



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 02:02 PM JST

PDB ID : 7D0C
EMDB ID : EMD-30530
Title : S protein of SARS-CoV-2 in complex bound with P5A-3A1
Authors : Yan, R.H.; Wang, R.K.; Yu, J.F.; Zhang, Y.Y.; Liu, N.; Wang, H.W.; Wang, X.Q.; Zhang, L.Q.; Zhou, Q.
Deposited on : 2020