:C	1:B:362:VAL:O	2.56	0.49
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.49
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.48
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.48
1:B:517:LEU:CD2	1:B:517:LEU:N	2.73	0.48
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.48
1:A:331:ASN:O	1:A:333:THR:N	2.46	0.48
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.48
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.48
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.48
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.48
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:B:519:HIS:ND1	1:C:41:LYS:HB2	2.29	0.48
1:C:676:THR:O	1:C:690:GLN:CB	2.46	0.48
1:C:325:SER:C	1:C:326:ILE:CG1	2.85	0.48
1:A:328:ARG:CZ	1:A:578:ASP:CG	2.87	0.48
1:A:393:THR:O	1:A:523:THR:CB	2.61	0.48
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.94	0.48
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.77	0.48
1:B:327:VAL:CG1	1:B:329:PHE:HD1	2.25	0.48
1:B:332:ILE:HG12	1:B:333:THR:N	2.27	0.48
1:A:319:ARG:CB	1:A:319:ARG:NH2	2.77	0.48
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.48
1:C:675:GLN:O	1:C:690:GLN:HG2	2.14	0.48
1:A:522:ALA:O	1:A:523:THR:OG1	2.27	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
1:A:41:LYS:N	1:A:41:LYS:CE	2.77	0.47
1:A:42:VAL:N	1:C:563:GLN:CG	2.70	0.47
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:C:690:GLN:CA	1:C:690:GLN:NE2	2.77	0.47
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.47
1:B:566:GLY:HA2	1:C:43:PHE:HB3	1.95	0.47
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.44	0.47
1:A:328:ARG:HH11	1:A:533:LEU:HG	1.63	0.47
1:A:388:ASN:CB	1:A:527:PRO:HD2	2.38	0.47
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.47
1:A:531:THR:HG22	1:A:532:ASN:N	2.29	0.47
1:A:985:ASP:OD1	1:A:985:ASP:N	2.45	0.47
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.47
1:C:333:THR:H	1:C:362:VAL:CG2	2.28	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.47
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.47
1:A:592:PHE:CE2	1:B:740:MET:CE	2.95	0.47
1:B:335:LEU:HA	1:B:362:VAL:O	2.14	0.47
1:B:560:LEU:O	1:B:562:PHE:N	2.47	0.47
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.47
1:C:326:ILE:HD11	1:C:539:VAL:CG2	2.45	0.47
1:A:393:THR:O	1:A:523:THR:HG21	2.14	0.47
1:A:524:VAL:C	1:A:525:CYS:SG	2.97	0.47
1:A:535:LYS:HB2	1:A:535:LYS:NZ	2.29	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.47
1:A:328:ARG:NH1	1:A:533:LEU:CB	2.78	0.47
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.79	0.47
1:C:333:THR:N	1:C:362:VAL:CG2	2.78	0.47
1:C:319:ARG:CG	1:C:319:ARG:NH2	2.73	0.47
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.47
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.47
1:C:528:LYS:C	1:C:530:SER:N	2.73	0.47
1:A:327:VAL:H	1:A:531:THR:HB	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.98	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:364:ASP:O	1:B:367:VAL:HG12	2.16	0.46
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:A:385:THR:HG1	1:A:386:LYS:HZ3	1.59	0.46
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.46
1:B:335:LEU:C	1:B:335:LEU:CD2	2.87	0.46
1:B:654:GLU:O	1:B:693:ILE:HA	2.15	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.46
1:A:328:ARG:HD3	1:A:580:GLN:HG3	1.97	0.46
1:A:392:PHE:O	1:A:523:THR:HB	2.15	0.46
1:B:570:ALA:HB2	1:C:963:VAL:CG1	2.46	0.46
1:A:854:LYS:C	1:A:855:PHE:CD1	2.86	0.46
1:B:325:SER:C	1:B:326:ILE:HG23	2.40	0.46
1:B:533:LEU:C	1:B:534:VAL:HG13	2.40	0.46
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
1:A:324:GLU:O	1:A:539:VAL:HG23	2.15	0.46
1:A:534:VAL:O	1:A:535:LYS:HB2	2.15	0.46
1:B:533:LEU:CD1	1:B:533:LEU:N	2.73	0.46
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.46
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.46
1:B:328:ARG:HE	1:B:533:LEU:CG	2.17	0.46
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.46
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.46
1:C:393:THR:HG21	1:C:520:ALA:HB2	1.96	0.46
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.46
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.46
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:A:535:LYS:HG2	1:A:536:ASN:N	2.30	0.46
1:B:500:THR:O	1:B:500:THR:OG1	2.31	0.46
1:B:528:LYS:O	1:B:529:LYS:HG2	2.16	0.46
1:C:533:LEU:C	1:C:534:VAL:HG13	2.41	0.46
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.46
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.46
1:C:45:SER:O	1:C:279:TYR:CB	2.64	0.46
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.46
1:B:516:GLU:HG2	1:C:200:TYR:OH	2.16	0.46
1:C:326:ILE:C	1:C:327:VAL:HG23	2.41	0.46
1:A:329:PHE:HE2	1:A:528:LYS:CB	2.20	0.45
1:A:520:ALA:CB	1:A:521:PRO:HD2	2.18	0.45
1:A:535:LYS:CG	1:A:536:ASN:OD1	2.63	0.45
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.45
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.45
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.45
1:C:334:ASN:C	1:C:336:CYS:H	2.24	0.45
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.45
1:C:517:LEU:CD2	1:C:517:LEU:N	2.79	0.45
1:A:576:VAL:CG2	1:A:587:ILE:HD11	2.46	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
1:B:322:PRO:CG	1:B:538:CYS:SG	3.04	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.97	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
1:C:333:THR:N	1:C:362:VAL:HG21	2.31	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
1:C:696:THR:O	1:C:697:MET:C	2.56	0.45
1:A:41:LYS:CD	1:A:41:LYS:H	2.29	0.45
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.41	0.45
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.45
1:B:127:VAL:HG11	3:B:1402:NAG:H61	1.98	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.78	0.45
1:B:316:SER:OG	1:B:317:ASN:N	2.49	0.45
1:B:393:THR:HA	1:B:523:THR:HB	1.97	0.45
1:C:127:VAL:HG11	3:C:1402:NAG:H61	1.98	0.45
1:C:646:ARG:HG3	1:C:646:ARG:O	2.17	0.45
1:A:325:SER:HB2	1:A:540:ASN:HB3	1.98	0.45
1:A:326:ILE:HD12	1:A:533:LEU:HA	1.98	0.45
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:323:THR:O	1:C:324:GLU:HG3	2.17	0.45
1:C:674:TYR:CE1	1:C:691:SER:HA	2.51	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:327:VAL:N	1:A:531:THR:HB	2.32	0.45
1:A:592:PHE:O	1:A:592:PHE:CG	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:OE2	1:A:534:VAL:HG11	2.16	0.45
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.57	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
1:A:127:VAL:HG11	3:A:1402:NAG:H61	1.98	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.45
1:B:388:ASN:CG	1:B:527:PRO:CD	2.90	0.45
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.44
1:A:321:GLN:HA	1:A:321:GLN:OE1	2.16	0.44
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.44
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.44
1:C:316:SER:C	1:C:317:ASN:CG	2.85	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:C:532:ASN:O	1:C:533:LEU:HB2	2.17	0.44
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.44
1:B:335:LEU:O	1:B:362:VAL:O	2.34	0.44
1:B:518:LEU:O	1:B:519:HIS:CD2	2.71	0.44
1:B:550:GLY:HA2	1:B:590:CYS:SG	2.57	0.44
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.44
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.44
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.44
1:B:382:VAL:HA	1:C:983:ARG:O	2.18	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:C:392:PHE:CB	1:C:517:LEU:CD2	2.68	0.44
1:C:393:THR:HG21	1:C:520:ALA:CB	2.47	0.44
1:A:328:ARG:HH11	1:A:533:LEU:HB3	1.81	0.44
1:B:333:THR:CG2	1:B:334:ASN:N	2.55	0.44
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.44
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.44
1:A:391:CYS:CB	1:A:525:CYS:HB3	2.48	0.44
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.44
1:B:592:PHE:O	1:B:592:PHE:CD1	2.70	0.44
1:C:326:ILE:O	1:C:327:VAL:HG23	2.16	0.44
1:C:392:PHE:CA	1:C:517:LEU:CD1	2.85	0.44
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.44
1:B:653:ALA:CB	1:B:692:ILE:HG22	2.48	0.44
1:C:393:THR:HA	1:C:523:THR:HB	2.00	0.44
1:A:392:PHE:O	1:A:523:THR:N	2.51	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.44
1:B:669:GLY:N	1:C:864:LEU:O	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.44
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.44
2:L:1:NAG:H61	2:L:2:NAG:N2	2.33	0.44
1:A:535:LYS:HE2	1:A:554:GLU:OE2	2.18	0.43
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.43
1:B:655:HIS:CD2	1:B:694:ALA:O	2.70	0.43
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.43
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.43
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.43
1:A:967:SER:CB	1:C:571:ASP:HB2	2.48	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.18	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.01	0.43
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.43
1:C:393:THR:CG2	1:C:520:ALA:HB2	2.47	0.43
1:C:393:THR:HA	1:C:523:THR:CB	2.49	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.43
1:B:317:ASN:OD1	1:C:737:ASP:OD2	2.36	0.43
1:B:325:SER:C	1:B:326:ILE:CG2	2.91	0.43
1:B:337:PRO:C	1:B:339:GLY:H	2.26	0.43
1:B:523:THR:O	1:B:524:VAL:C	2.60	0.43
1:B:532:ASN:ND2	1:B:533:LEU:N	2.60	0.43
1:B:986:PRO:CB	1:B:987:PRO:HD3	2.46	0.43
1:C:323:THR:N	1:C:538:CYS:O	2.43	0.43
1:B:329:PHE:CD1	1:B:528:LYS:CB	3.00	0.43
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.43
1:C:41:LYS:HD3	1:C:41:LYS:N	2.33	0.43
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.43
1:B:127:VAL:HG21	3:B:1402:NAG:H5	2.01	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:C:309:GLU:H	1:C:309:GLU:HG2	1.71	0.43
2:S:1:NAG:H61	2:S:2:NAG:N2	2.33	0.43
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.43
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.43
1:A:335:LEU:C	1:A:362:VAL:O	2.61	0.43
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.33	0.43
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.82	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CB	1:B:528:LYS:HE3	2.48	0.43
1:B:337:PRO:C	1:B:339:GLY:N	2.77	0.43
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.43
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.43
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.43
1:B:528:LYS:CG	1:B:529:LYS:H	2.32	0.43
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.43
2:E:1:NAG:H61	2:E:2:NAG:N2	2.33	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.43
1:B:327:VAL:CG1	1:B:329:PHE:CD1	3.02	0.43
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.43
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.43
1:B:528:LYS:HE3	1:B:528:LYS:HB3	1.80	0.43
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.42
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
3:B:1409:NAG:O4	3:B:1410:NAG:O5	2.28	0.42
1:C:41:LYS:N	1:C:41:LYS:CD	2.82	0.42
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.42
1:C:326:ILE:O	1:C:327:VAL:CG2	2.67	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:A:338:PHE:C	1:A:340:GLU:N	2.75	0.42
1:B:546:LEU:HD11	1:B:565:PHE:CG	2.53	0.42
1:A:967:SER:HB2	1:C:571:ASP:HB2	2.01	0.42
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.42
1:B:322:PRO:HG3	1:B:538:CYS:SG	2.59	0.42
1:C:735:SER:OG	1:C:859:THR:HG22	2.17	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:C:357:ARG:H	1:C:357:ARG:HG3	1.62	0.42
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.42
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42
1:B:566:GLY:CA	1:C:43:PHE:HB3	2.50	0.42
1:C:127:VAL:HG21	3:C:1402:NAG:H5	2.01	0.42
1:A:326:ILE:HD13	1:A:533:LEU:HA	2.01	0.42
1:C:328:ARG:NE	1:C:533:LEU:HD22	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.42
1:A:330:PRO:O	1:A:331:ASN:C	2.63	0.42
1:A:565:PHE:O	1:B:42:VAL:CA	2.57	0.42
1:C:335:LEU:CA	1:C:362:VAL:HB	2.49	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
2:T:1:NAG:H3	2:T:1:NAG:H83	2.02	0.42
1:A:390:LEU:O	1:A:525:CYS:HB3	2.20	0.42
1:A:393:THR:HA	1:A:523:THR:CB	2.50	0.42
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.42
1:B:328:ARG:NH2	1:B:532:ASN:HA	2.34	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:B:810:SER:O	1:B:810:SER:OG	2.35	0.42
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:B:319:ARG:NH2	1:C:740:MET:HE1	2.32	0.42
1:C:323:THR:C	1:C:324:GLU:CG	2.89	0.42
1:A:565:PHE:O	1:B:43:PHE:N	2.51	0.42
1:A:654:GLU:O	1:A:694:ALA:N	2.53	0.42
1:C:327:VAL:HB	1:C:531:THR:OG1	2.20	0.42
1:A:328:ARG:HH11	1:A:533:LEU:CB	2.33	0.41
1:A:675:GLN:O	1:A:690:GLN:NE2	2.48	0.41
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.41
1:C:521:PRO:HB3	1:C:562:PHE:O	2.20	0.41
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.41
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.41
1:A:699:LEU:HD12	1:B:872:GLN:CD	2.45	0.41
1:A:770:ILE:HD13	1:A:770:ILE:HG21	1.76	0.41
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.41
1:A:985:ASP:CG	1:C:383:SER:HB2	2.45	0.41
1:B:323:THR:O	1:B:324:GLU:CG	2.51	0.41
1:B:521:PRO:O	1:B:522:ALA:CB	2.69	0.41
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.41
1:C:280:ASN:OD1	1:C:281:GLU:N	2.50	0.41
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.41
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.41
1:B:393:THR:O	1:B:523:THR:CG2	2.58	0.41
1:C:317:ASN:N	1:C:317:ASN:ND2	2.68	0.41
1:C:907:ASN:HD22	1:C:907:ASN:HA	1.64	0.41
1:A:703:ASN:HB2	1:B:787:GLN:CD	2.26	0.41
1:B:525:CYS:HB3	1:B:526:GLY:H	1.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG21	3:A:1402:NAG:H5	2.01	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.41
1:C:331:ASN:O	1:C:332:ILE:CB	2.68	0.41
1:A:41:LYS:HB3	1:C:563:GLN:CA	2.41	0.41
1:B:335:LEU:HD22	1:B:336:CYS:O	2.19	0.41
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:323:THR:O	1:A:324:GLU:HG2	2.20	0.41
1:B:333:THR:CG2	1:B:334:ASN:H	2.05	0.41
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.41
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.41
1:C:533:LEU:C	1:C:534:VAL:CG1	2.94	0.41
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.41
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:C:41:LYS:HD3	1:C:41:LYS:H	1.85	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:295:PRO:HB3	1:C:597:VAL:HG22	2.02	0.41
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.41
1:C:740:MET:HE2	1:C:740:MET:HB2	1.91	0.41
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.41
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.41
1:A:206:LYS:HZ3	1:A:208:THR:HG23	1.86	0.41
1:A:524:VAL:CG2	1:A:525:CYS:N	2.84	0.41
1:A:535:LYS:CD	1:A:536:ASN:OD1	2.68	0.41
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.41
1:B:48:LEU:H	1:B:48:LEU:CD1	2.33	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:332:ILE:CG1	1:B:333:THR:N	2.84	0.41
1:B:655:HIS:HA	1:B:694:ALA:O	2.21	0.41
1:C:45:SER:O	1:C:47:VAL:N	2.54	0.41
1:C:325:SER:HB2	1:C:540:ASN:HB3	2.01	0.41
1:C:406:GLU:CG	1:C:418:ILE:HG13	2.50	0.41
1:C:521:PRO:O	1:C:522:ALA:CB	2.64	0.41
1:C:532:ASN:C	1:C:532:ASN:ND2	2.73	0.41
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.91	0.41
1:A:89:GLY:HA2	1:A:194:PHE:O	2.21	0.41
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.41
1:A:854:LYS:O	1:A:855:PHE:CD1	2.71	0.41
1:A:1123:SER:O	1:A:1123:SER:OG	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:HG11	1:B:329:PHE:CD1	2.55	0.41
1:B:931:ILE:HD13	1:B:931:ILE:HA	1.88	0.41
1:C:45:SER:OG	1:C:281:GLU:HA	2.21	0.41
1:C:46:SER:C	1:C:47:VAL:HG13	2.46	0.41
1:C:48:LEU:H	1:C:48:LEU:CD1	2.33	0.41
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.41
1:C:324:GLU:CD	1:C:539:VAL:HG23	2.46	0.41
1:C:327:VAL:HG12	1:C:530:SER:HA	2.02	0.41
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.41
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.41
1:A:187:LYS:N	1:A:187:LYS:HE2	2.36	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:406:GLU:CG	1:B:418:ILE:HG13	2.50	0.40
1:B:533:LEU:C	1:B:534:VAL:CG1	2.94	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:335:LEU:O	1:C:336:CYS:HB2	2.22	0.40
1:A:213:VAL:HG23	1:A:214:ARG:N	2.36	0.40
1:A:347:PHE:CD1	1:A:509:ARG:HD3	2.56	0.40
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.40
1:B:964:LYS:HE3	1:B:964:LYS:HB2	1.77	0.40
1:B:984:LEU:HD23	1:B:988:GLU:HB3	2.03	0.40
1:C:591:SER:C	1:C:592:PHE:CD1	2.98	0.40
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.40
1:A:46:SER:C	1:A:47:VAL:HG13	2.46	0.40
1:A:1132:ILE:H	1:A:1132:ILE:HG13	1.36	0.40
1:B:89:GLY:HA2	1:B:194:PHE:O	2.22	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40
1:C:166:CYS:HB3	1:C:169:GLU:OE1	2.21	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.40
1:B:226:LEU:HB3	1:B:227:VAL:HG23	2.03	0.40
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.90	0.40
1:C:322:PRO:HA	1:C:538:CYS:SG	2.62	0.40
1:C:371:SER:C	1:C:373:SER:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	952/1283 (74%)	831 (87%)	93 (10%)	28 (3%)	3	26
1	B	951/1283 (74%)	819 (86%)	107 (11%)	25 (3%)	4	27
1	C	951/1283 (74%)	814 (86%)	102 (11%)	35 (4%)	2	21
All	All	2854/3849 (74%)	2464 (86%)	302 (11%)	88 (3%)	5	25

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	332	ILE
1	A	524	VAL
1	A	534	VAL
1	A	691	SER
1	A	701	ALA
1	B	48	LEU
1	B	329	PHE
1	B	335	LEU
1	B	519	HIS
1	B	524	VAL
1	B	531	THR
1	C	48	LEU
1	C	329	PHE
1	C	332	ILE
1	C	519	HIS
1	C	529	LYS
1	C	814	LYS
1	A	41	LYS
1	A	46	SER
1	A	331	ASN
1	A	339	GLY
1	A	518	LEU
1	A	520	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	41	LYS
1	B	46	SER
1	B	320	VAL
1	B	332	ILE
1	B	528	LYS
1	B	534	VAL
1	B	742	ILE
1	B	743	CYS
1	C	41	LYS
1	C	46	SER
1	C	319	ARG
1	C	533	LEU
1	C	534	VAL
1	C	592	PHE
1	C	697	MET
1	C	810	SER
1	A	43	PHE
1	A	521	PRO
1	A	522	ALA
1	A	695	TYR
1	A	710	ASN
1	B	43	PHE
1	B	336	CYS
1	B	522	ALA
1	B	532	ASN
1	C	43	PHE
1	C	327	VAL
1	C	518	LEU
1	C	522	ALA
1	A	44	ARG
1	A	324	GLU
1	A	329	PHE
1	A	336	CYS
1	A	349	SER
1	A	535	LYS
1	B	44	ARG
1	B	349	SER
1	B	746	SER
1	C	44	ARG
1	C	316	SER
1	C	349	SER
1	C	527	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	591	SER
1	C	691	SER
1	C	813	SER
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	B	40	ASP
1	B	42	VAL
1	B	47	VAL
1	B	324	GLU
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL
1	C	535	LYS
1	A	337	PRO
1	C	318	PHE
1	C	336	CYS
1	C	811	LYS
1	C	812	PRO
1	C	330	PRO
1	C	520	ALA
1	A	527	PRO

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	851/1122 (76%)	732 (86%)	119 (14%)	3	19
1	B	850/1122 (76%)	752 (88%)	98 (12%)	5	24
1	C	850/1122 (76%)	742 (87%)	108 (13%)	4	21
All	All	2551/3366 (76%)	2226 (87%)	325 (13%)	6	21

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	41	LYS
1	A	46	SER
1	A	48	LEU
1	A	66	HIS
1	A	81	ASN
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	171	VAL
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	231	ILE
1	A	282	ASN
1	A	289	VAL
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	317	ASN
1	A	319	ARG
1	A	320	VAL
1	A	323	THR
1	A	324	GLU
1	A	328	ARG
1	A	334	ASN
1	A	335	LEU
1	A	336	CYS
1	A	375	SER
1	A	382	VAL
1	A	383	SER
1	A	388	ASN
1	A	389	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	390	LEU
1	A	403	ARG
1	A	406	GLU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	529	LYS
1	A	530	SER
1	A	533	LEU
1	A	535	LYS
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	576	VAL
1	A	583	GLU
1	A	585	LEU
1	A	590	CYS
1	A	599	THR
1	A	602	THR
1	A	608	VAL
1	A	673	SER
1	A	692	ILE
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	705	VAL
1	A	719	THR
1	A	722	VAL
1	A	729	VAL
1	A	730	SER
1	A	738	CYS
1	A	746	SER
1	A	772	VAL
1	A	773	GLU
1	A	785	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	939	SER
1	A	951	VAL
1	A	960	ASN
1	A	967	SER
1	A	973	ILE
1	A	976	VAL
1	A	991	VAL
1	A	994	ASP
1	A	998	THR
1	A	1005	GLN
1	A	1018	ILE
1	A	1039	ARG
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1114	ILE
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1142	GLN
1	A	1144	GLU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	66	HIS
1	B	81	ASN
1	B	97	LYS
1	B	109	THR
1	B	116	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	118	LEU
1	B	122	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	171	VAL
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	231	ILE
1	B	282	ASN
1	B	289	VAL
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	315	THR
1	B	320	VAL
1	B	328	ARG
1	B	331	ASN
1	B	335	LEU
1	B	357	ARG
1	B	375	SER
1	B	382	VAL
1	B	383	SER
1	B	389	ASP
1	B	390	LEU
1	B	403	ARG
1	B	406	GLU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	500	THR
1	B	514	SER
1	B	516	GLU
1	B	517	LEU
1	B	518	LEU
1	B	519	HIS
1	B	528	LYS
1	B	530	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	531	THR
1	B	533	LEU
1	B	535	LYS
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	576	VAL
1	B	583	GLU
1	B	585	LEU
1	B	599	THR
1	B	602	THR
1	B	608	VAL
1	B	673	SER
1	B	710	ASN
1	B	729	VAL
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	772	VAL
1	B	779	GLN
1	B	787	GLN
1	B	791	THR
1	B	811	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	991	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1081	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1133	VAL
1	B	1141	LEU
1	C	40	ASP
1	C	41	LYS
1	C	46	SER
1	C	48	LEU
1	C	66	HIS
1	C	81	ASN
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	141	LEU
1	C	143	VAL
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	171	VAL
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	231	ILE
1	C	282	ASN
1	C	289	VAL
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	317	ASN
1	C	319	ARG
1	C	323	THR
1	C	324	GLU
1	C	326	ILE
1	C	333	THR
1	C	335	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	357	ARG
1	C	375	SER
1	C	382	VAL
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	403	ARG
1	C	406	GLU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	500	THR
1	C	514	SER
1	C	516	GLU
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	529	LYS
1	C	532	ASN
1	C	535	LYS
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	576	VAL
1	C	583	GLU
1	C	585	LEU
1	C	588	THR
1	C	591	SER
1	C	592	PHE
1	C	599	THR
1	C	602	THR
1	C	608	VAL
1	C	673	SER
1	C	690	GLN
1	C	692	ILE
1	C	693	ILE
1	C	696	THR
1	C	697	MET
1	C	699	LEU
1	C	727	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	768	THR
1	C	770	ILE
1	C	778	THR
1	C	787	GLN
1	C	791	THR
1	C	814	LYS
1	C	856	ASN
1	C	878	LEU
1	C	907	ASN
1	C	922	LEU
1	C	929	SER
1	C	931	ILE
1	C	934	ILE
1	C	937	SER
1	C	968	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1018	ILE
1	C	1027	THR
1	C	1063	LEU
1	C	1077	THR
1	C	1092	GLU
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	450	ASN
1	A	498	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	556	ASN
1	A	613	GLN
1	A	644	GLN
1	A	658	ASN
1	A	675	GLN
1	A	703	ASN
1	A	755	GLN
1	A	762	GLN
1	A	787	GLN
1	A	901	GLN
1	A	914	ASN
1	A	926	GLN
1	A	949	GLN
1	A	969	ASN
1	A	992	GLN
1	A	1010	GLN
1	A	1054	GLN
1	A	1125	ASN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	317	ASN
1	B	422	ASN
1	B	440	ASN
1	B	450	ASN
1	B	498	GLN
1	B	519	HIS
1	B	532	ASN
1	B	542	ASN
1	B	556	ASN
1	B	613	GLN
1	B	644	GLN
1	B	655	HIS
1	B	658	ASN
1	B	675	GLN
1	B	690	GLN
1	B	703	ASN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	920	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	926	GLN
1	B	949	GLN
1	B	957	GLN
1	B	960	ASN
1	B	992	GLN
1	B	1011	GLN
1	B	1101	HIS
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	317	ASN
1	C	422	ASN
1	C	440	ASN
1	C	450	ASN
1	C	498	GLN
1	C	519	HIS
1	C	532	ASN
1	C	542	ASN
1	C	556	ASN
1	C	644	GLN
1	C	658	ASN
1	C	675	GLN
1	C	690	GLN
1	C	703	ASN
1	C	764	ASN
1	C	779	GLN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	992	GLN
1	C	1010	GLN
1	C	1011	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
1	C	1125	ASN
1	C	1135	ASN

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 ⓘ

44 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	0.52	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	E	1	2,1	14,14,15	0.55	0	17,19,21	0.58	0
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	F	1	2,1	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.49	0
2	NAG	G	1	2,1	14,14,15	0.36	0	17,19,21	0.74	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	1.40	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
2	NAG	H	2	2	14,14,15	0.42	0	17,19,21	1.49	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.68	0
2	NAG	J	1	2,1	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
2	NAG	J	2	2	14,14,15	0.16	0	17,19,21	0.49	0
2	NAG	K	1	2,1	14,14,15	0.52	0	17,19,21	0.51	0
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	L	1	2,1	14,14,15	0.55	0	17,19,21	0.57	0
2	NAG	L	2	2	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	M	1	2,1	14,14,15	0.30	0	17,19,21	0.42	0
2	NAG	M	2	2	14,14,15	0.40	0	17,19,21	0.37	0
2	NAG	N	1	2,1	14,14,15	0.36	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	O	1	2,1	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
2	NAG	O	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	P	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	P	2	2	14,14,15	0.35	0	17,19,21	0.73	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.39	0
2	NAG	R	1	2,1	14,14,15	0.53	0	17,19,21	0.51	0
2	NAG	R	2	2	14,14,15	0.26	0	17,19,21	0.60	0
2	NAG	S	1	2,1	14,14,15	0.56	0	17,19,21	0.58	0
2	NAG	S	2	2	14,14,15	0.30	0	17,19,21	0.48	0
2	NAG	T	1	2,1	14,14,15	0.23	0	17,19,21	1.44	2 (11%)
2	NAG	T	2	2	14,14,15	0.19	0	17,19,21	0.52	0
2	NAG	U	1	2,1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
2	NAG	U	2	2	14,14,15	0.38	0	17,19,21	0.47	0
2	NAG	V	1	2,1	14,14,15	0.38	0	17,19,21	0.40	0
2	NAG	V	2	2	14,14,15	0.20	0	17,19,21	0.77	0
2	NAG	W	1	2,1	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	W	2	2	14,14,15	0.59	0	17,19,21	1.38	2 (11%)
2	NAG	X	1	2,1	14,14,15	0.60	0	17,19,21	0.45	0
2	NAG	X	2	2	14,14,15	0.34	0	17,19,21	1.44	2 (11%)
2	NAG	Y	1	2,1	14,14,15	0.38	0	17,19,21	0.47	0
2	NAG	Y	2	2	14,14,15	0.24	0	17,19,21	0.51	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
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	6/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	3/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	6/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	6/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	5/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	NAG	O5-C1	-2.54	1.39	1.43
2	I	1	NAG	O5-C1	-2.46	1.39	1.43
2	H	1	NAG	O5-C1	-2.22	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1	NAG	C2-N2-C7	4.96	129.54	122.90
2	H	2	NAG	C2-N2-C7	4.71	129.22	122.90
2	X	2	NAG	C2-N2-C7	4.64	129.12	122.90
2	W	2	NAG	C2-N2-C7	4.58	129.04	122.90
2	G	2	NAG	C2-N2-C7	4.56	129.01	122.90
2	N	1	NAG	C1-O5-C5	3.37	116.70	112.19
2	H	2	NAG	C1-C2-N2	2.61	114.55	110.43
2	G	2	NAG	C1-C2-N2	2.59	114.51	110.43
2	X	2	NAG	C1-C2-N2	2.48	114.34	110.43
2	P	1	NAG	O4-C4-C3	-2.35	104.84	110.38
2	U	1	NAG	C1-O5-C5	2.30	115.26	112.19
2	O	1	NAG	C1-O5-C5	2.29	115.25	112.19
2	T	1	NAG	C1-C2-N2	2.14	113.80	110.43
2	H	2	NAG	C1-O5-C5	2.12	115.03	112.19
2	J	1	NAG	C1-O5-C5	2.09	114.99	112.19
2	P	2	NAG	C1-O5-C5	2.07	114.97	112.19
2	W	2	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	2	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	P	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	W	2	NAG	C8-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	X	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	T	1	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C3-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	V	2	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	Y	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	V	2	NAG	C1-C2-N2-C7
2	W	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7
2	S	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	S	2	NAG	C3-C2-N2-C7
2	T	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 19 short contacts:

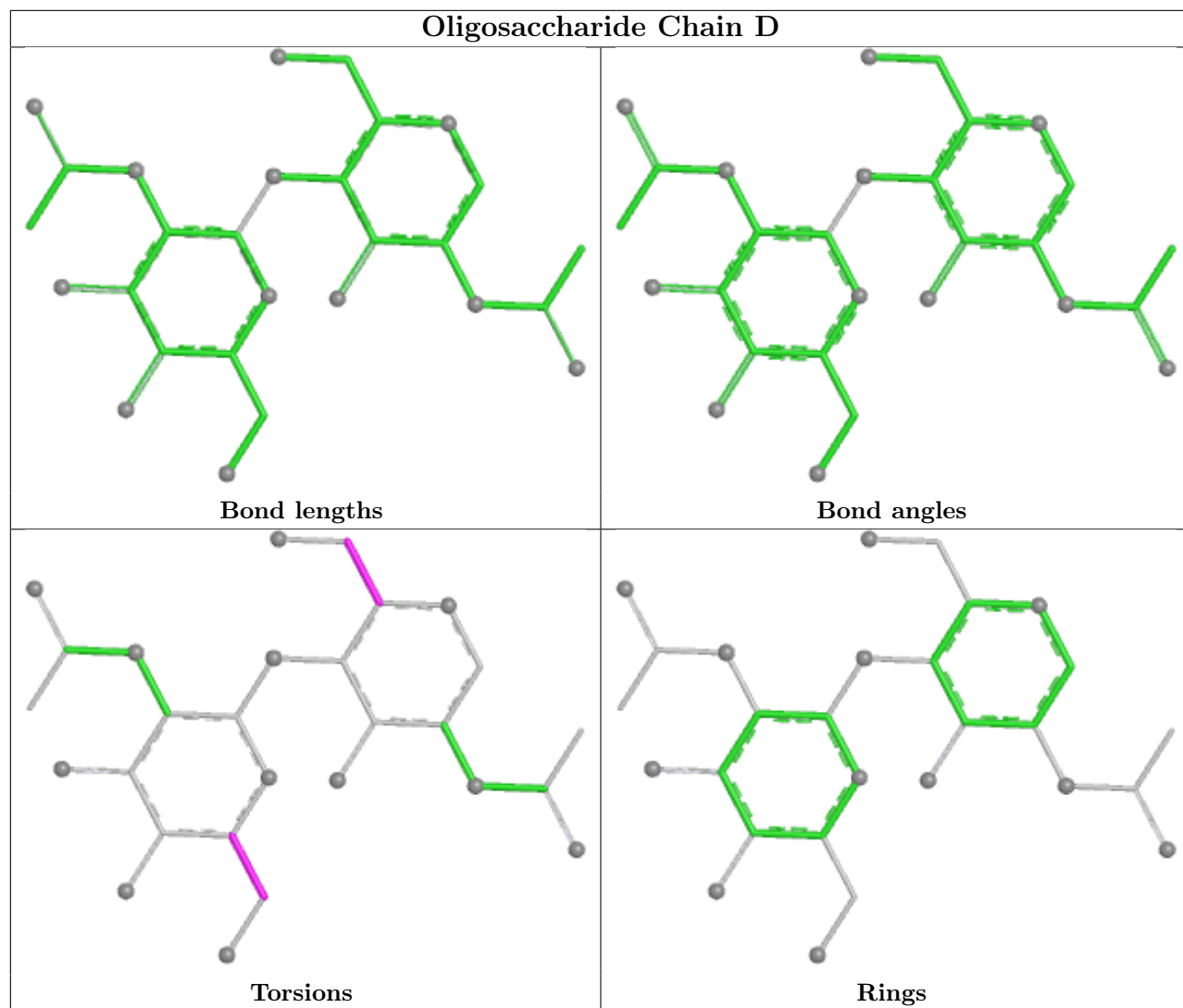
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	2	NAG	1	0

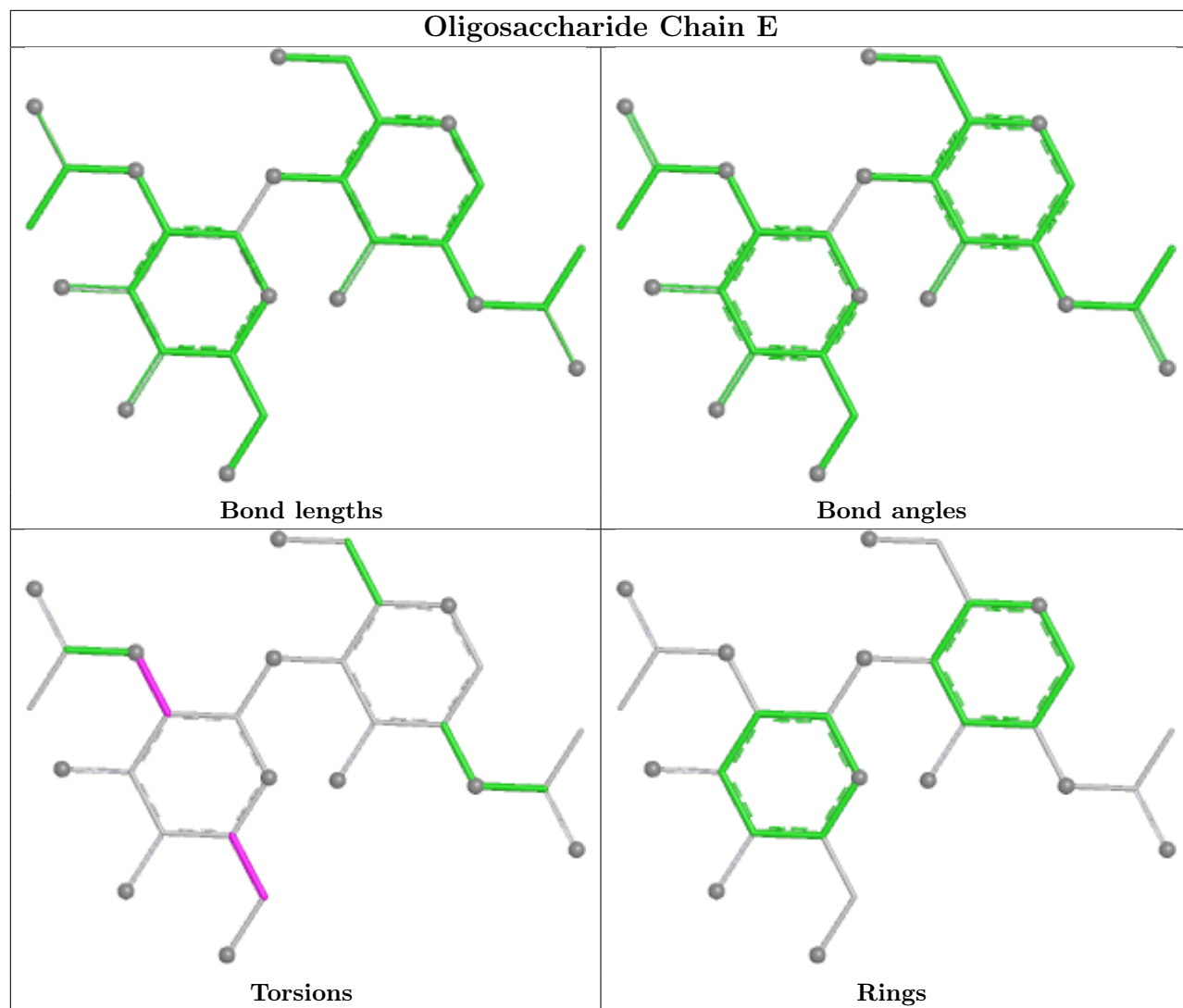
Continued on next page...

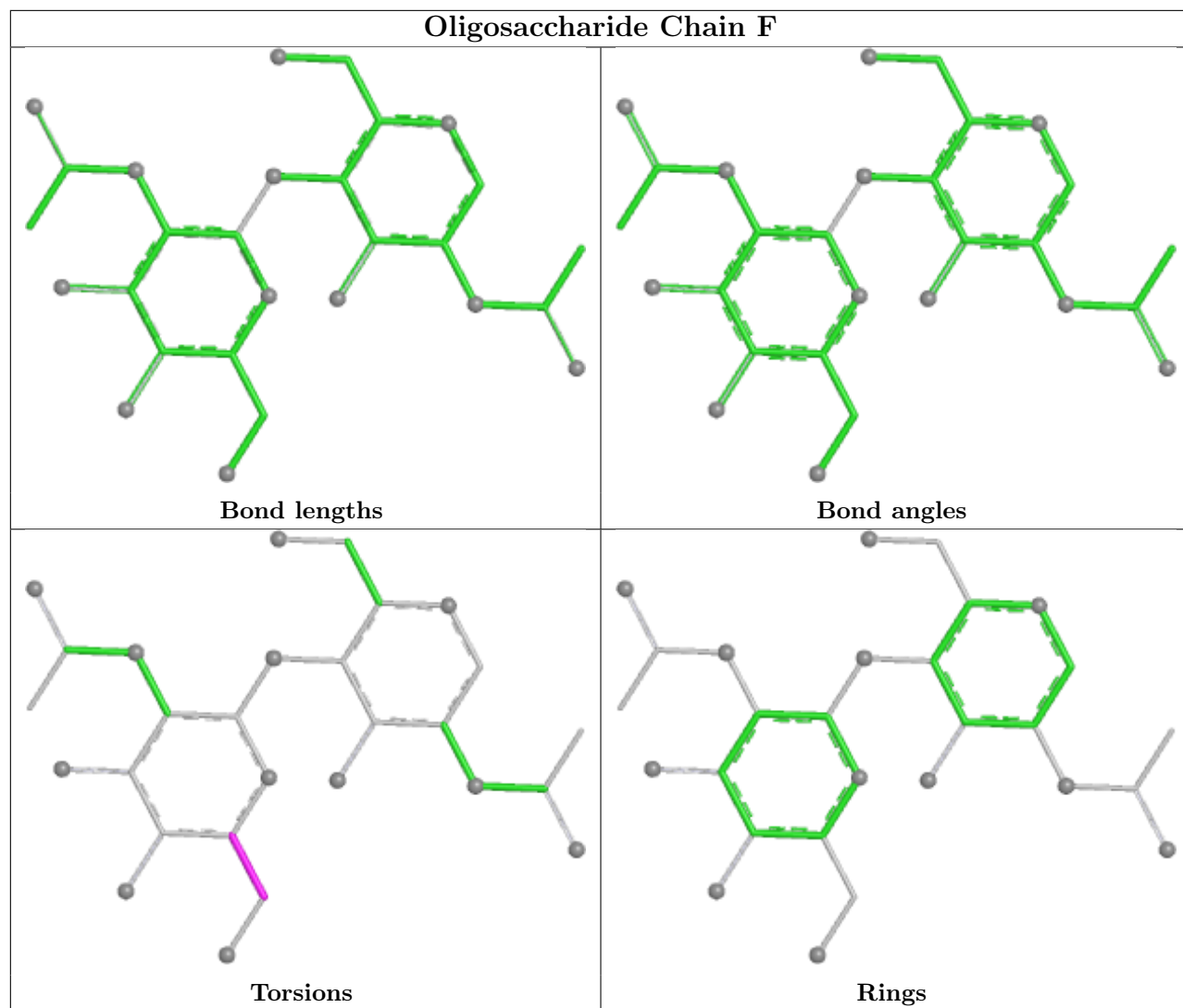
Continued from previous page...

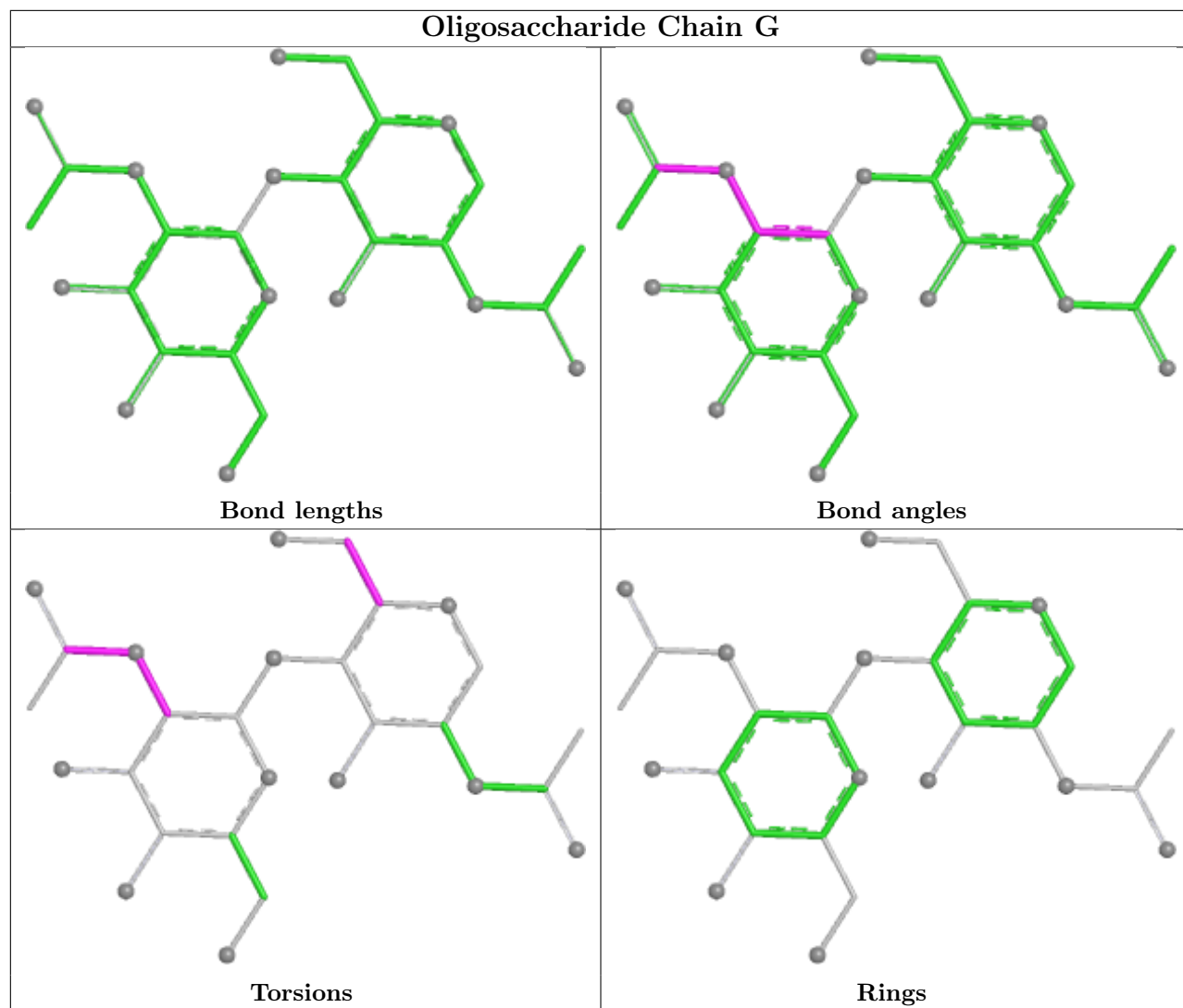
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
2	E	1	NAG	3	0
2	L	1	NAG	3	0
2	H	2	NAG	1	0
2	P	1	NAG	1	0
2	G	2	NAG	1	0
2	T	1	NAG	1	0
2	K	1	NAG	3	0
2	P	2	NAG	1	0
2	S	2	NAG	2	0
2	X	1	NAG	1	0
2	L	2	NAG	2	0
2	W	2	NAG	1	0
2	S	1	NAG	3	0

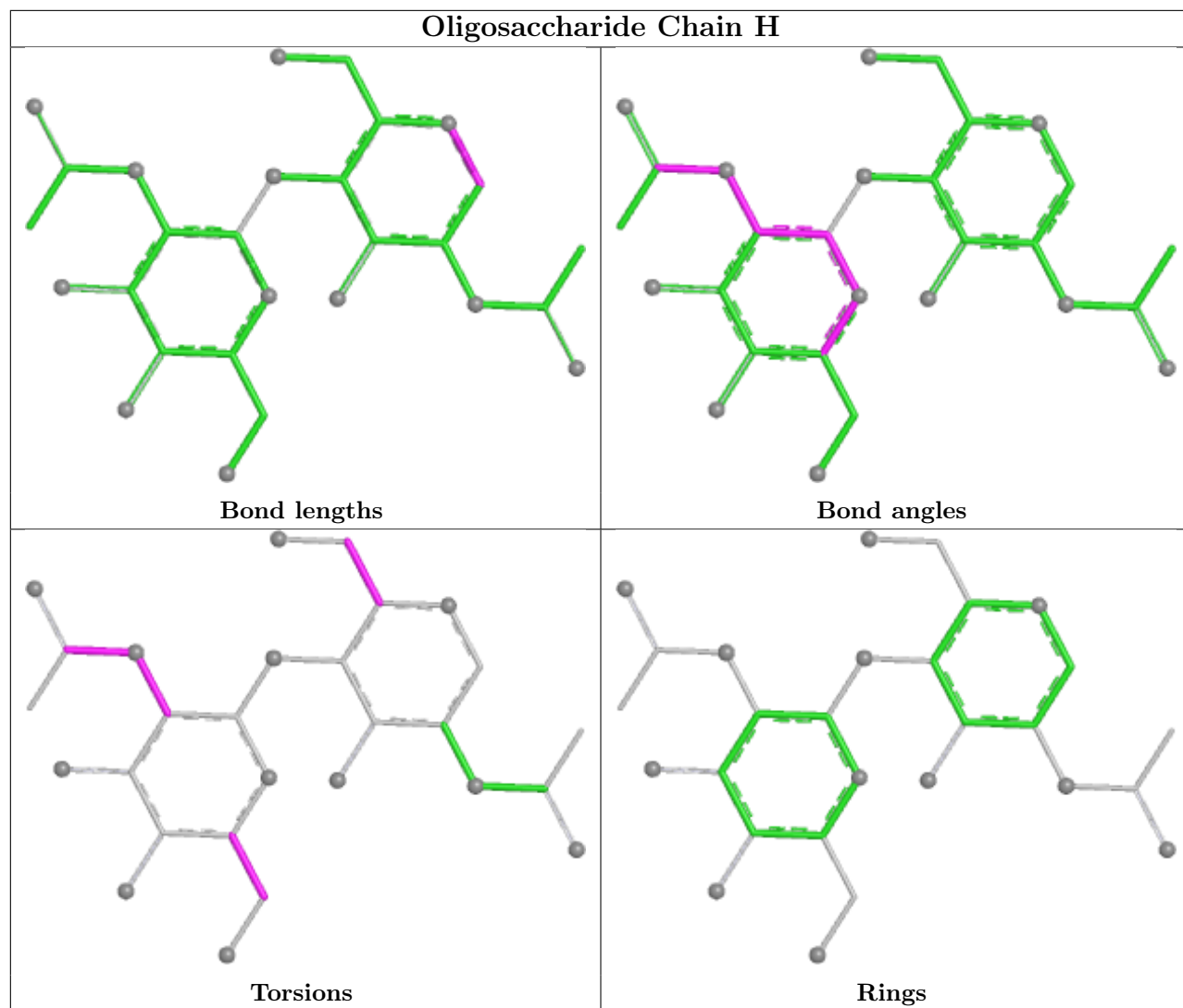
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

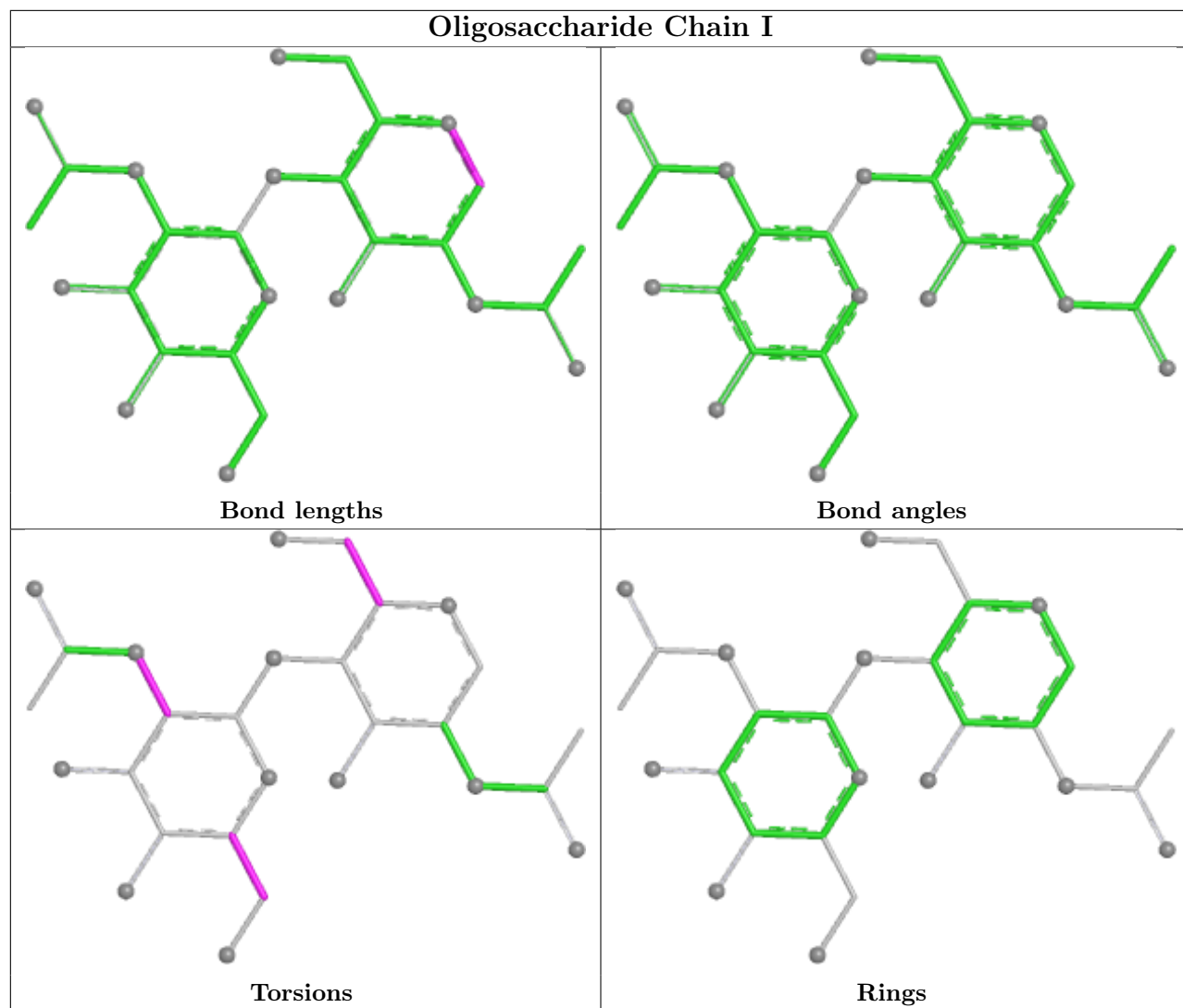


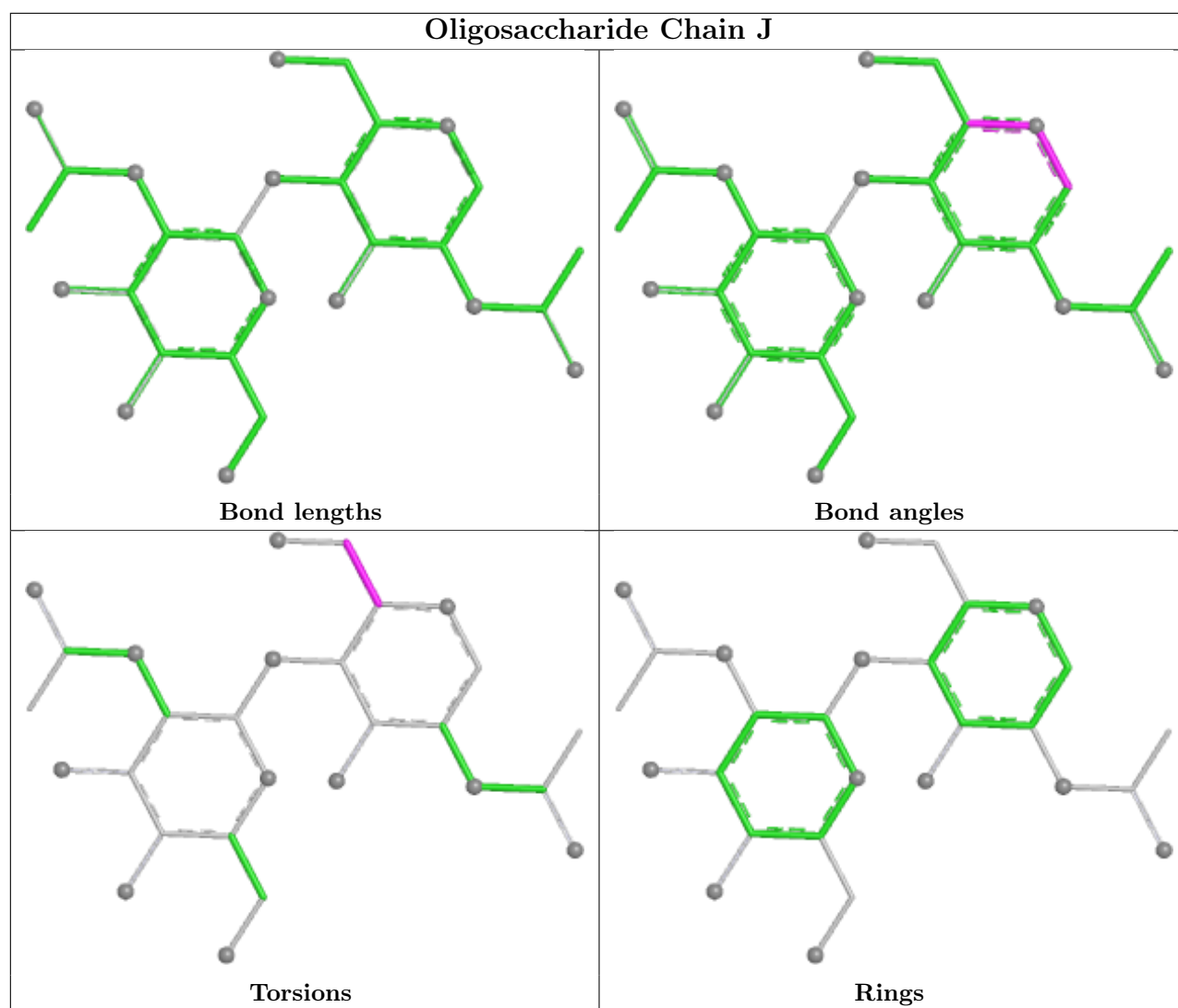


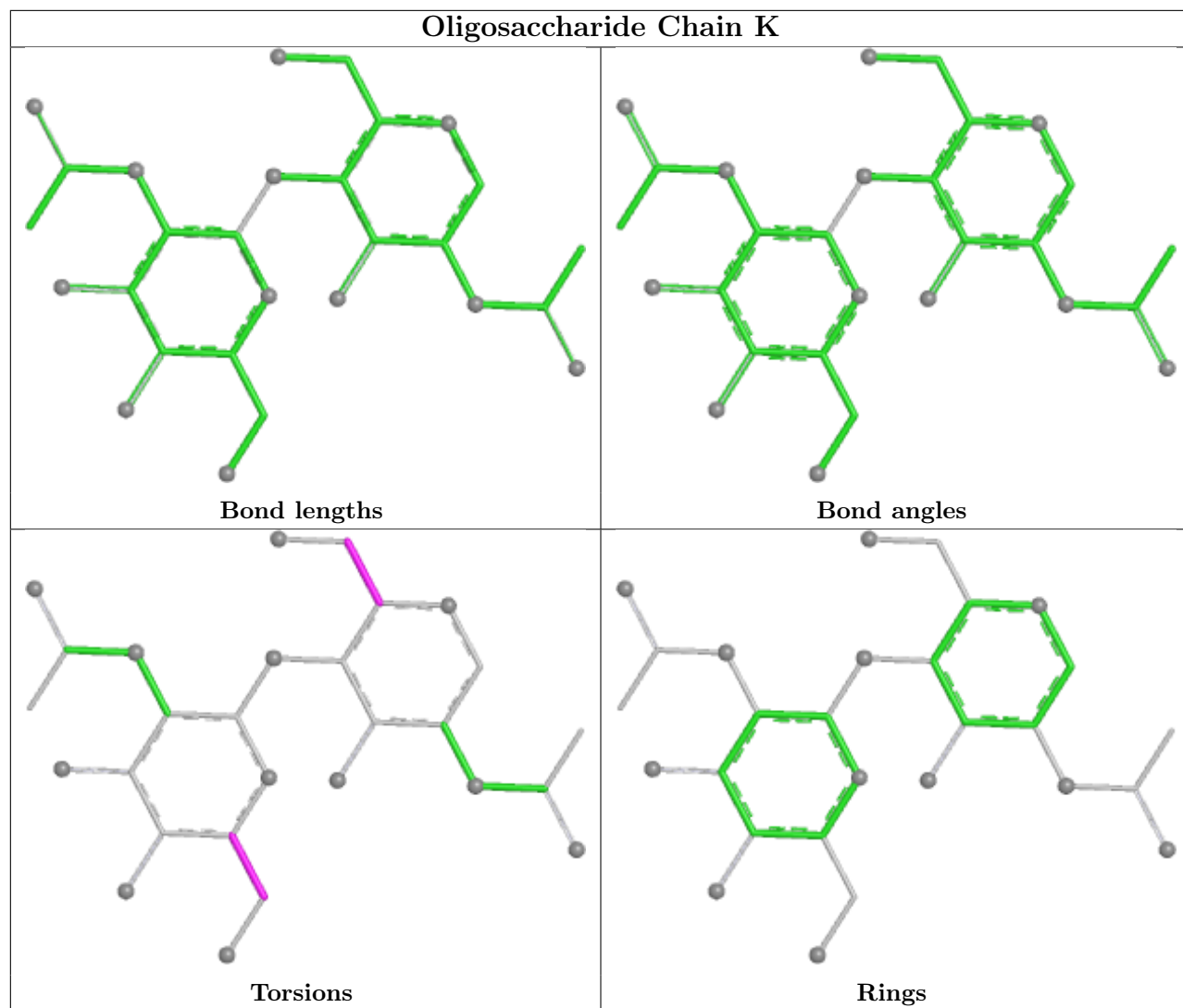


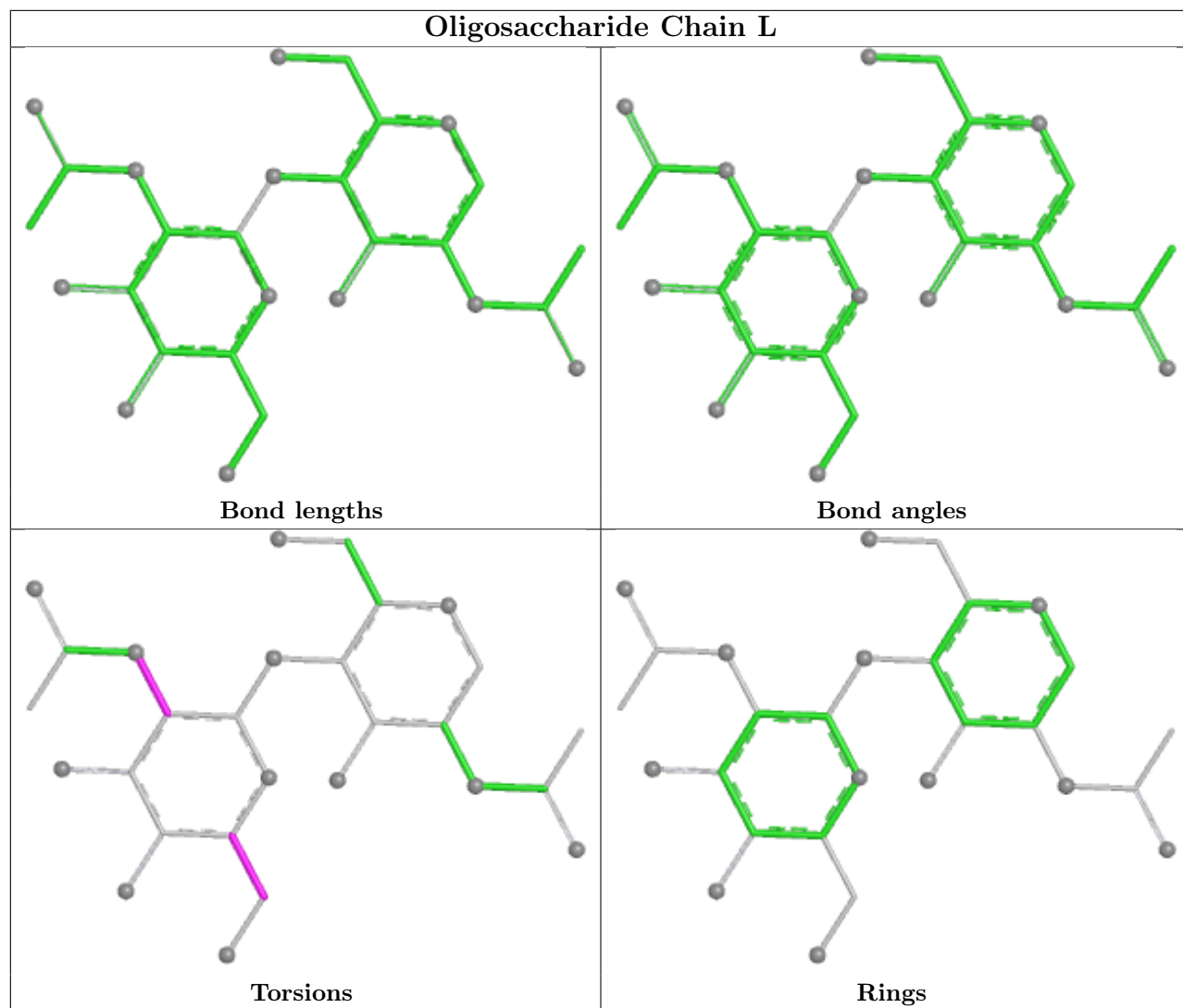


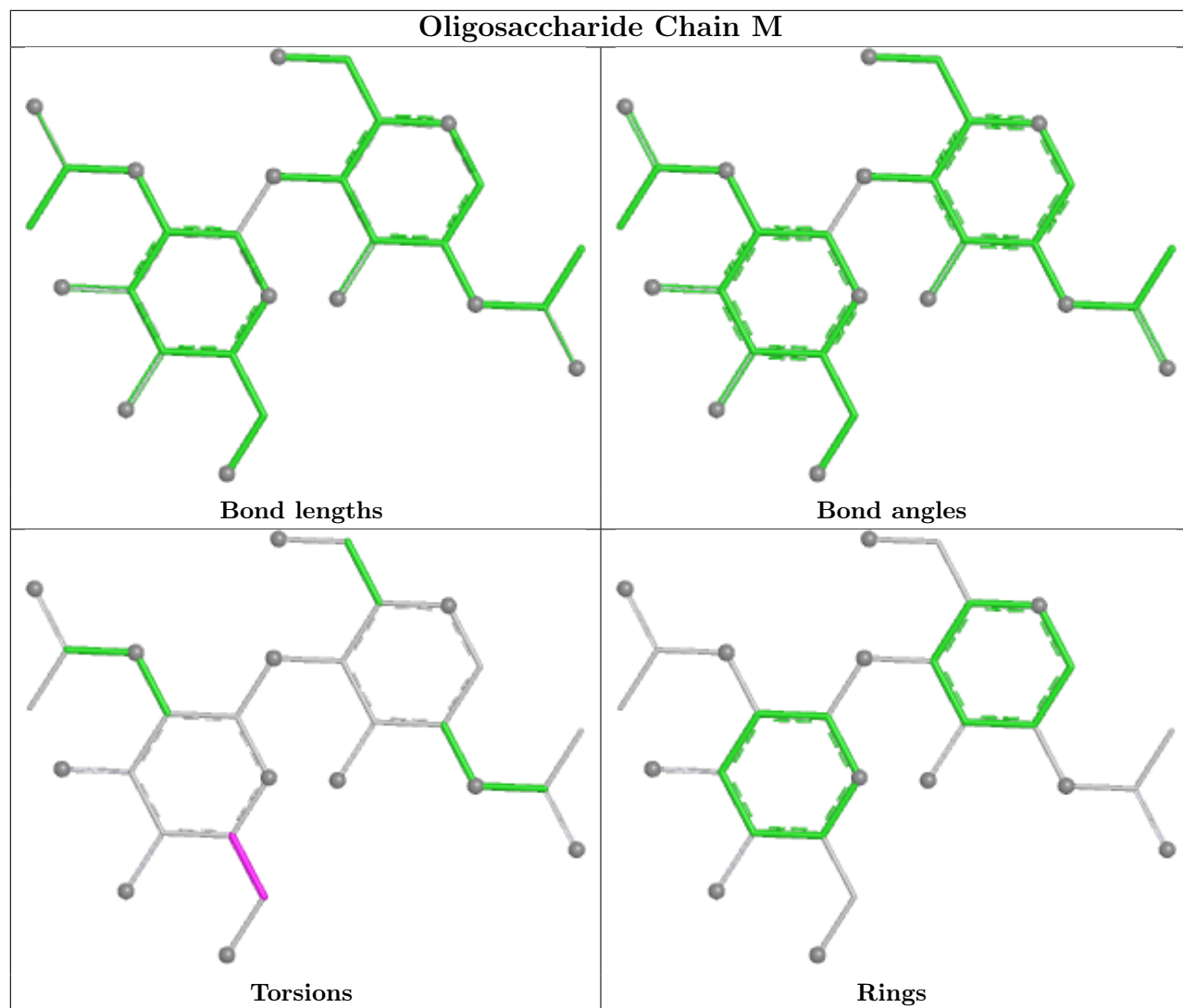


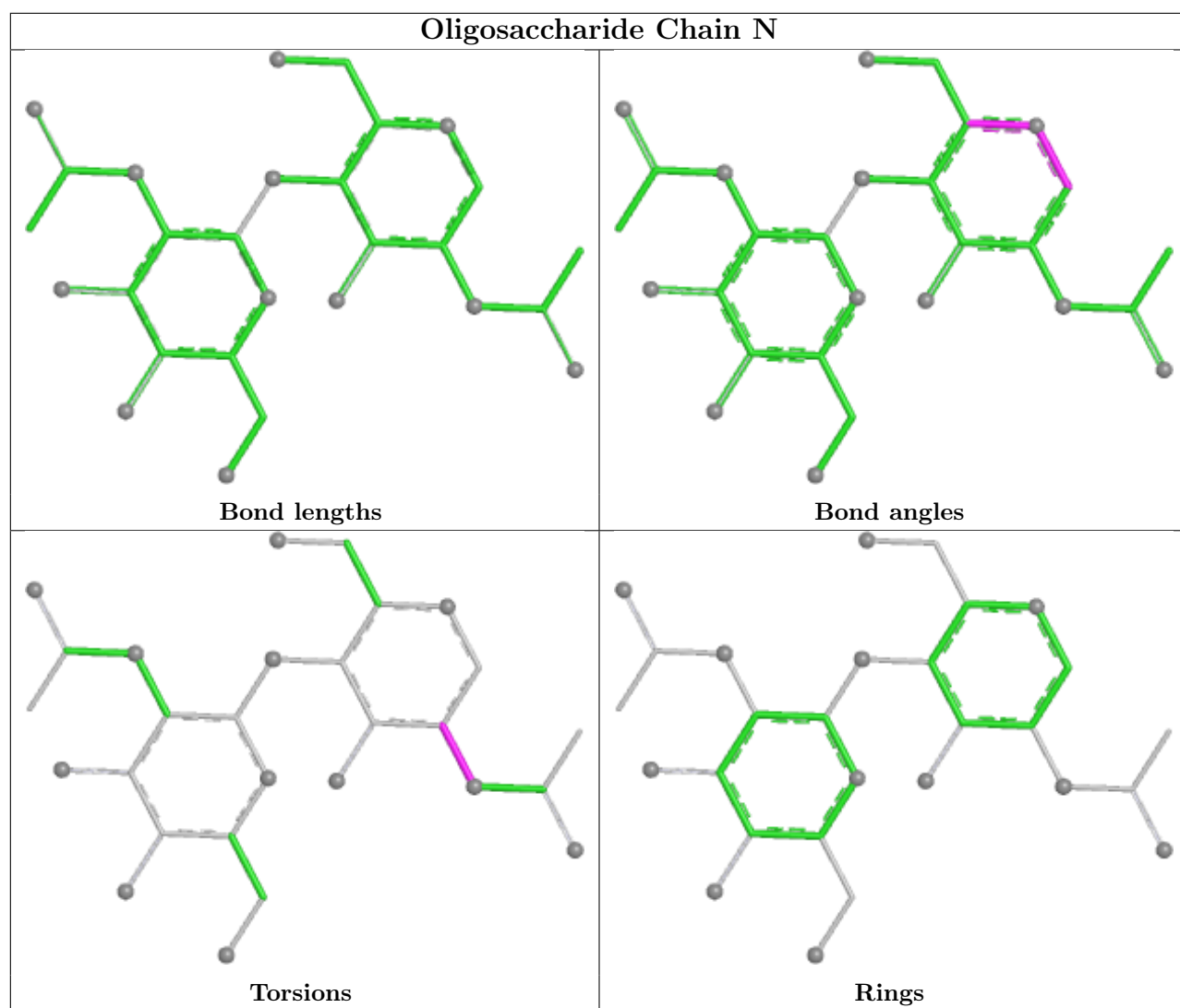


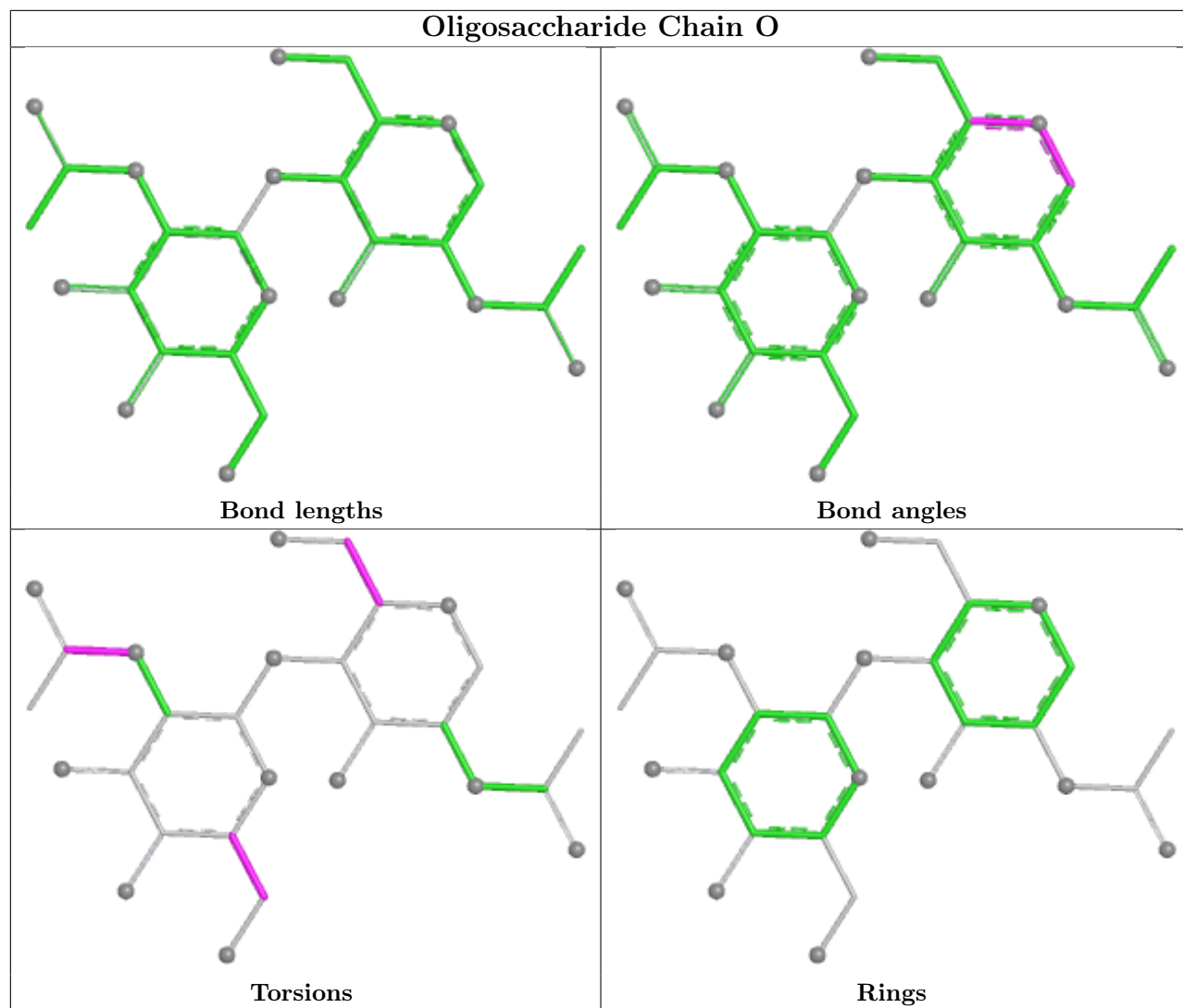


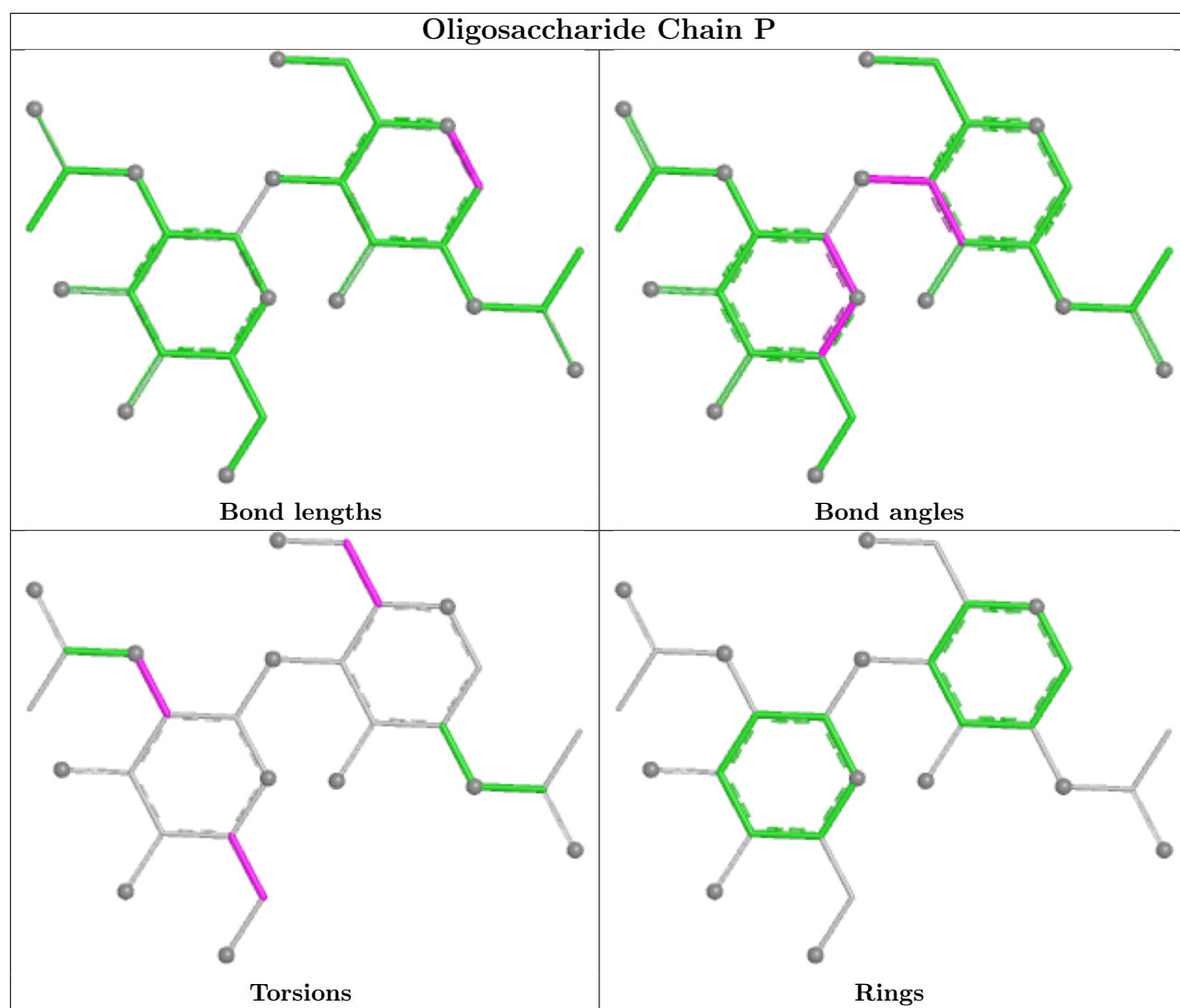


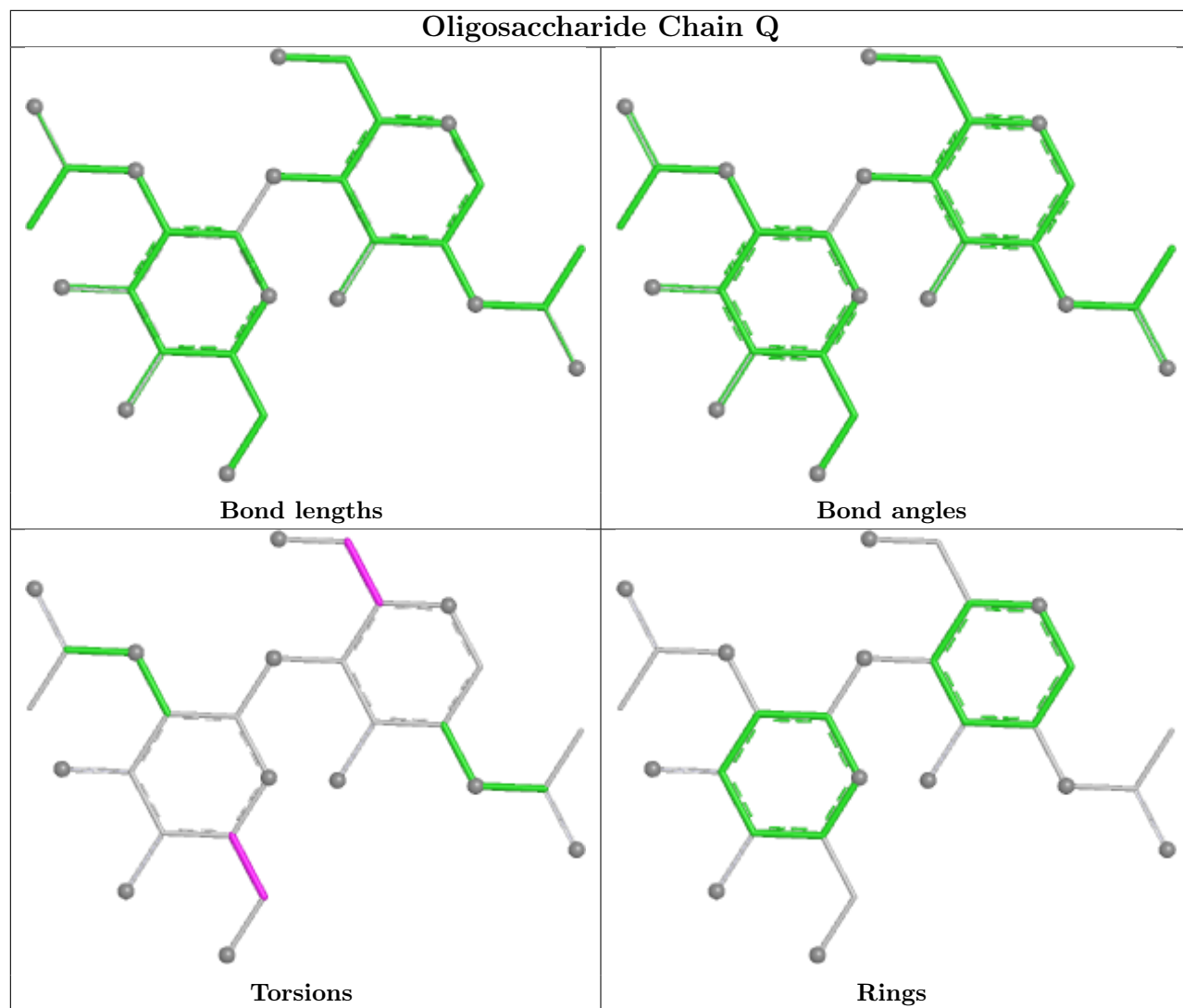


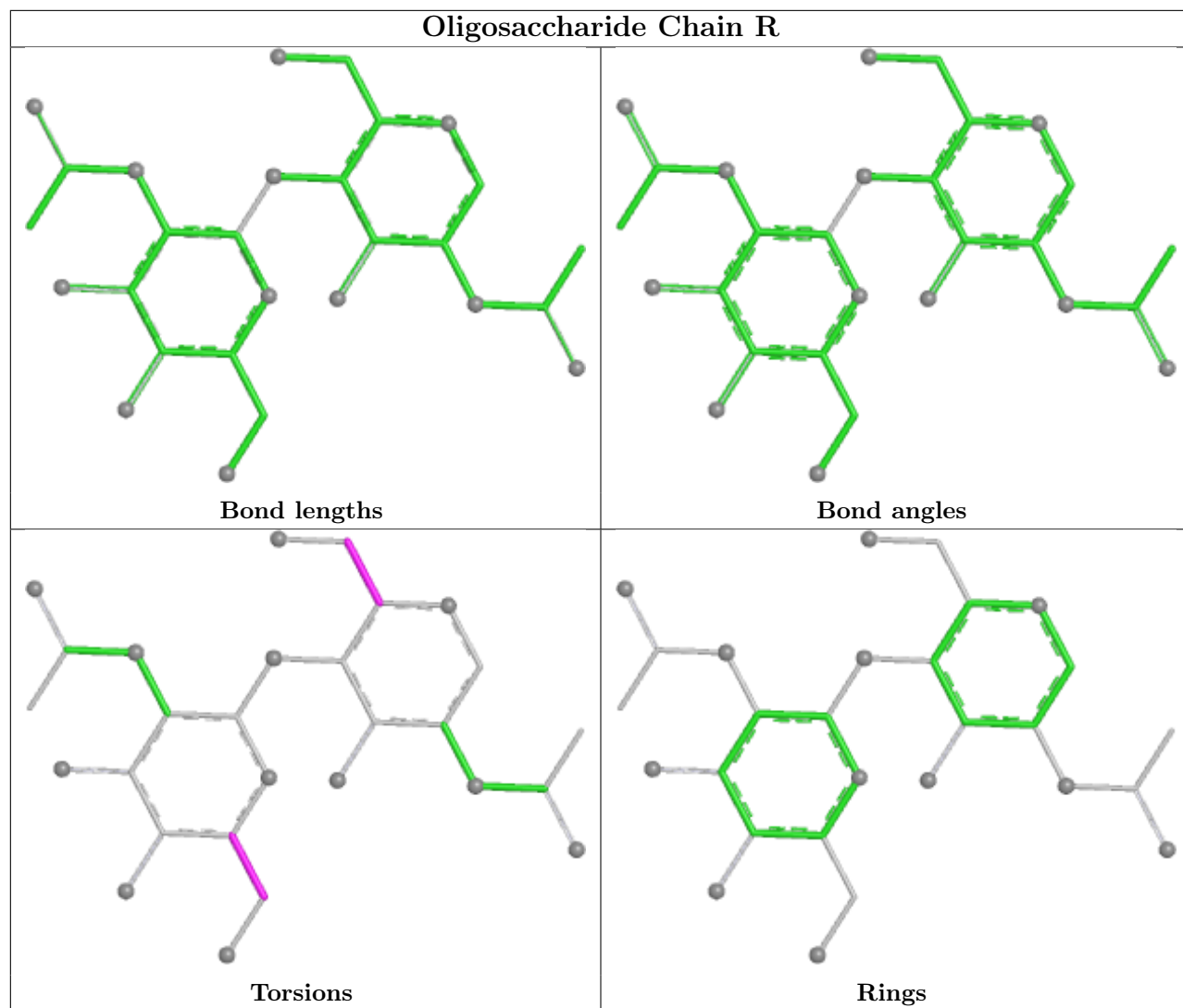


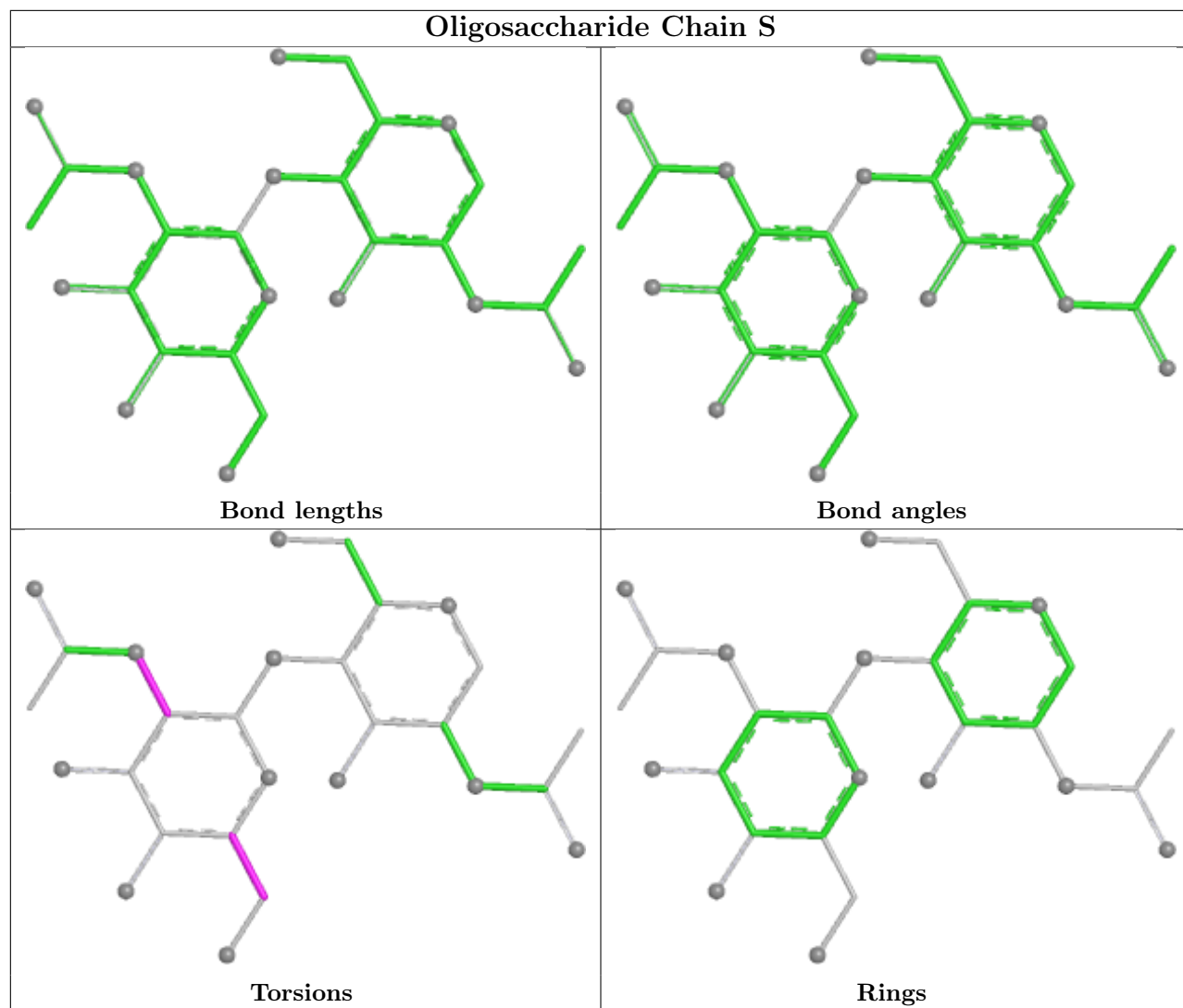


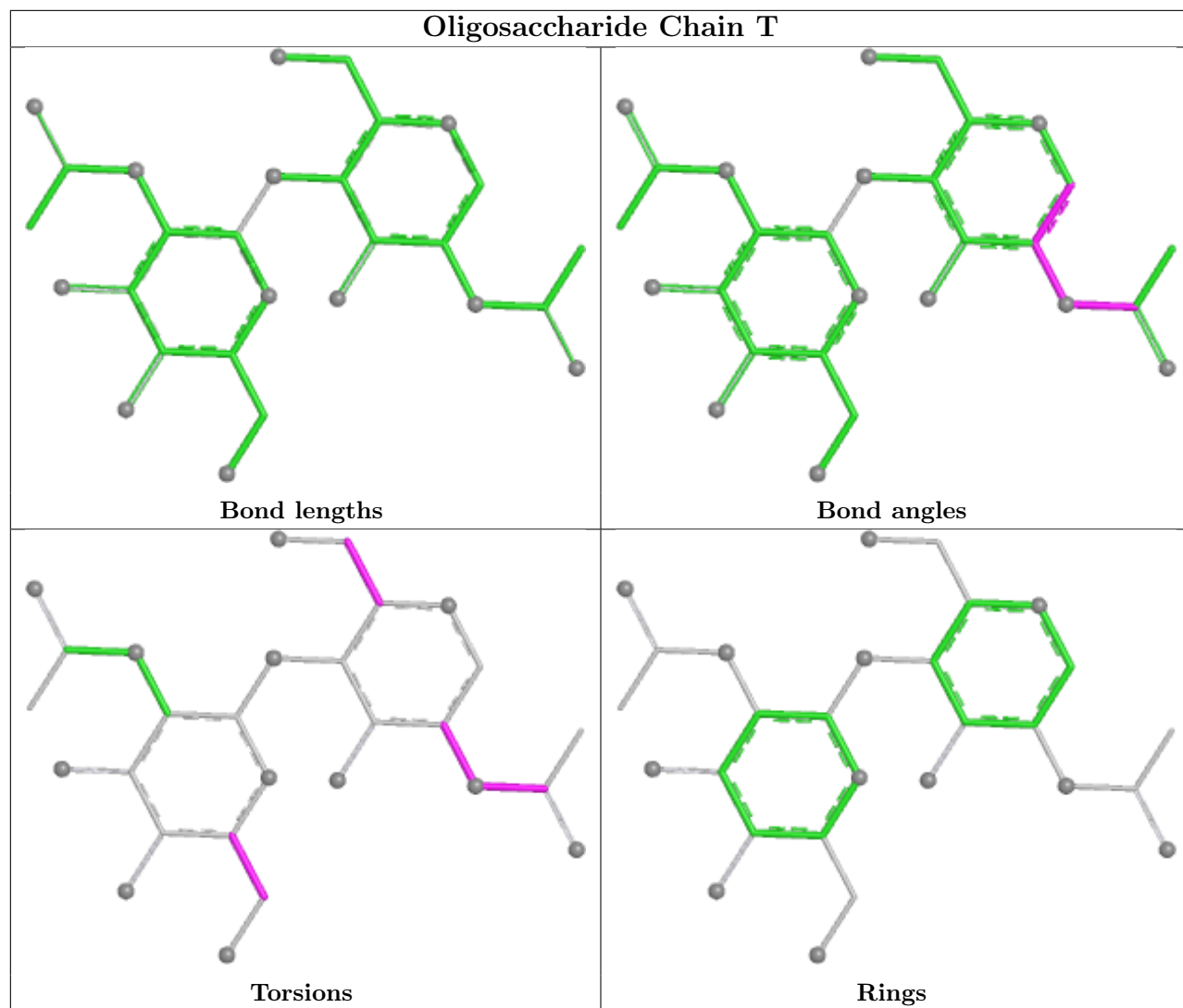


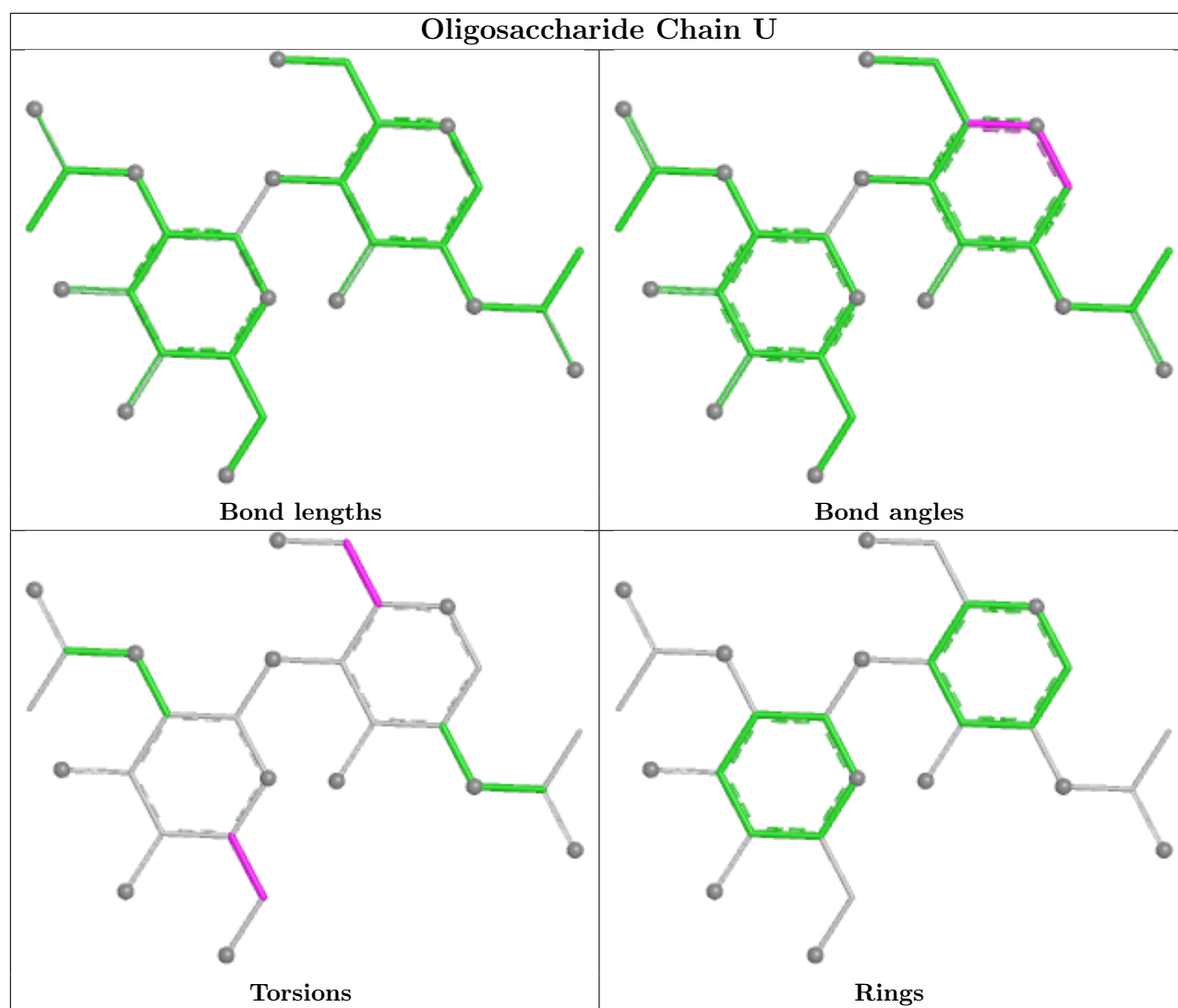


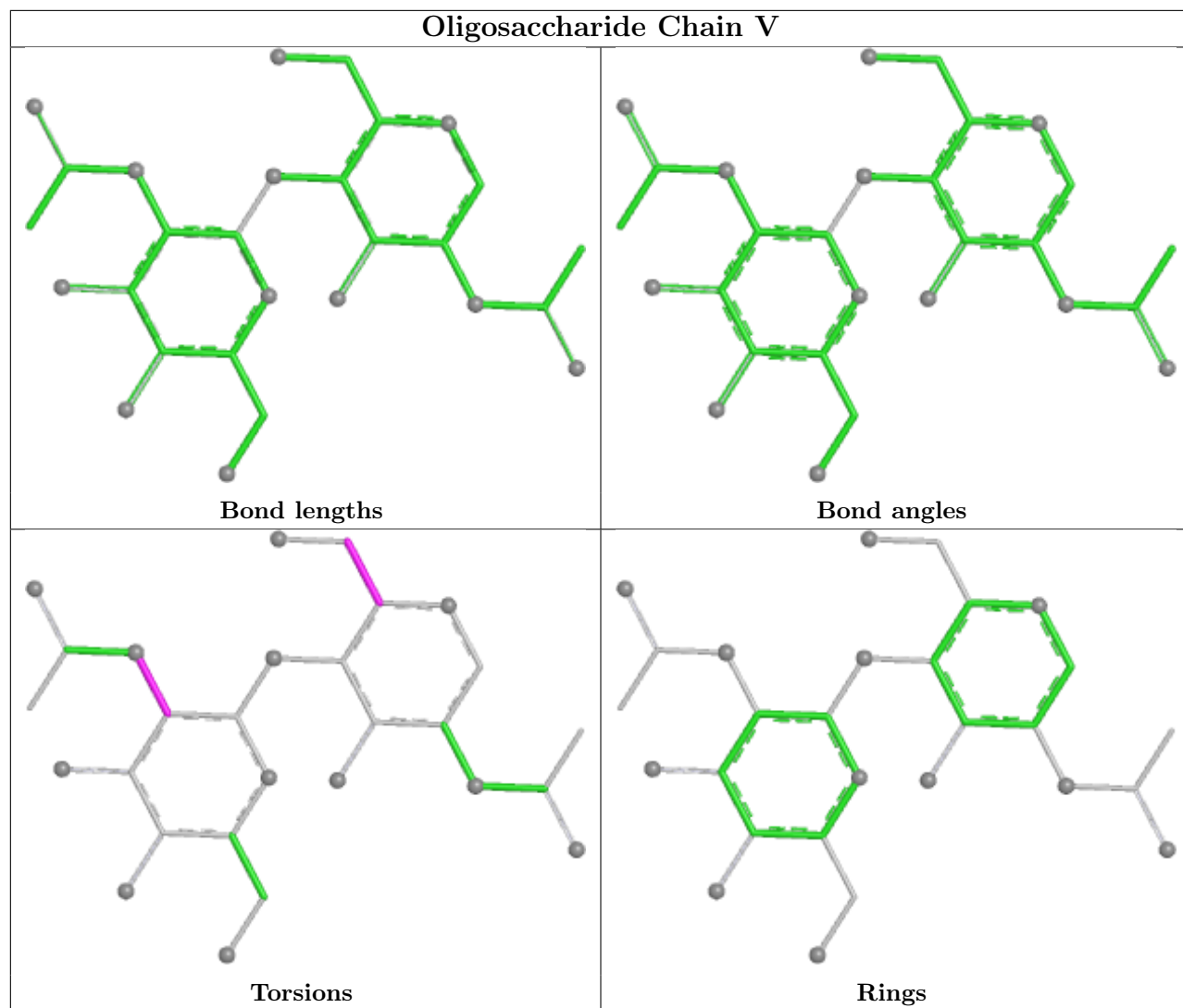


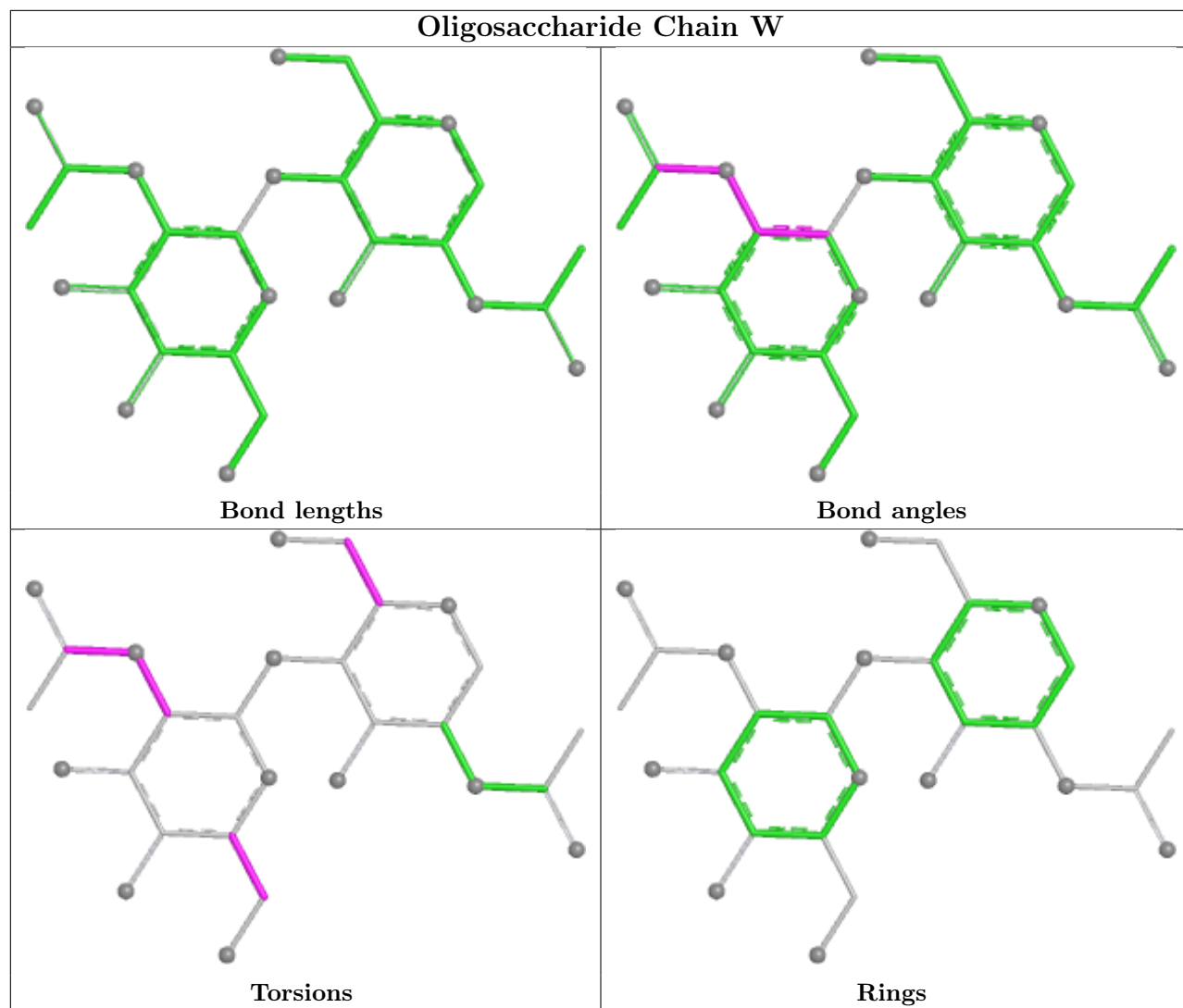


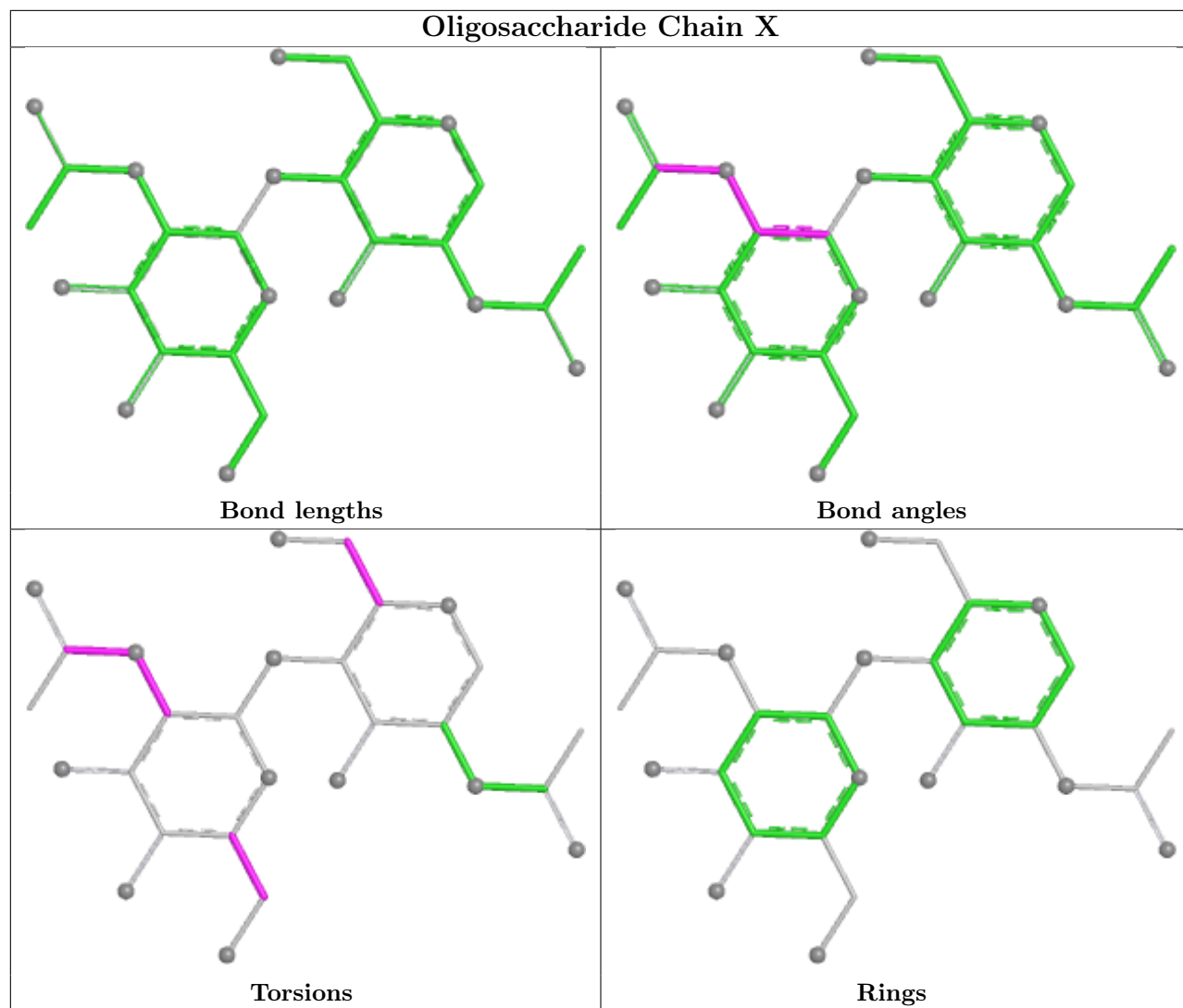


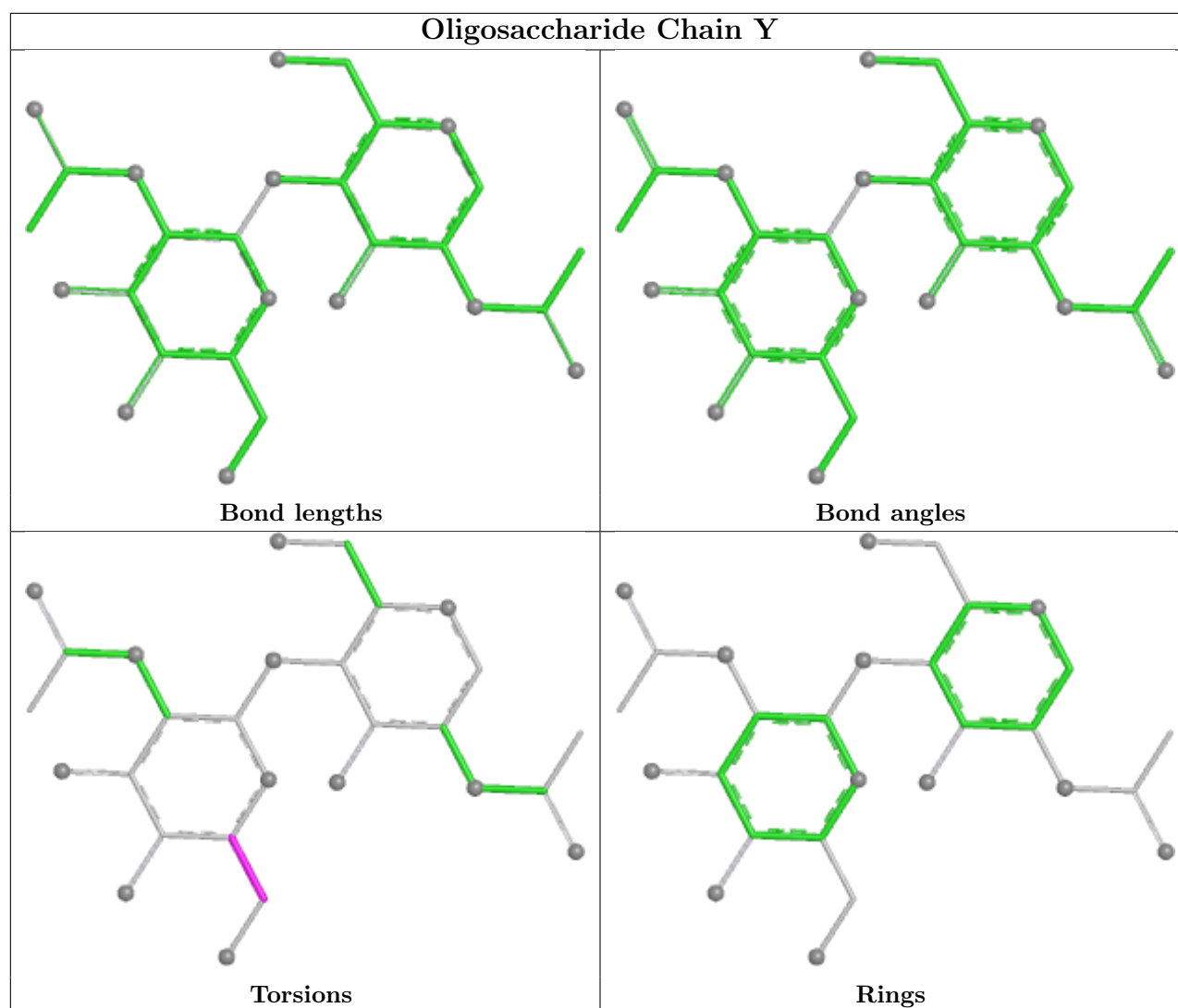












5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	A	1408	1	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	C	1403	1	14,14,15	0.19	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1401	1	14,14,15	0.32	0	17,19,21	0.35	0
3	NAG	B	1409	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
3	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	C	1407	1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	A	1409	1	14,14,15	0.51	0	17,19,21	0.37	0
3	NAG	A	1405	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
3	NAG	C	1404	1	14,14,15	0.49	0	17,19,21	0.54	0
3	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	C	1408	1	14,14,15	0.33	0	17,19,21	0.40	0
3	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.66	0
3	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.67	0
3	NAG	A	1404	1	14,14,15	0.49	0	17,19,21	0.54	0
3	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	C	1405	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
3	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
3	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.66	0
3	NAG	C	1406	1	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	B	1410	-	14,14,15	0.36	0	17,19,21	0.43	0
3	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.39	0
3	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
3	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.34	0
3	NAG	B	1404	1	14,14,15	0.51	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1409	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1405	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1405	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1405	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1404	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1405	NAG	C2-N2-C7	4.62	129.10	122.90
3	C	1405	NAG	C2-N2-C7	4.60	129.07	122.90
3	A	1405	NAG	C2-N2-C7	4.60	129.07	122.90
3	B	1409	NAG	C8-C7-N2	2.29	119.92	116.12
3	B	1409	NAG	C2-N2-C7	-2.20	119.96	122.90
3	C	1405	NAG	C1-C2-N2	2.12	113.78	110.43
3	A	1405	NAG	C1-C2-N2	2.10	113.74	110.43
3	B	1405	NAG	C1-C2-N2	2.10	113.74	110.43

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1406	NAG	O5-C5-C6-O6
3	B	1406	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1406	NAG	O5-C5-C6-O6
3	A	1402	NAG	O5-C5-C6-O6
3	A	1404	NAG	O5-C5-C6-O6
3	B	1402	NAG	O5-C5-C6-O6
3	B	1404	NAG	O5-C5-C6-O6
3	C	1404	NAG	O5-C5-C6-O6
3	C	1405	NAG	O5-C5-C6-O6
3	A	1401	NAG	O5-C5-C6-O6
3	C	1401	NAG	O5-C5-C6-O6
3	C	1402	NAG	O5-C5-C6-O6
3	A	1402	NAG	C4-C5-C6-O6
3	B	1402	NAG	C4-C5-C6-O6
3	C	1402	NAG	C4-C5-C6-O6
3	A	1405	NAG	O5-C5-C6-O6
3	B	1401	NAG	O5-C5-C6-O6
3	B	1405	NAG	O5-C5-C6-O6
3	A	1409	NAG	C4-C5-C6-O6
3	A	1405	NAG	C4-C5-C6-O6
3	B	1405	NAG	C4-C5-C6-O6
3	C	1405	NAG	C4-C5-C6-O6
3	B	1408	NAG	O5-C5-C6-O6
3	A	1408	NAG	O5-C5-C6-O6
3	C	1408	NAG	O5-C5-C6-O6
3	A	1409	NAG	O5-C5-C6-O6
3	A	1406	NAG	C4-C5-C6-O6
3	B	1406	NAG	C4-C5-C6-O6
3	C	1406	NAG	C4-C5-C6-O6
3	A	1405	NAG	C8-C7-N2-C2
3	A	1405	NAG	O7-C7-N2-C2
3	B	1405	NAG	C8-C7-N2-C2
3	B	1405	NAG	O7-C7-N2-C2
3	C	1405	NAG	C8-C7-N2-C2
3	C	1405	NAG	O7-C7-N2-C2
3	A	1404	NAG	C4-C5-C6-O6
3	B	1404	NAG	C4-C5-C6-O6
3	C	1404	NAG	C4-C5-C6-O6
3	A	1403	NAG	C4-C5-C6-O6
3	B	1403	NAG	C4-C5-C6-O6
3	C	1403	NAG	C4-C5-C6-O6
3	A	1403	NAG	O5-C5-C6-O6
3	B	1403	NAG	O5-C5-C6-O6
3	C	1403	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1408	NAG	C4-C5-C6-O6
3	C	1408	NAG	C4-C5-C6-O6
3	A	1408	NAG	C4-C5-C6-O6
3	A	1401	NAG	C4-C5-C6-O6
3	B	1401	NAG	C4-C5-C6-O6
3	C	1401	NAG	C4-C5-C6-O6
3	A	1405	NAG	C1-C2-N2-C7
3	B	1405	NAG	C1-C2-N2-C7
3	C	1405	NAG	C1-C2-N2-C7
3	A	1405	NAG	C3-C2-N2-C7
3	B	1405	NAG	C3-C2-N2-C7
3	C	1405	NAG	C3-C2-N2-C7

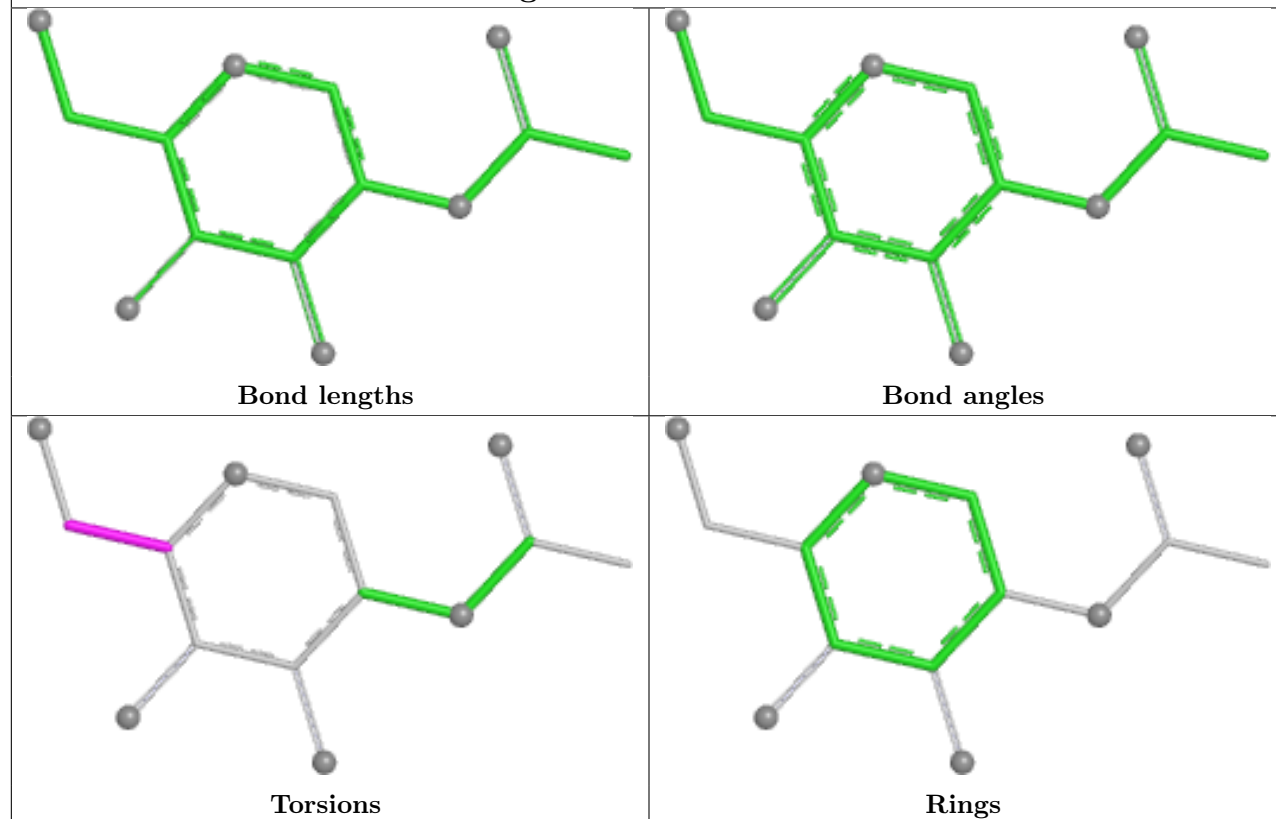
There are no ring outliers.

8 monomers are involved in 18 short contacts:

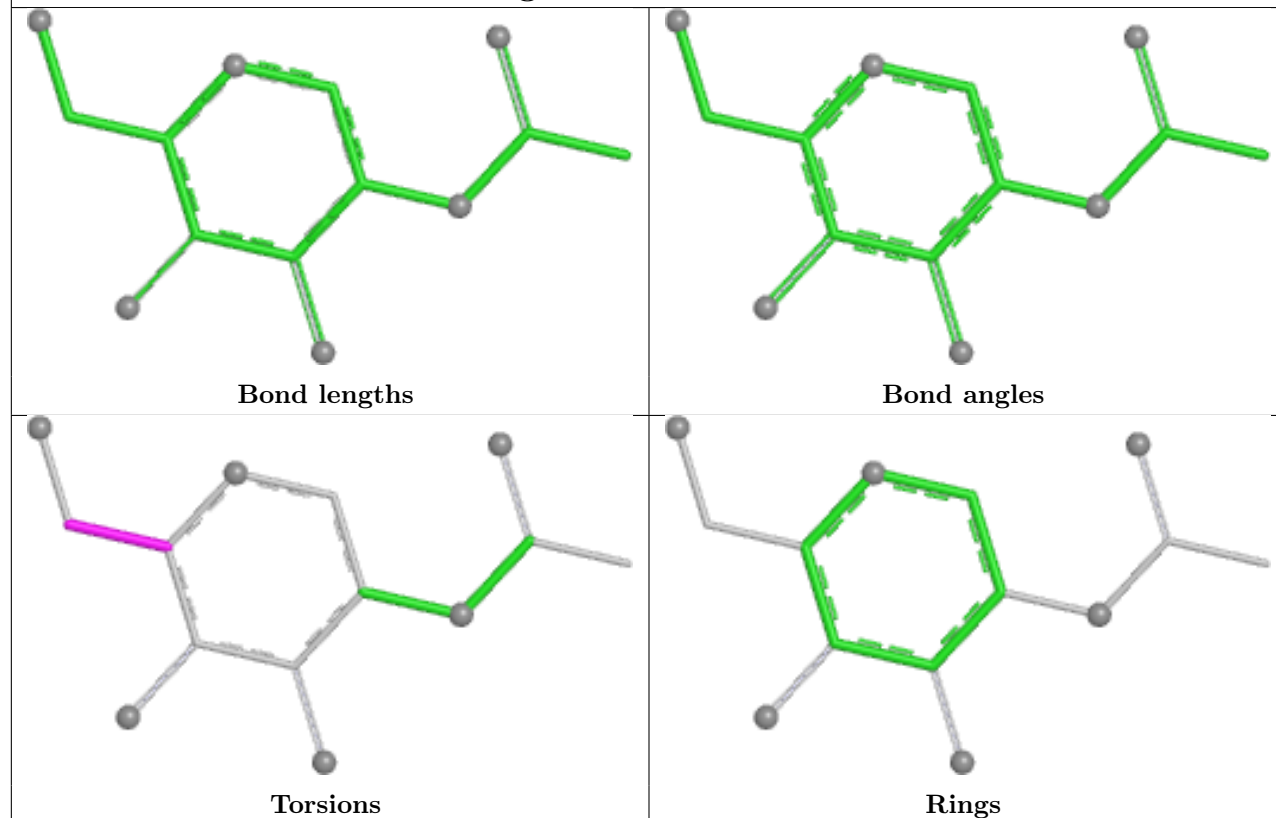
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1409	NAG	4	0
3	A	1405	NAG	1	0
3	B	1402	NAG	3	0
3	C	1402	NAG	3	0
3	C	1405	NAG	3	0
3	B	1405	NAG	1	0
3	A	1402	NAG	3	0
3	B	1410	NAG	4	0

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.

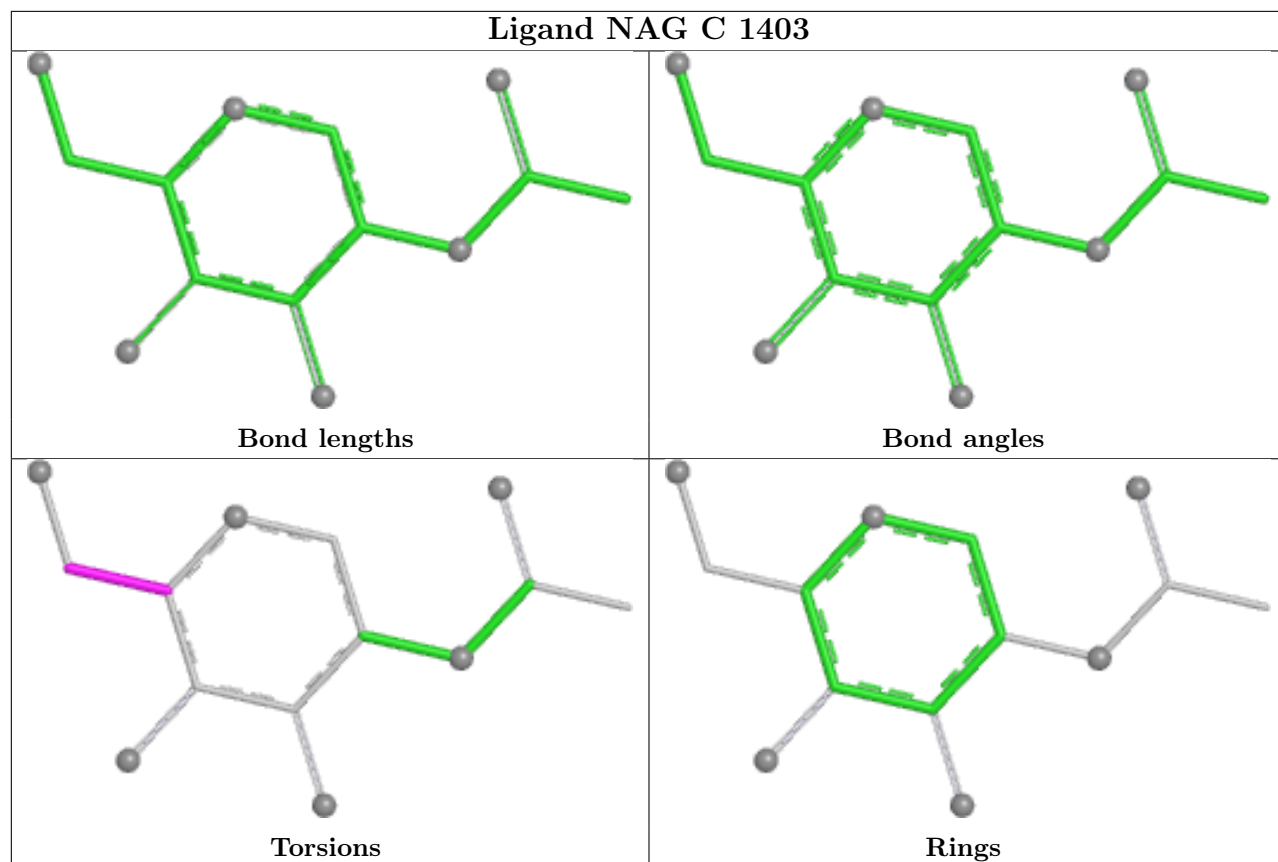
Ligand NAG B 1406



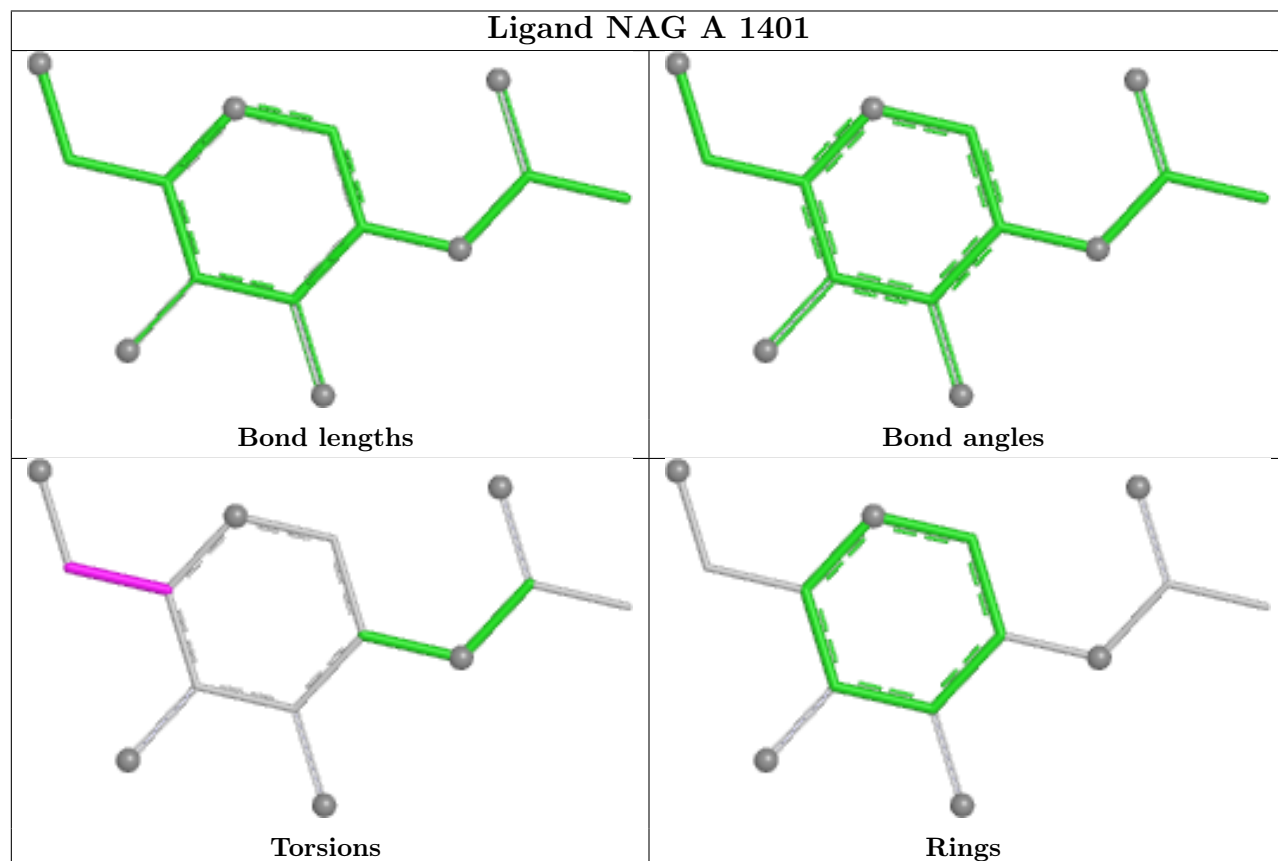
Ligand NAG A 1408

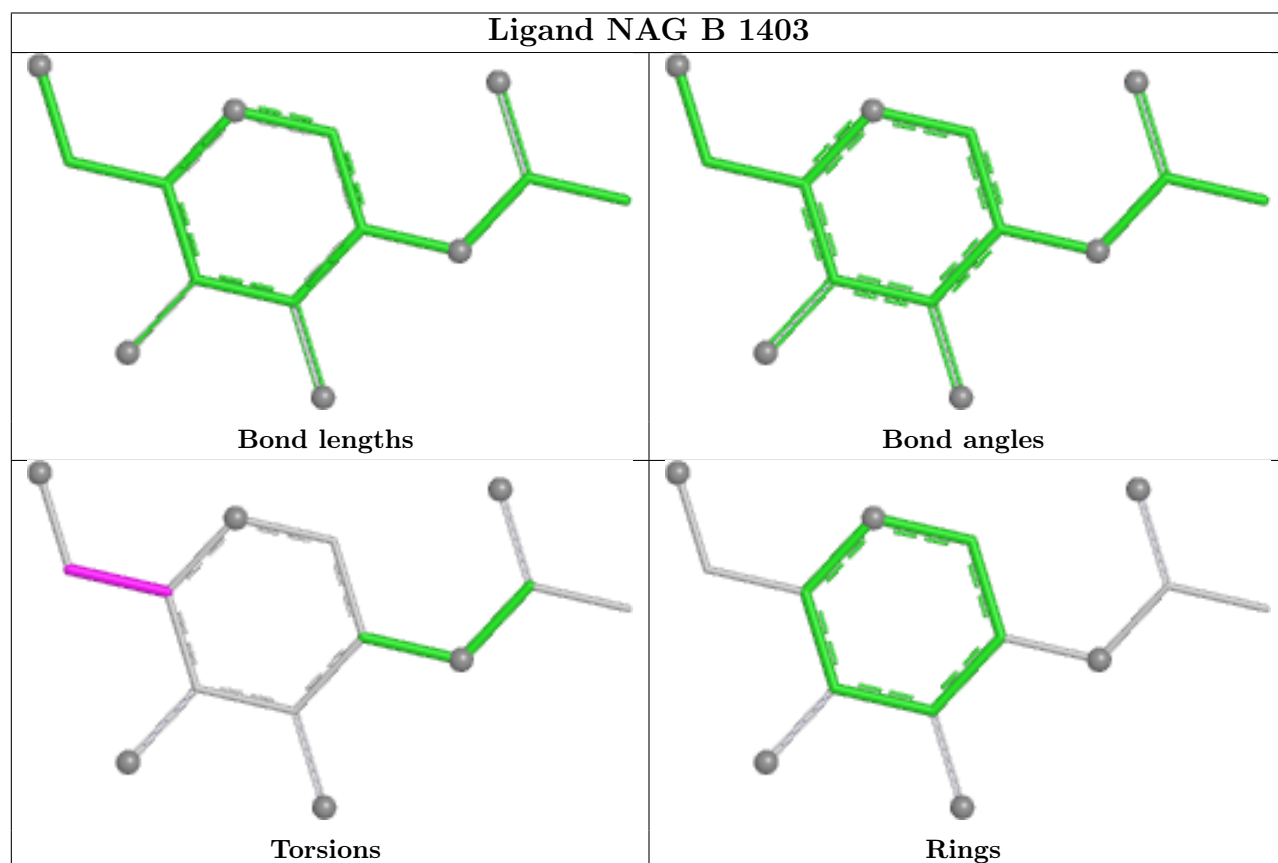
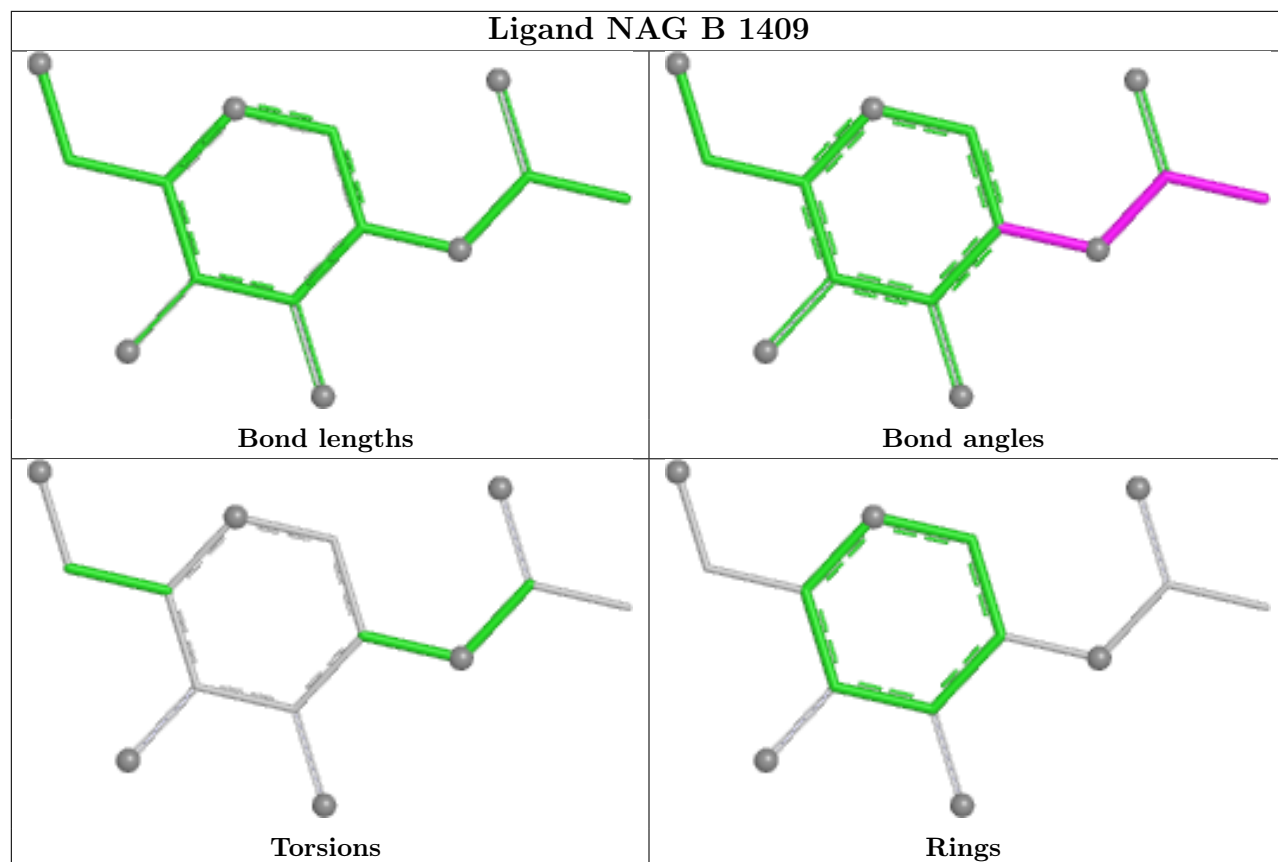


Ligand NAG C 1403

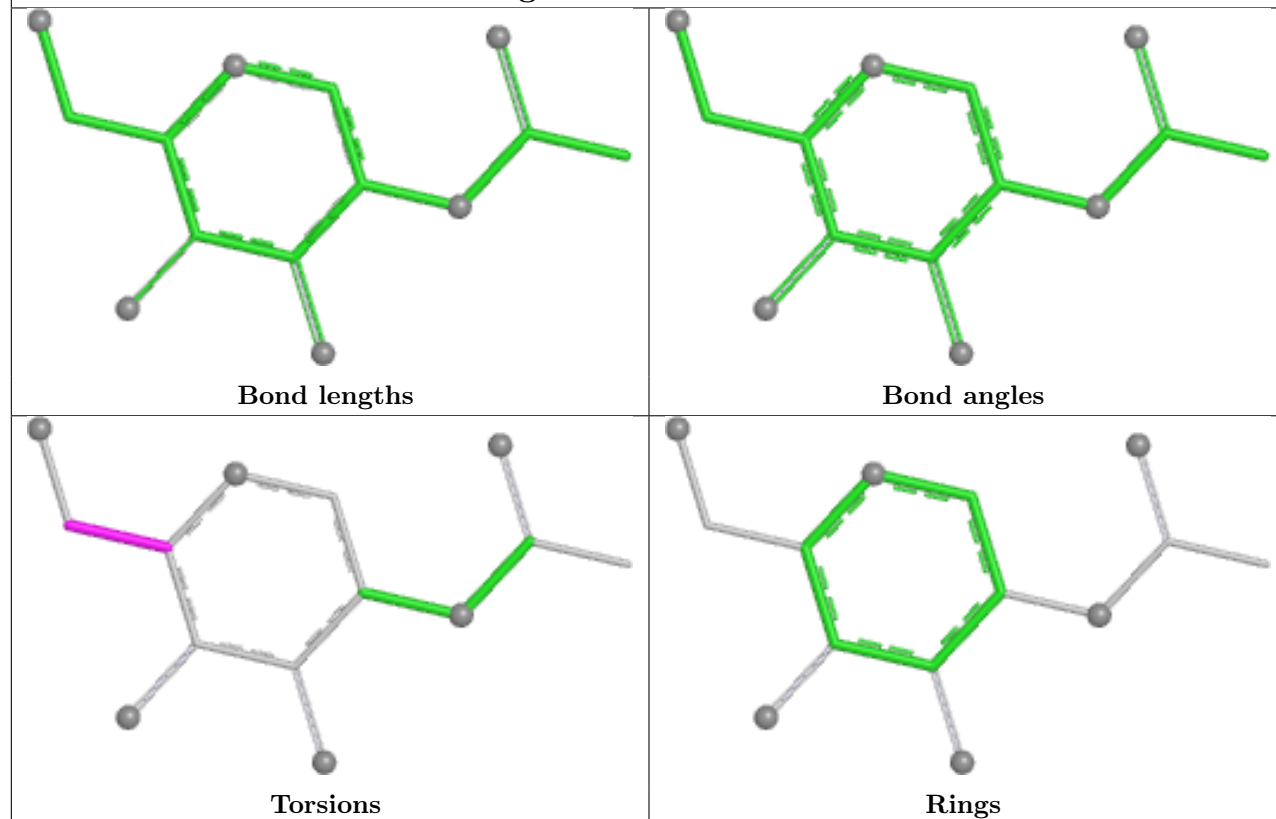


Ligand NAG A 1401

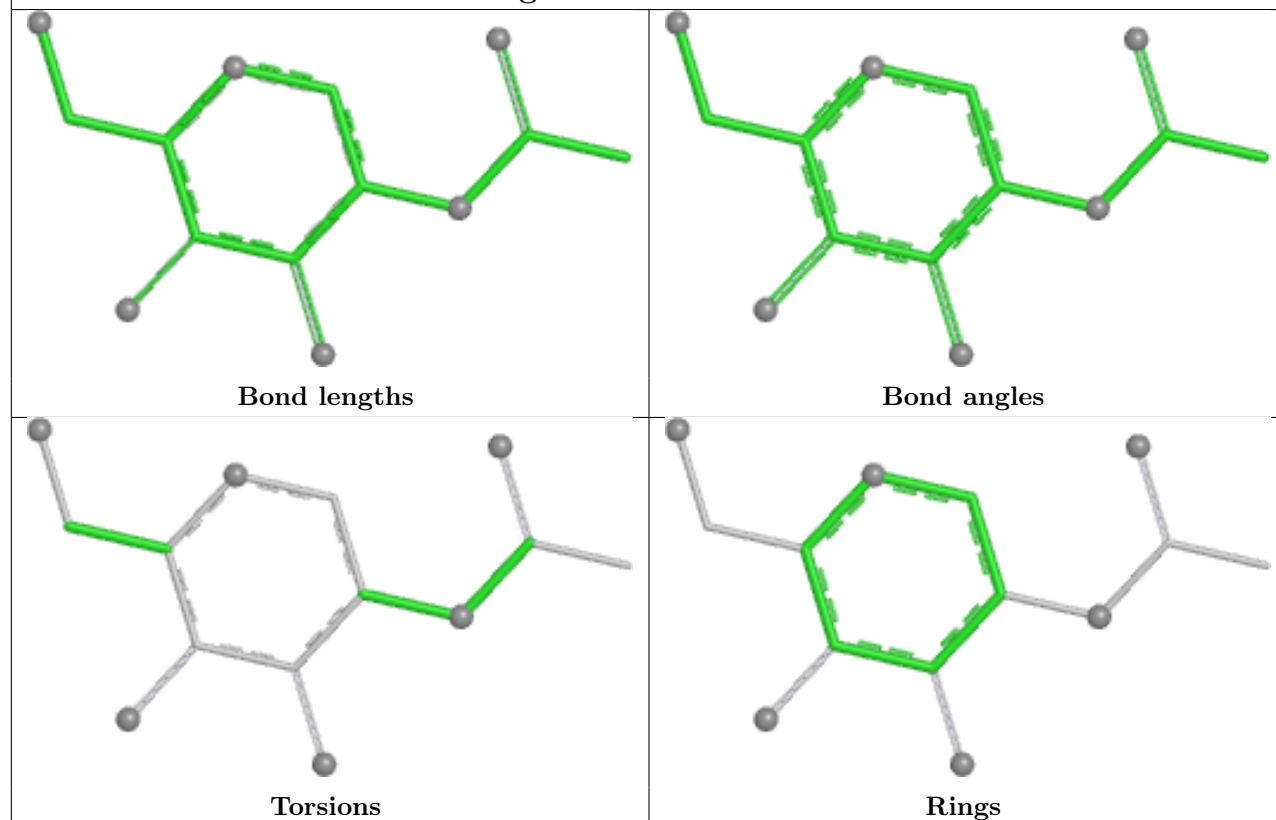




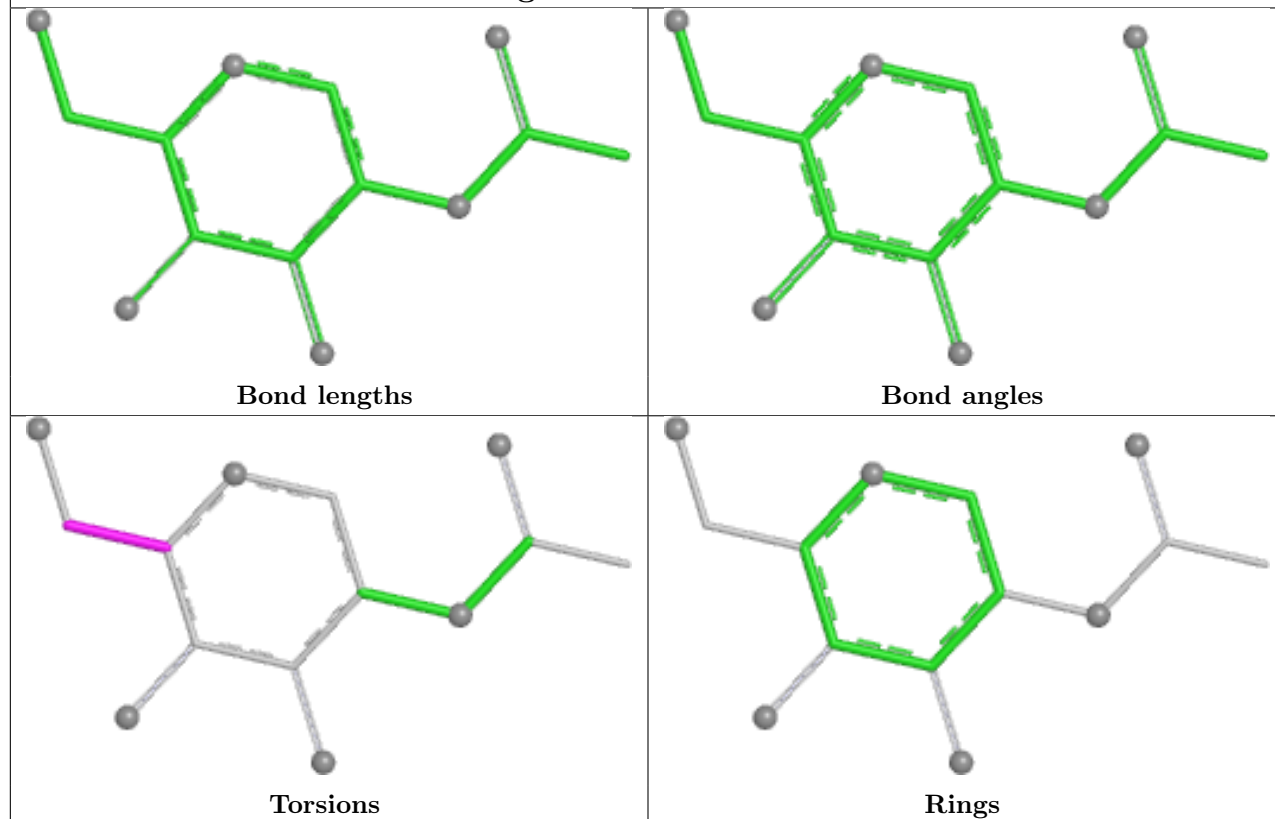
Ligand NAG A 1406



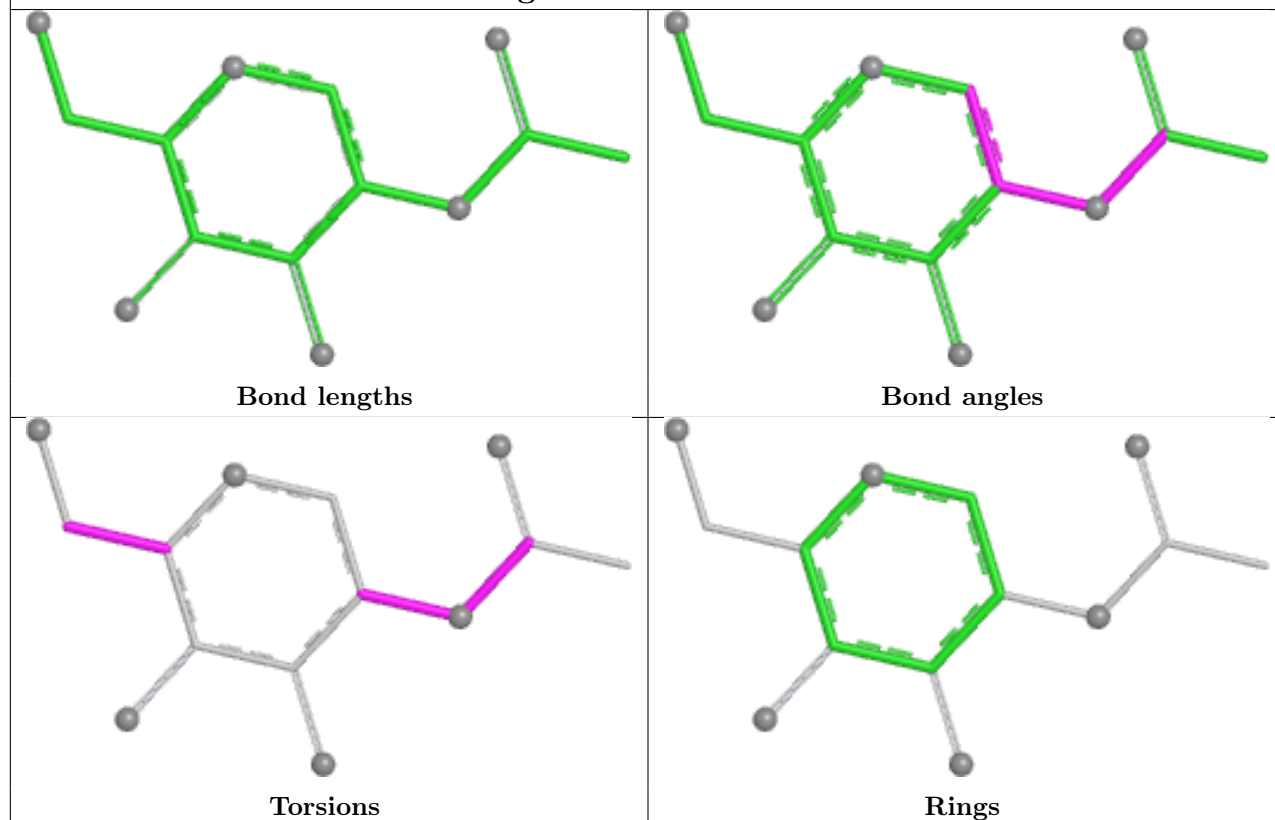
Ligand NAG C 1407



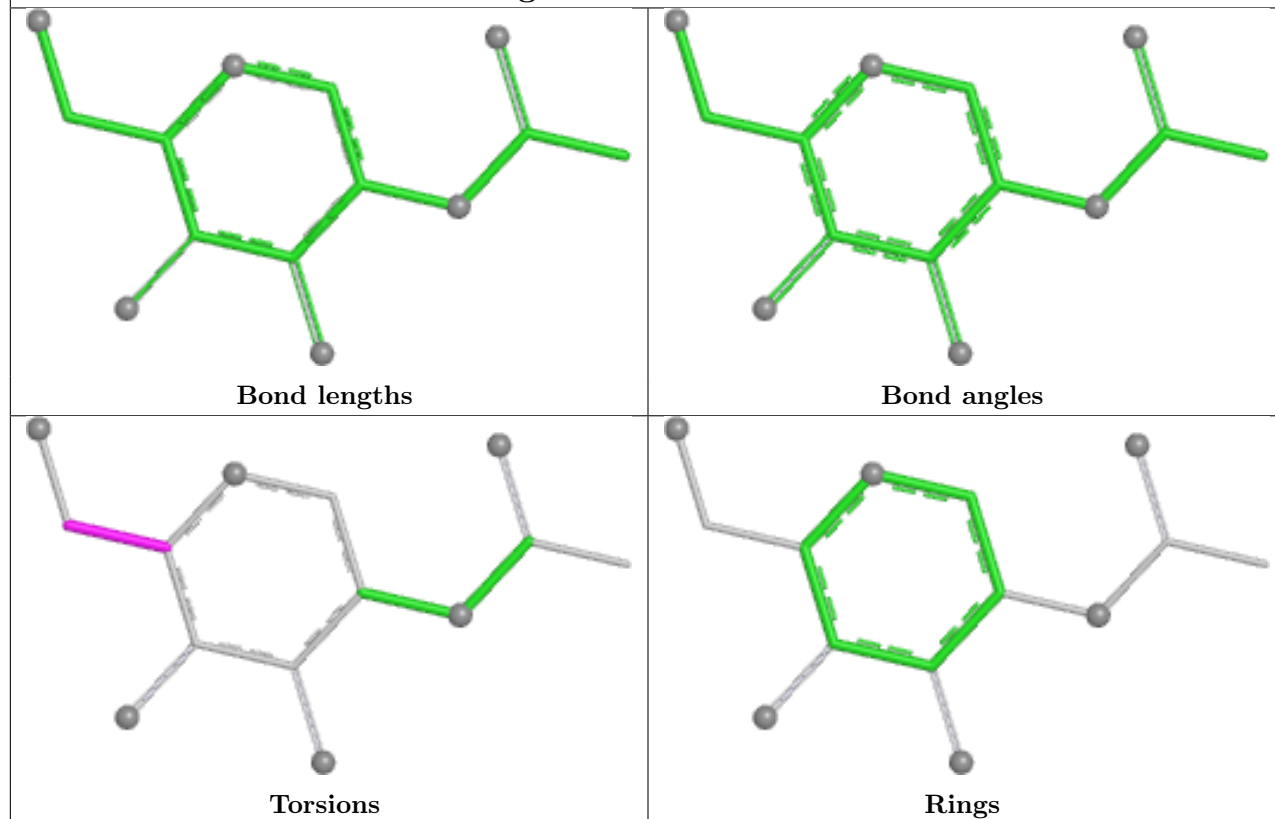
Ligand NAG A 1409



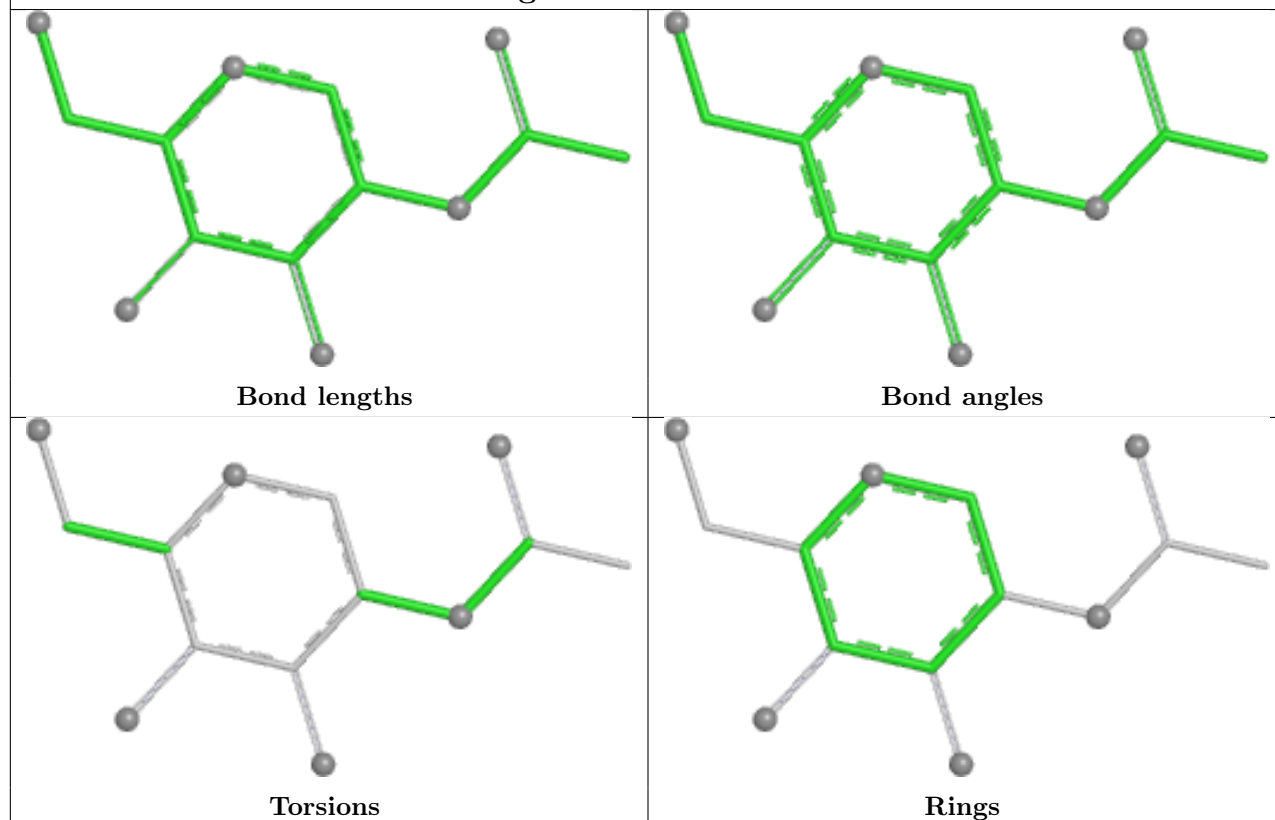
Ligand NAG A 1405



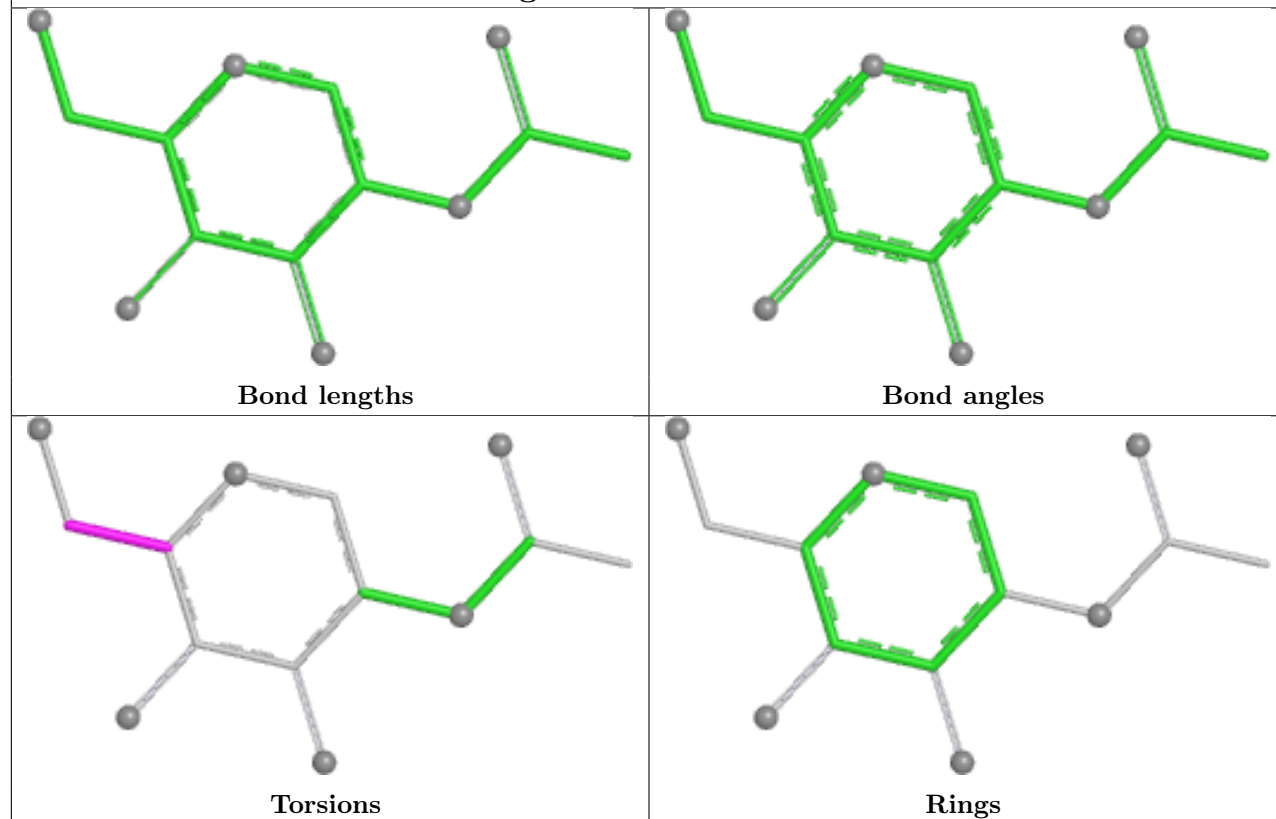
Ligand NAG C 1404



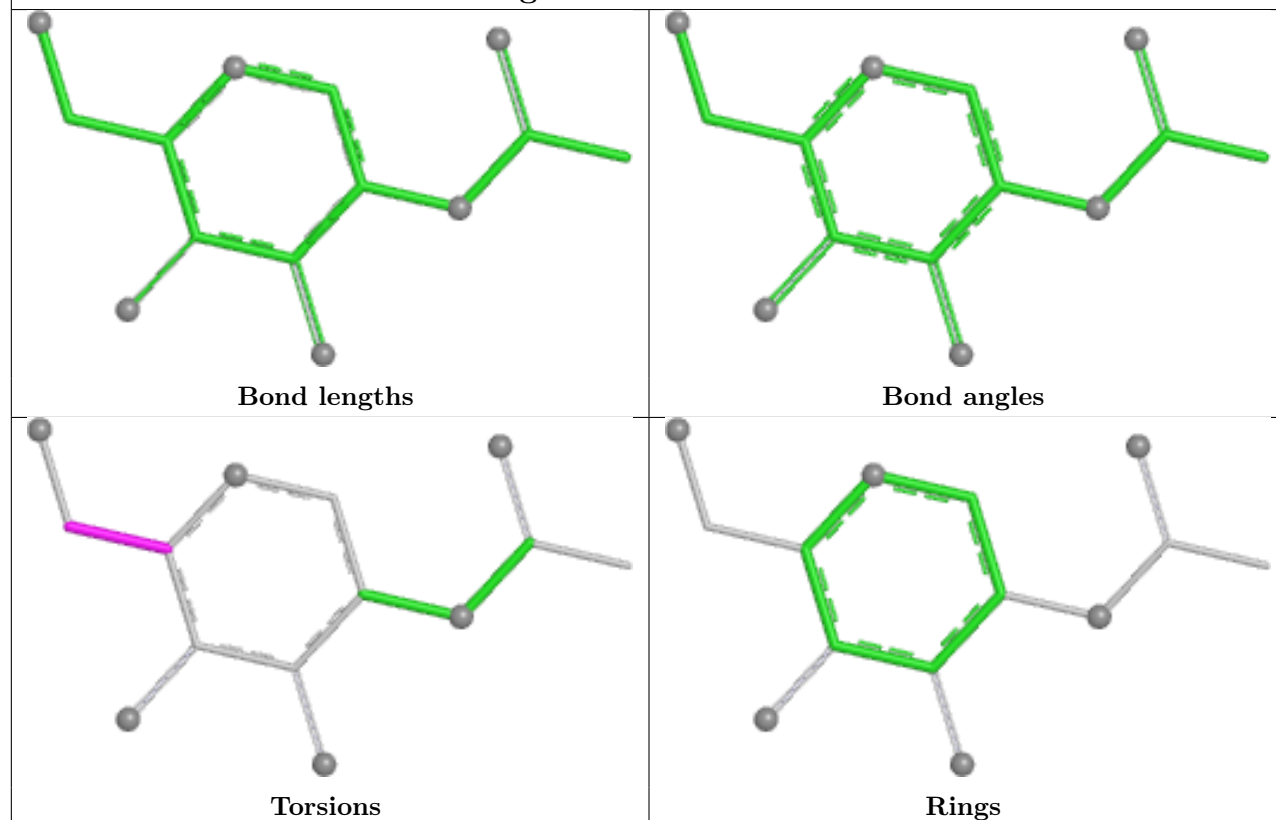
Ligand NAG B 1407



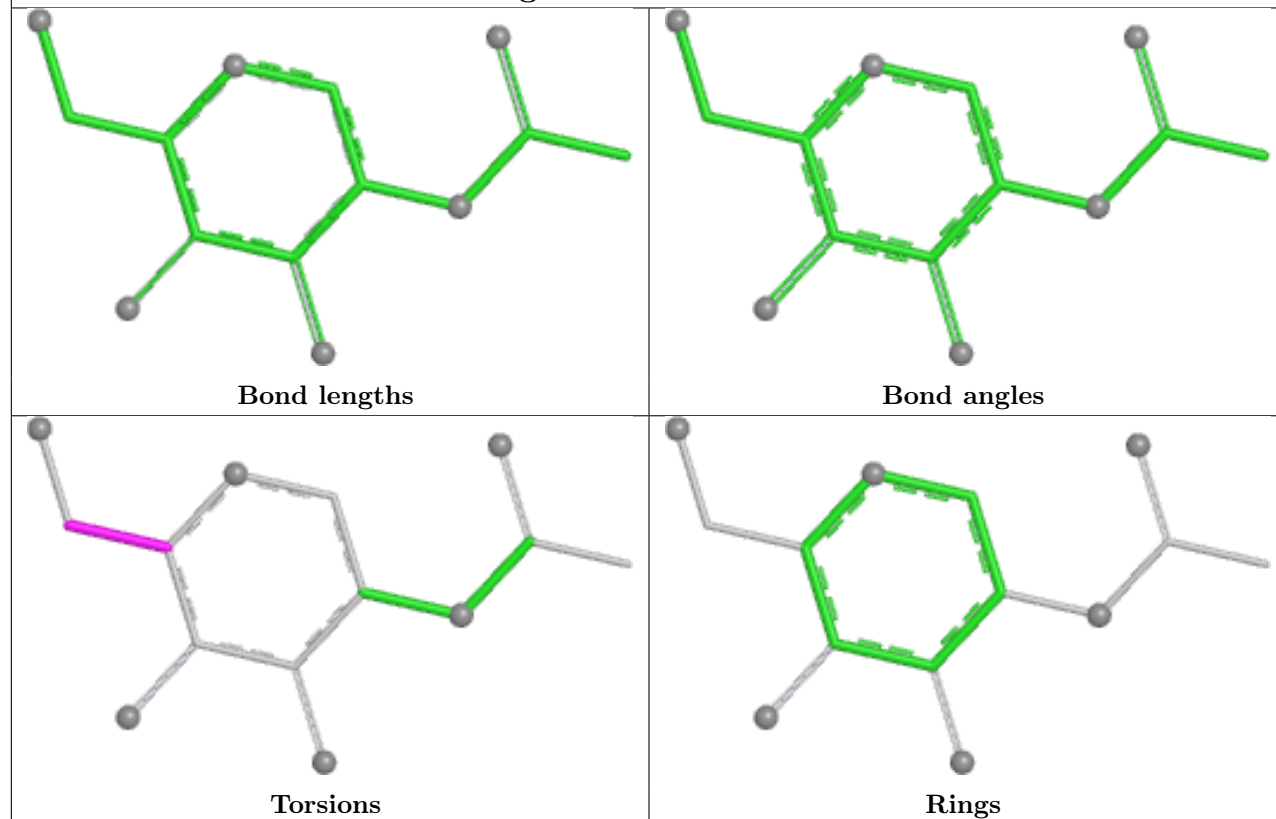
Ligand NAG C 1408



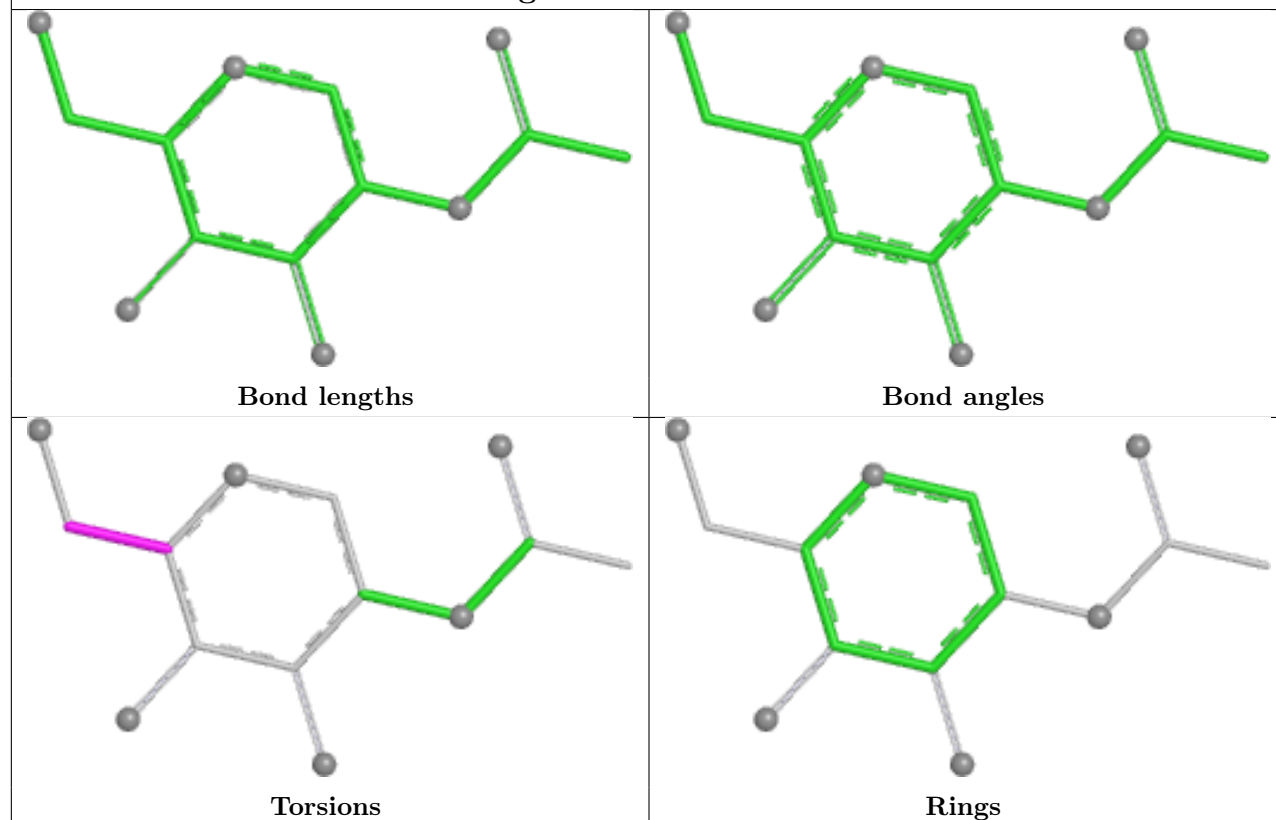
Ligand NAG B 1402



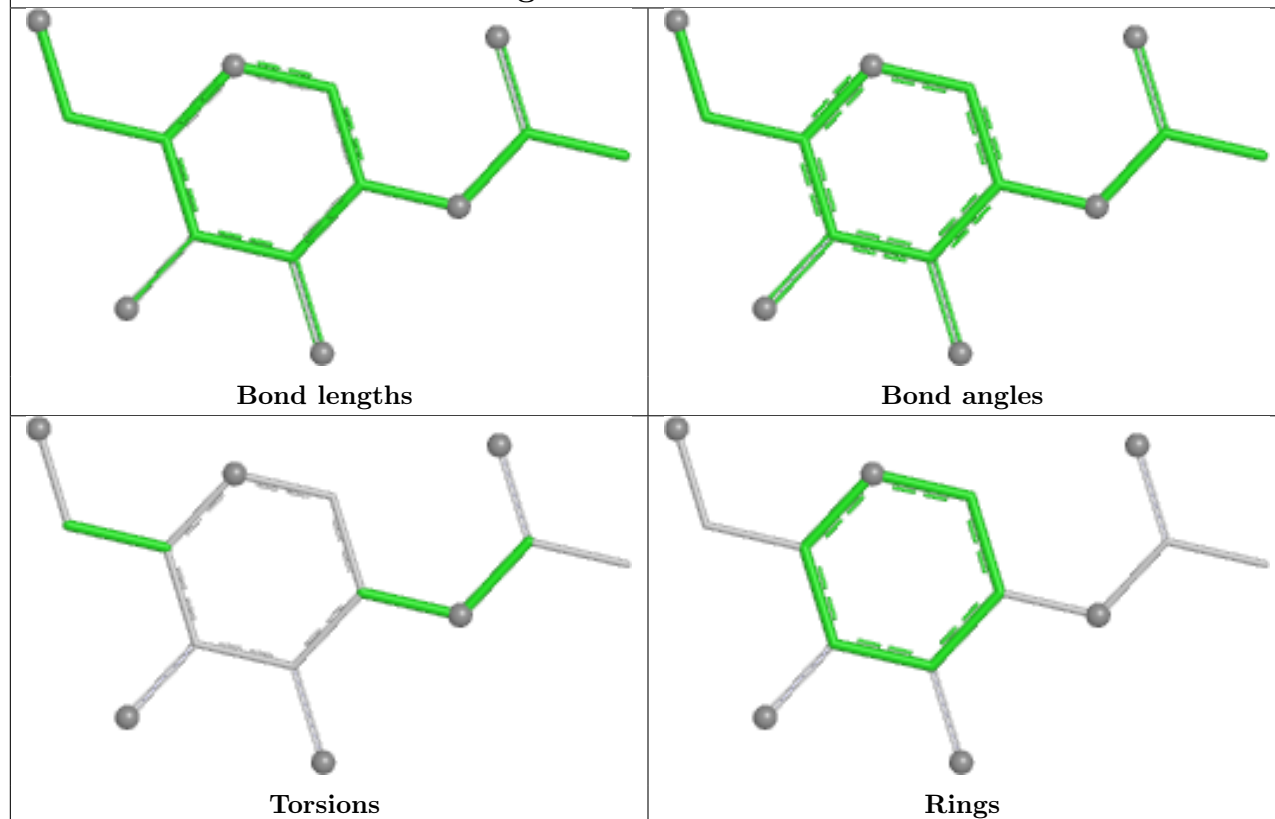
Ligand NAG C 1402



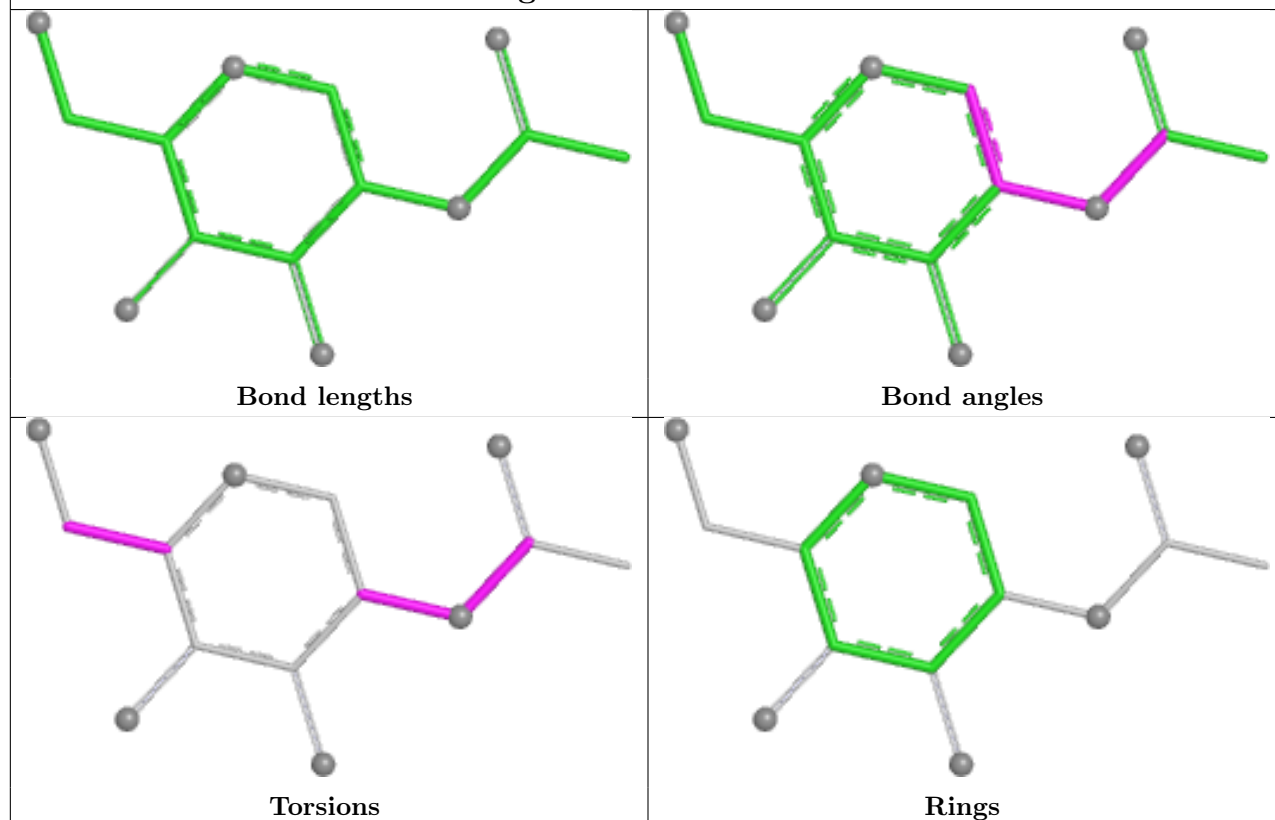
Ligand NAG A 1404

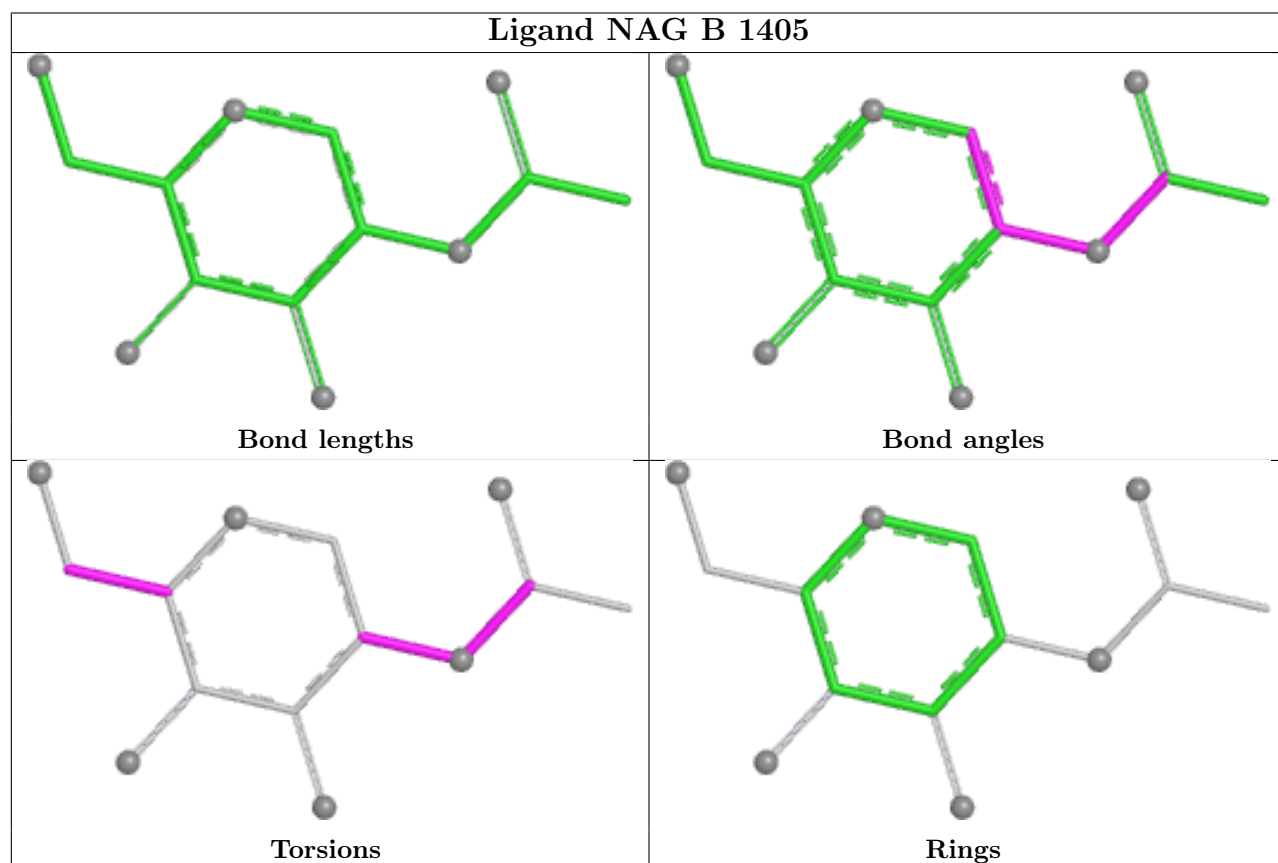
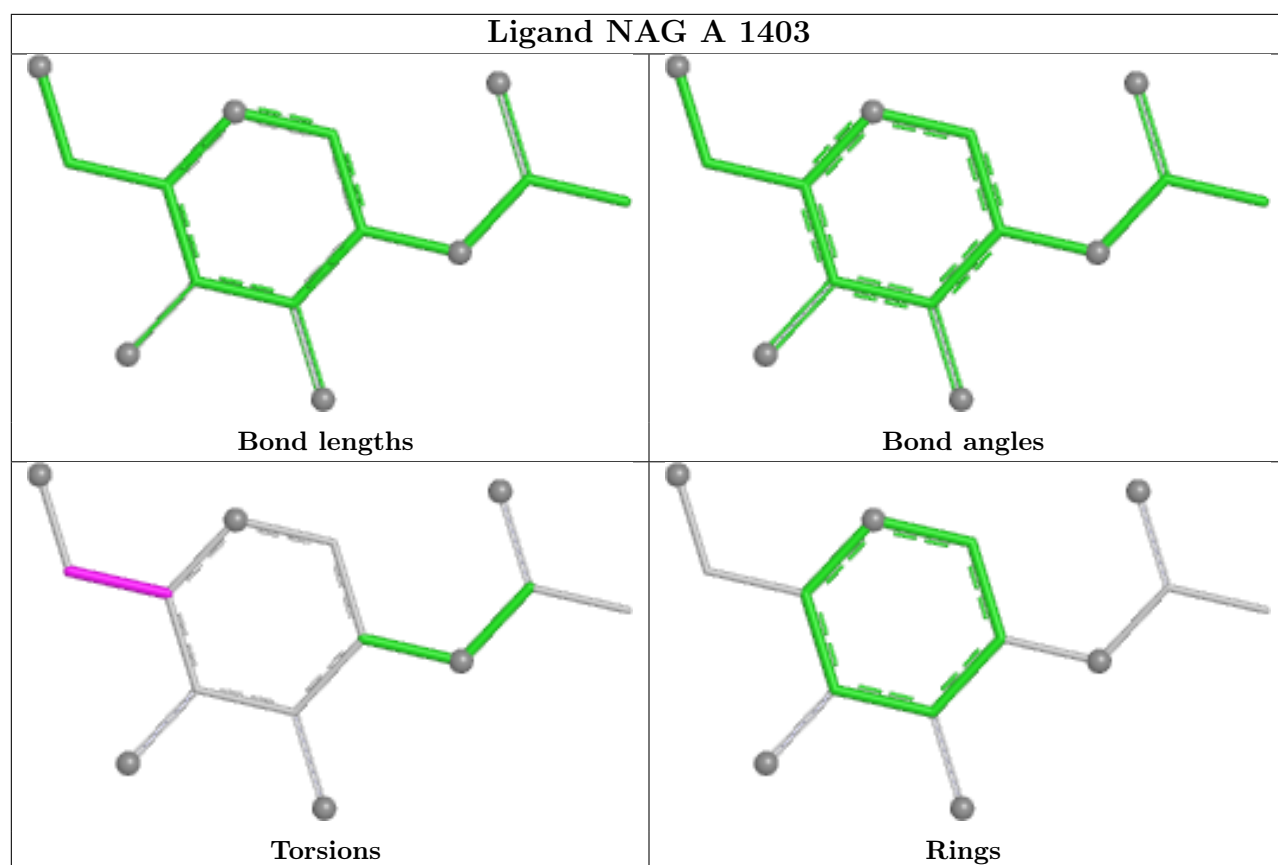


Ligand NAG A 1407

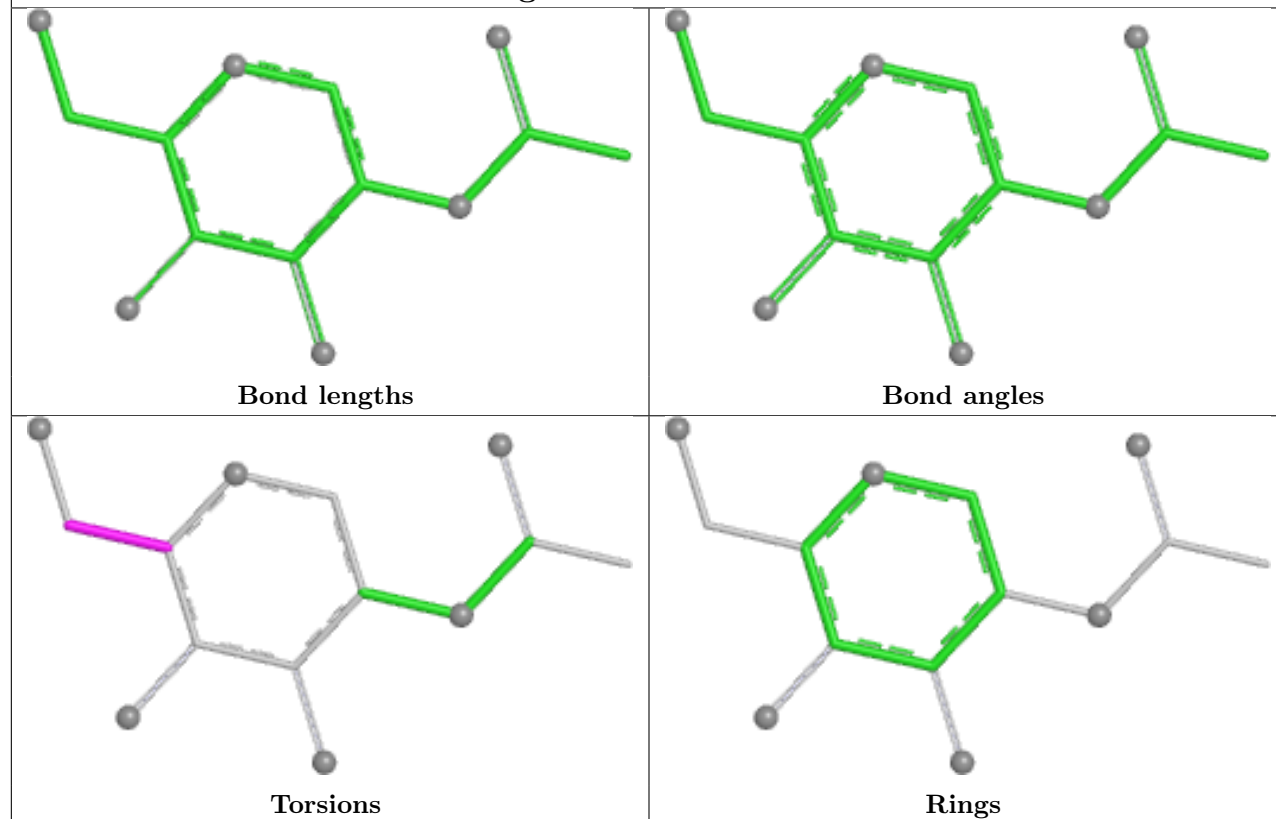


Ligand NAG C 1405

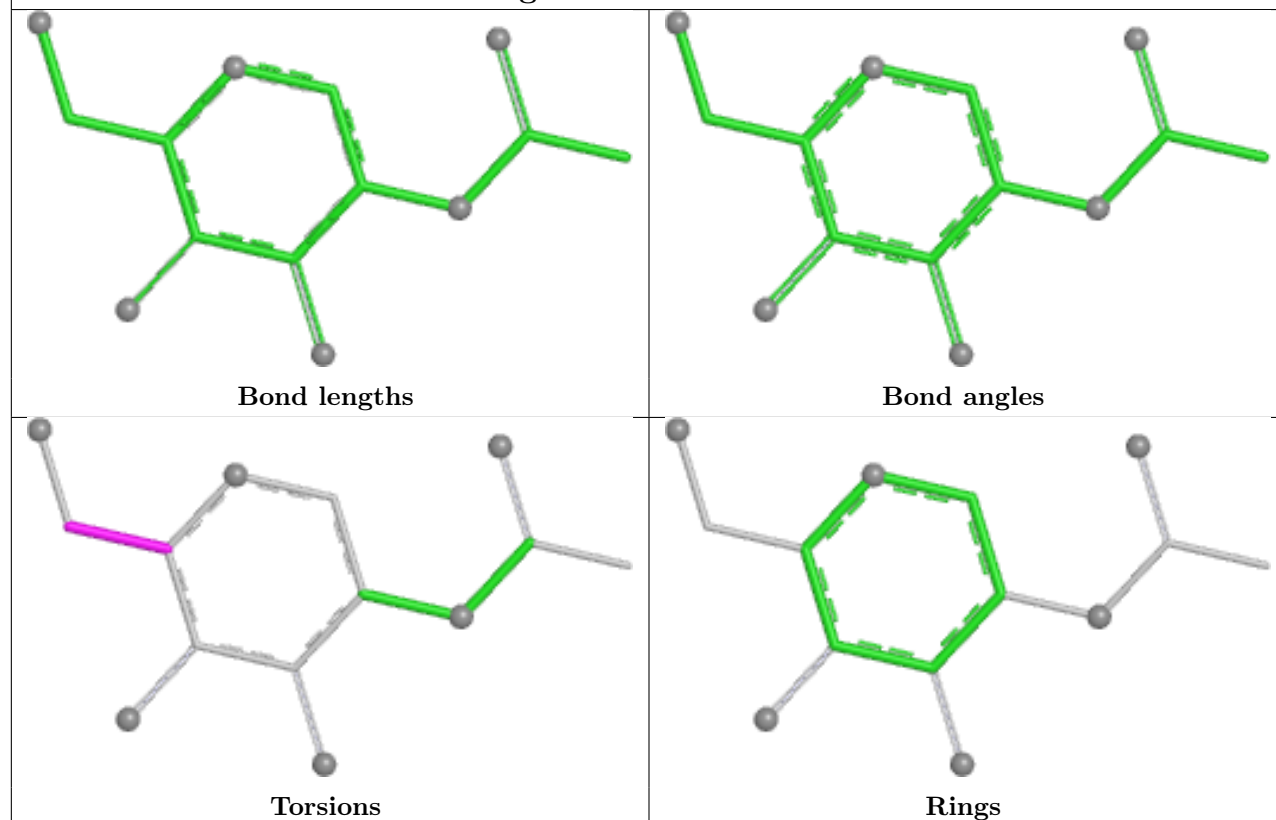




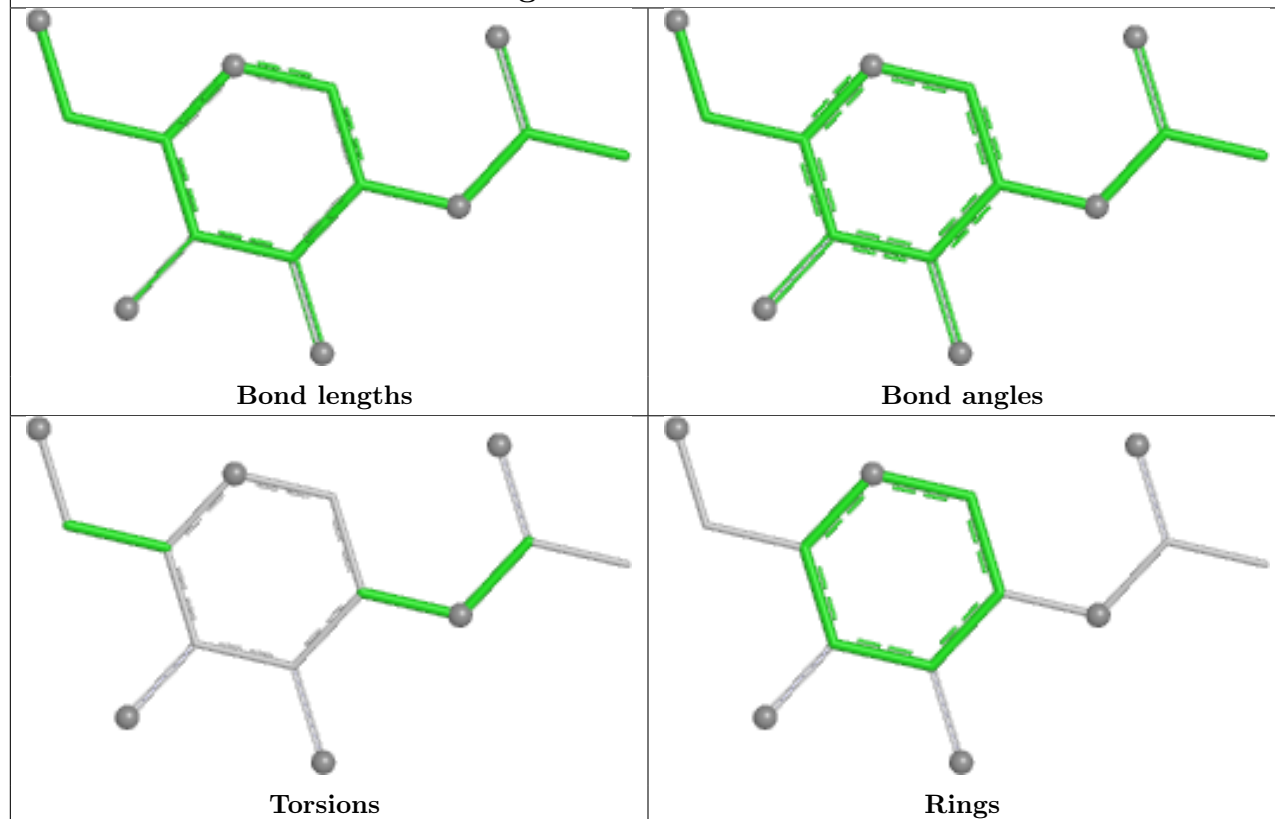
Ligand NAG A 1402



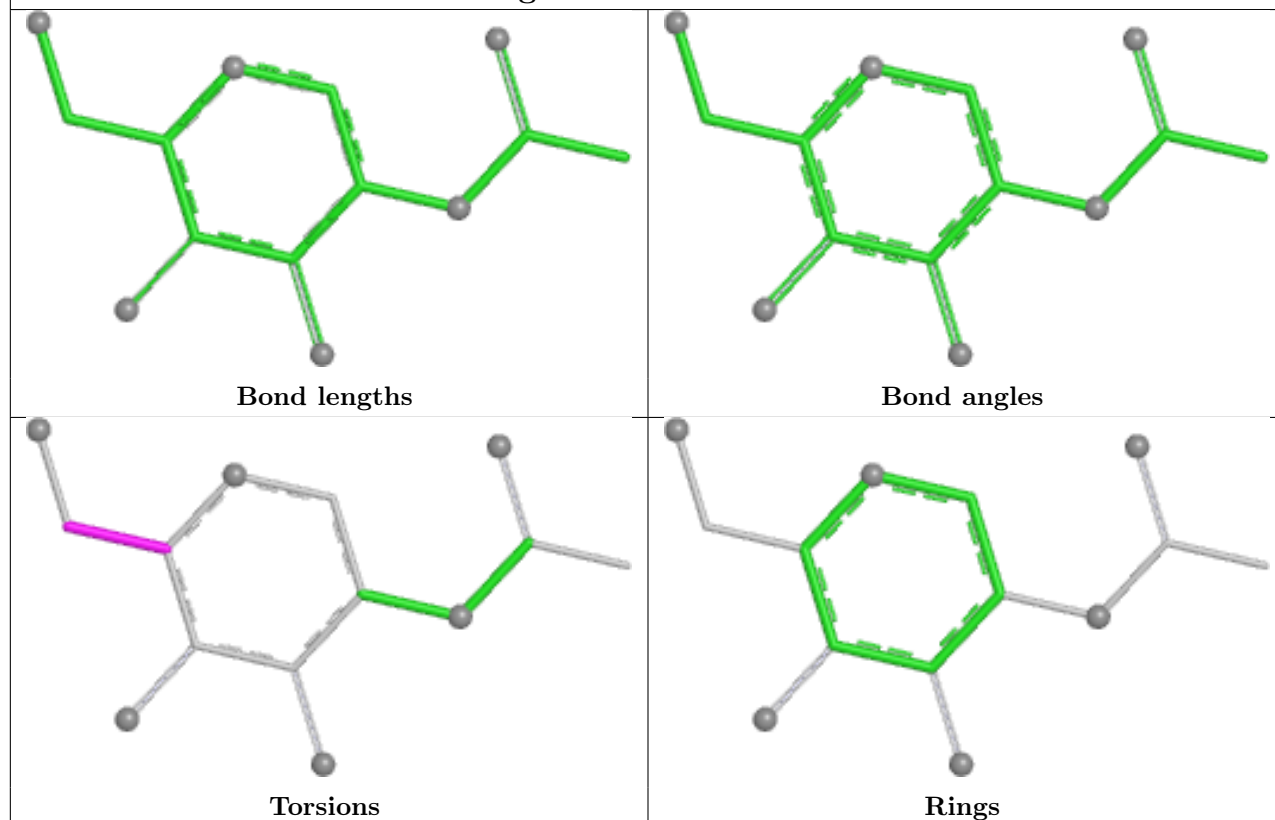
Ligand NAG C 1406



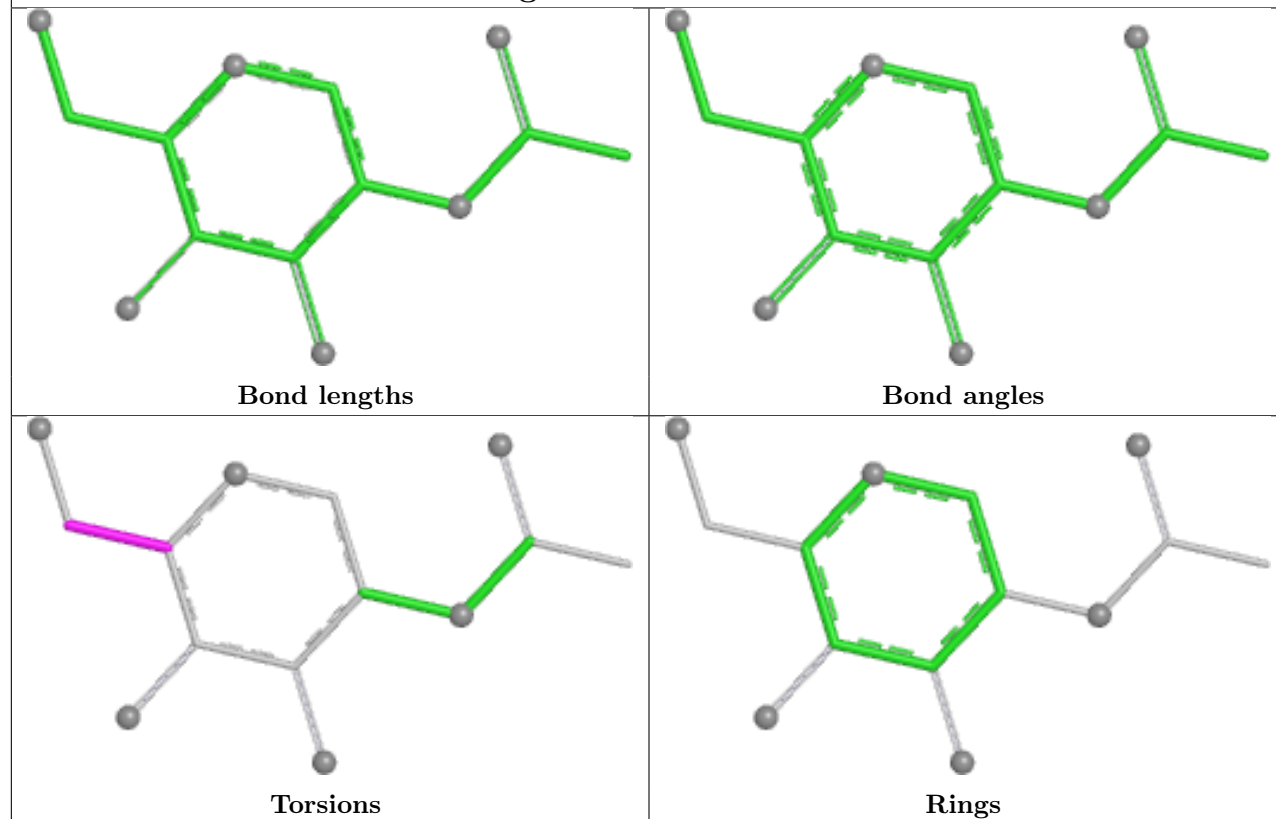
Ligand NAG B 1410



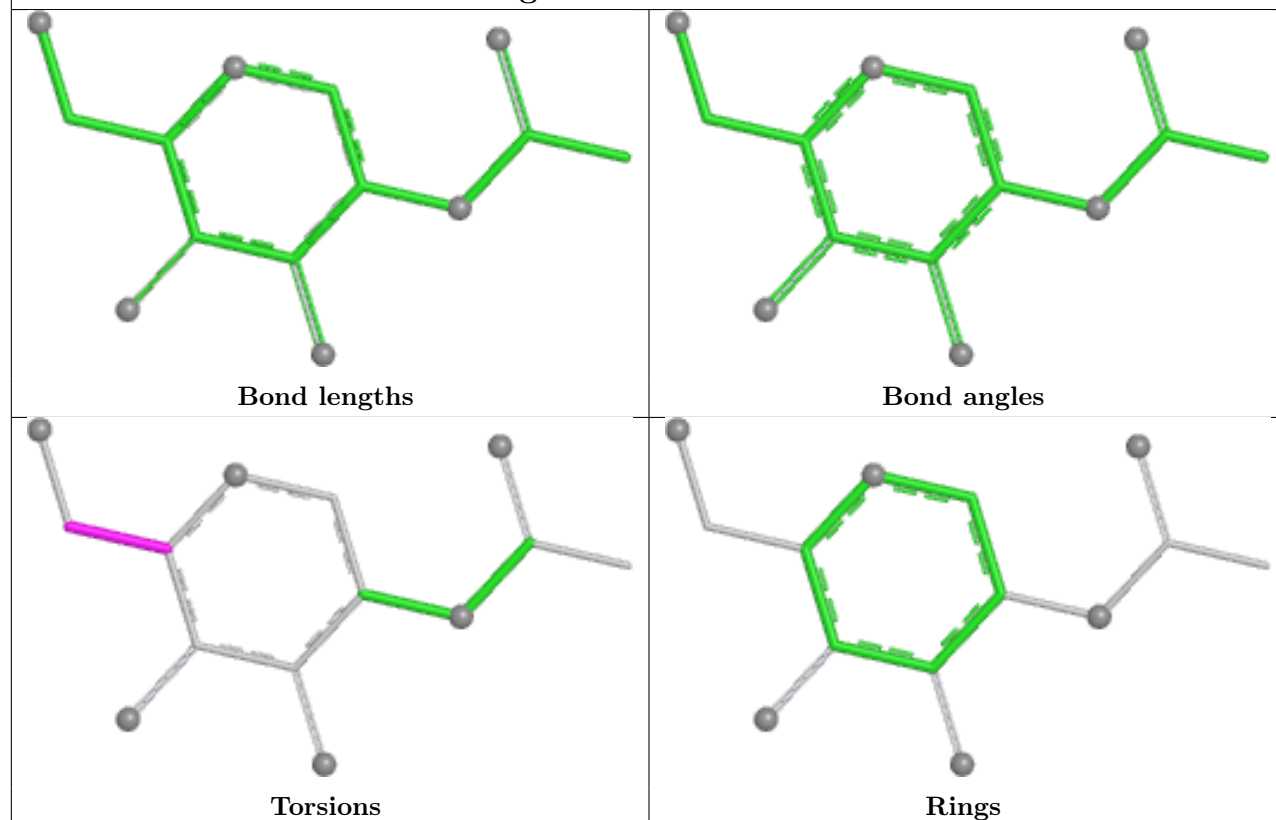
Ligand NAG B 1408

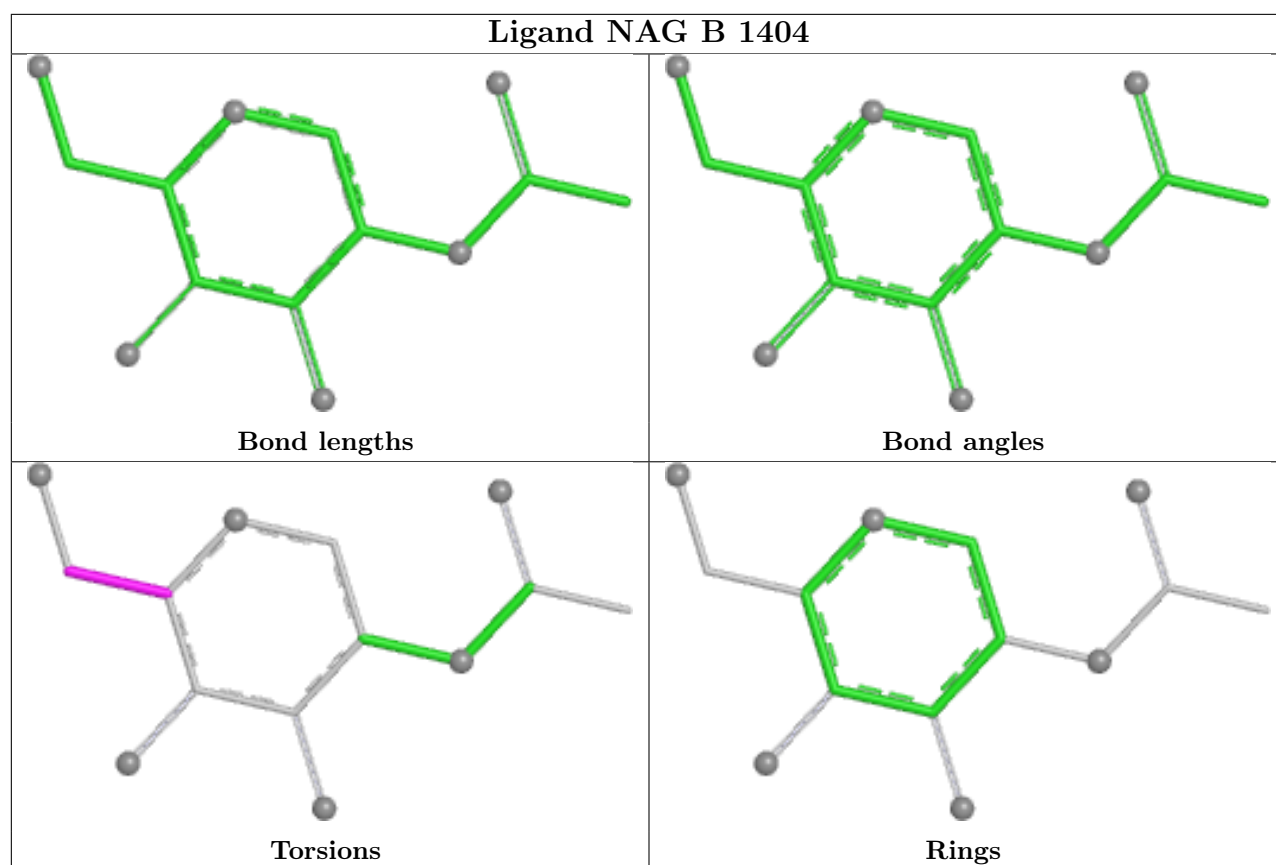


Ligand NAG C 1401



Ligand NAG B 1401





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.

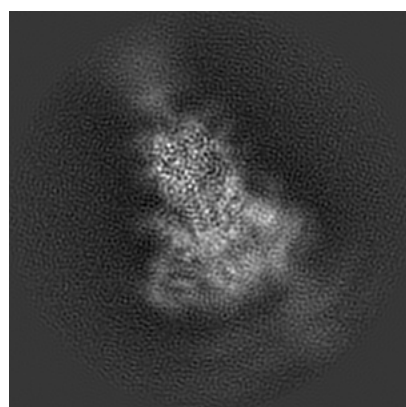
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30894. These allow visual inspection of the internal detail of the map and identification of artifacts.

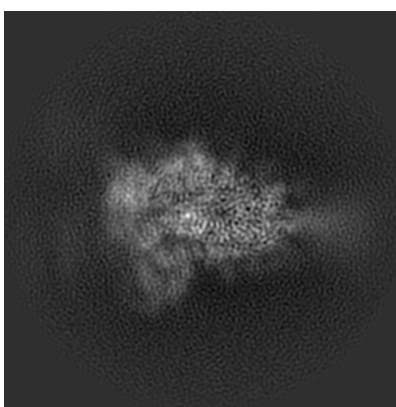
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

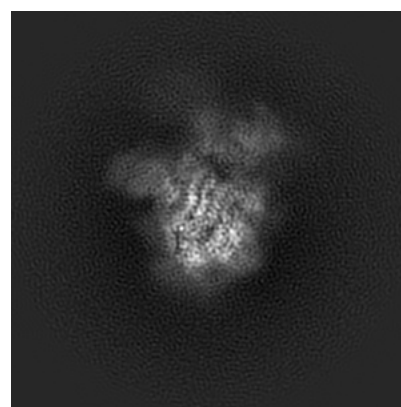
6.1.1 Primary map



X



Y

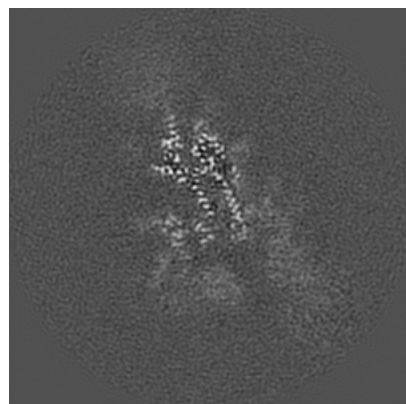


Z

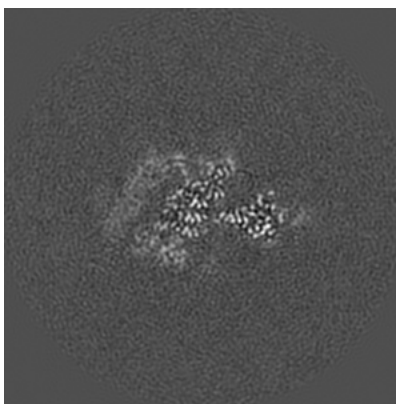
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

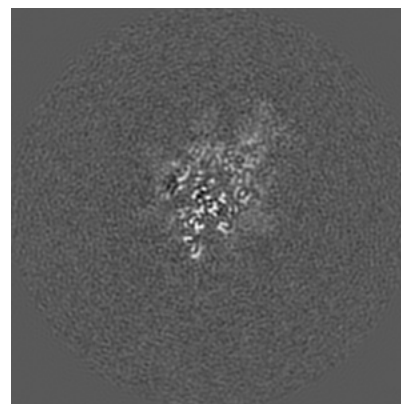
6.2.1 Primary map



X Index: 144



Y Index: 144

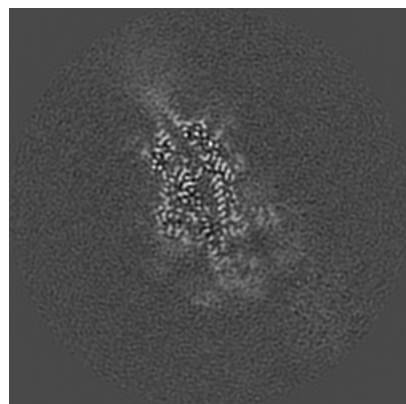


Z Index: 144

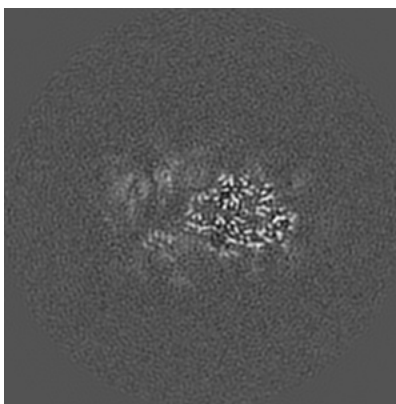
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

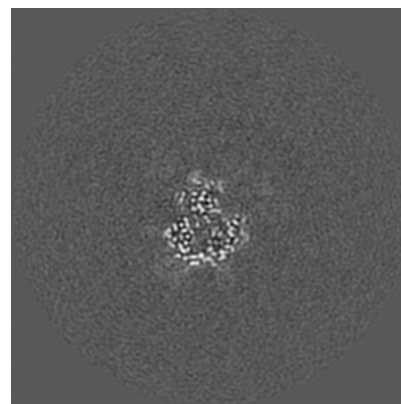
6.3.1 Primary map



X Index: 131



Y Index: 133

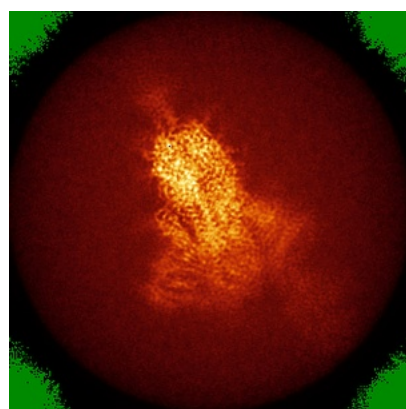


Z Index: 173

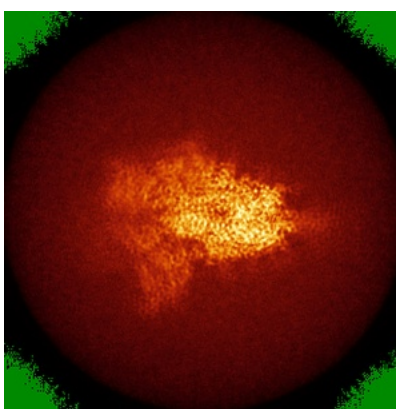
The images above show the largest variance slices of the map in three orthogonal directions.

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

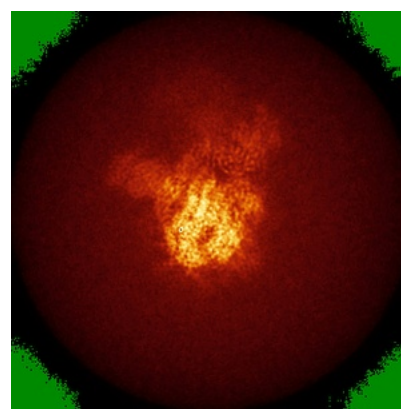
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

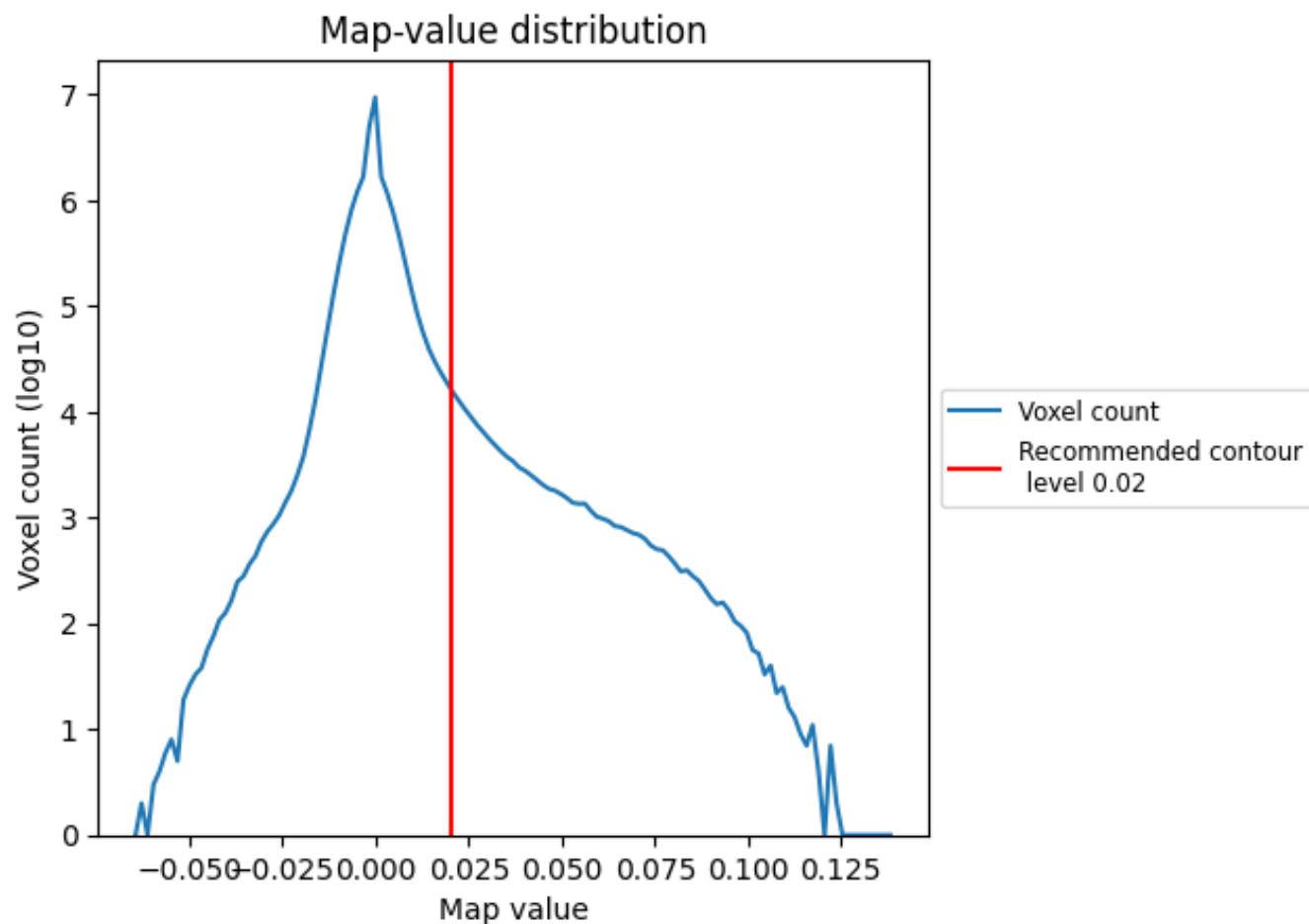
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

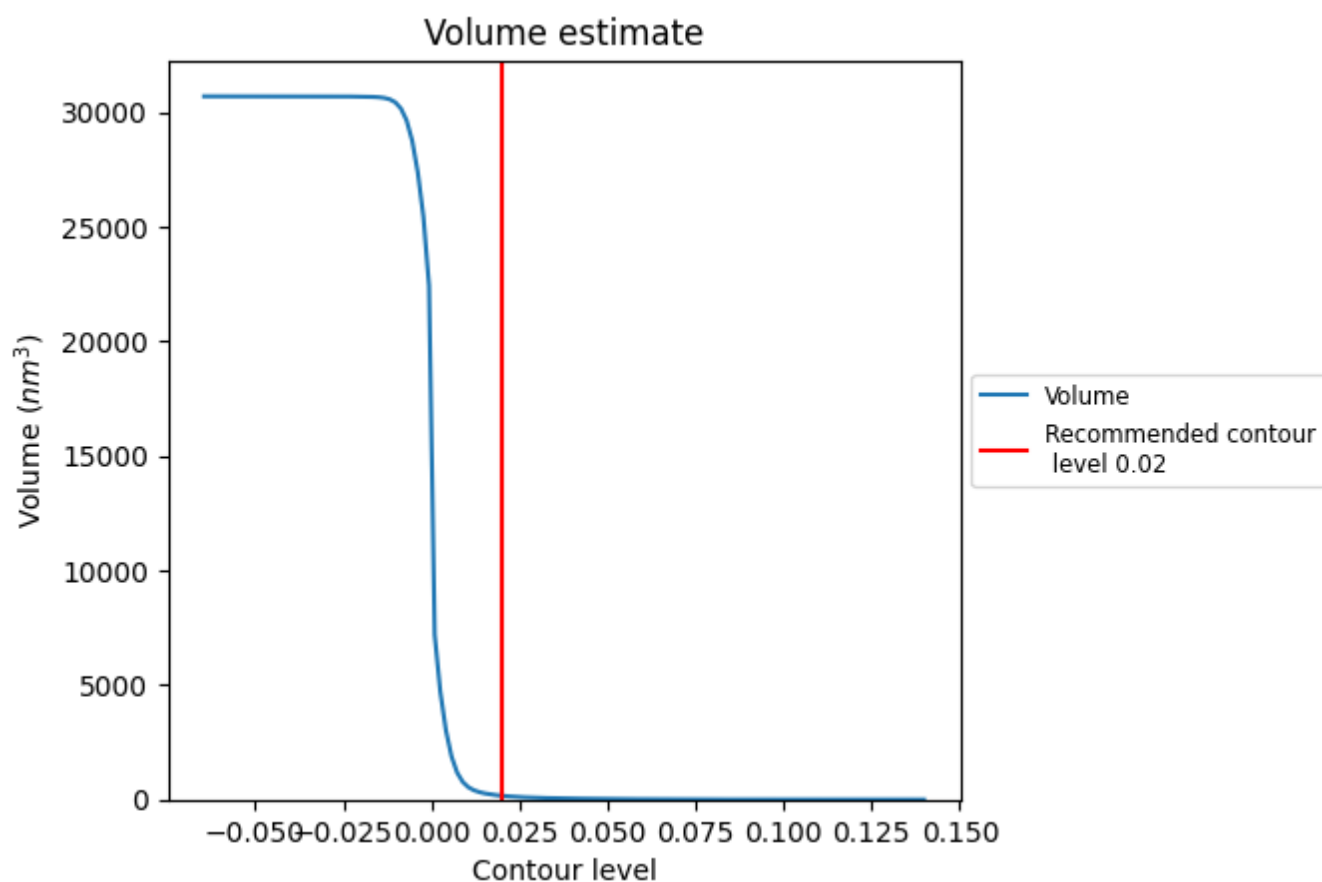
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

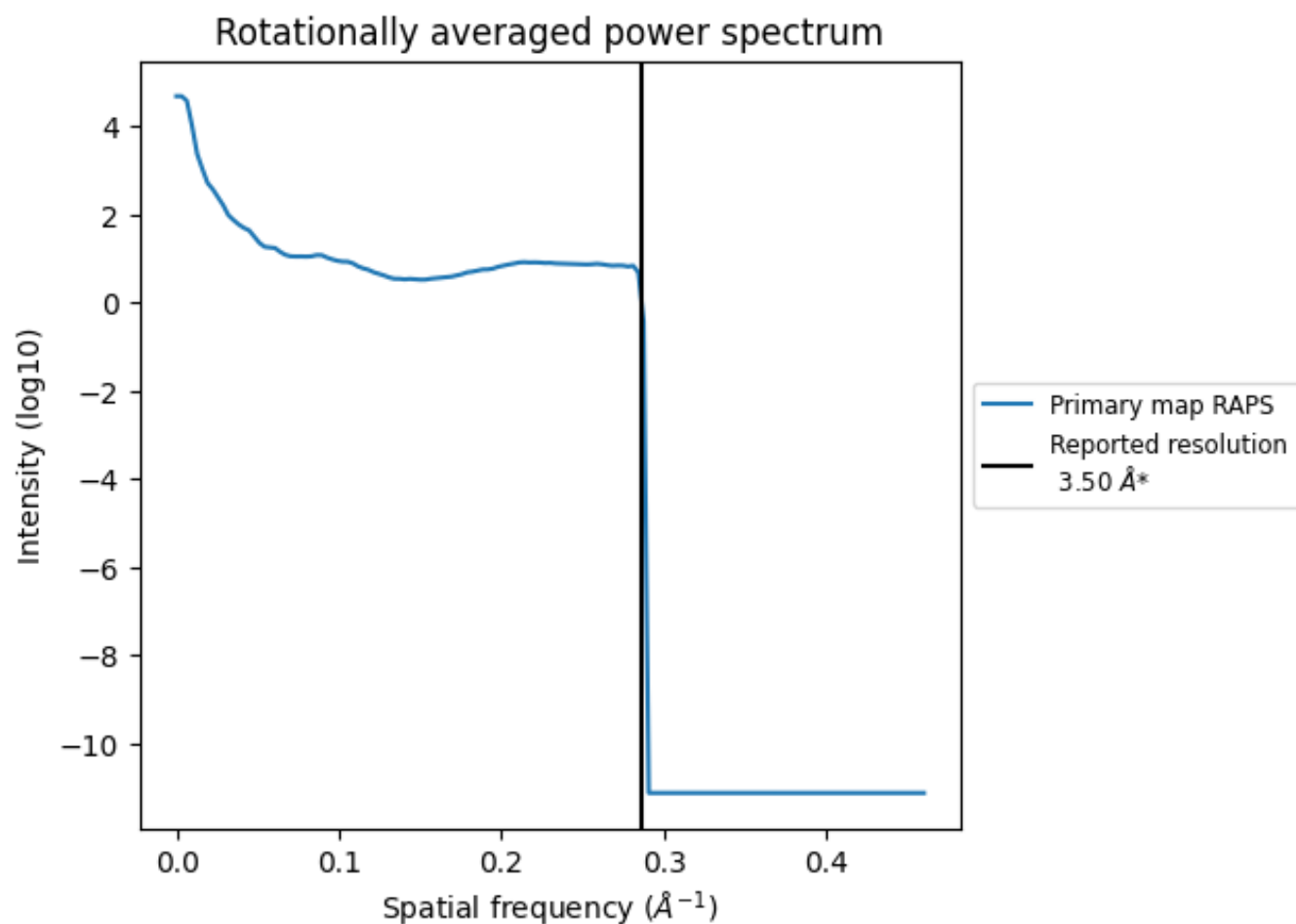
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 0.286 Å⁻¹

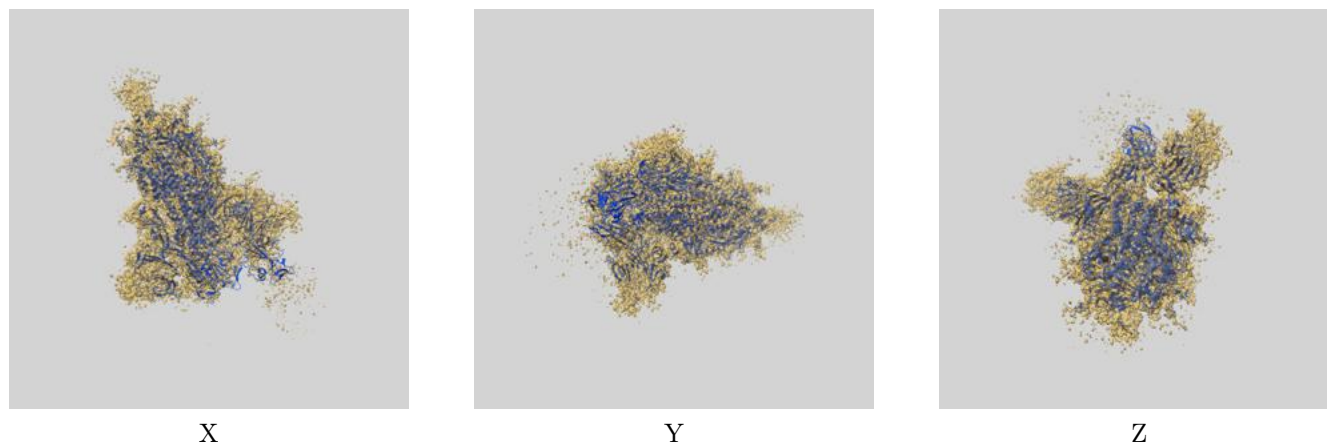
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

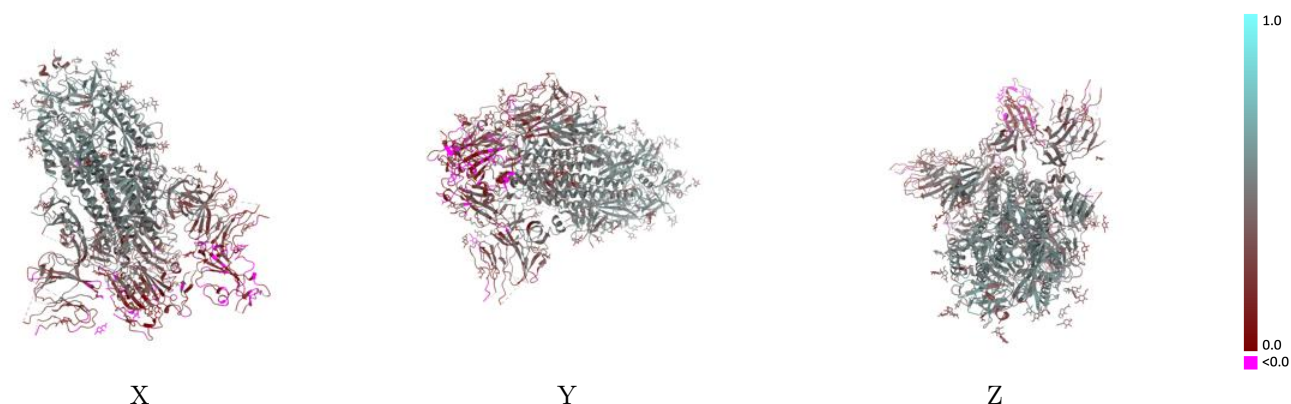
This section contains information regarding the fit between EMDB map EMD-30894 and PDB model 7DX3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)

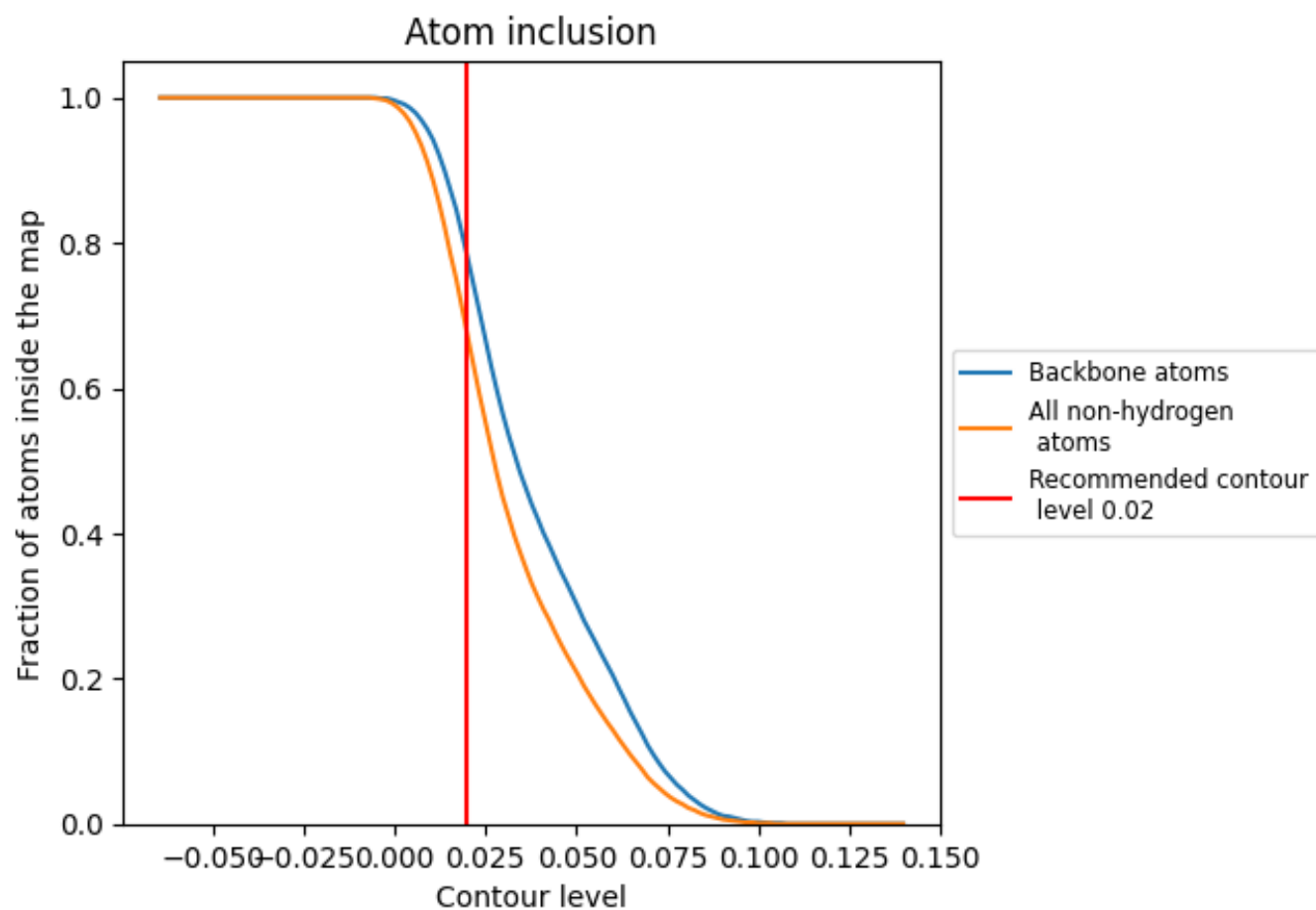


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 67% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6740	 0.3890
A	 0.6470	 0.3780
B	 0.6840	 0.3930
C	 0.7010	 0.4030
D	 0.3210	 0.1940
E	 0.0710	 -0.0210
F	 0.7140	 0.4660
G	 0.6790	 0.3440
H	 0.3570	 0.3050
I	 0.7500	 0.4590
J	 0.7500	 0.3920
K	 0.2860	 0.1990
L	 0.2860	 0.0980
M	 0.5360	 0.3650
N	 0.7500	 0.3560
O	 0.6790	 0.4010
P	 0.8930	 0.4500
Q	 0.7860	 0.4160
R	 0.1430	 0.1380
S	 0.1070	 0.0220
T	 0.5000	 0.3580
U	 0.7140	 0.4250
V	 0.7500	 0.4090
W	 0.5360	 0.3170
X	 0.7860	 0.3290
Y	 0.6430	 0.3340

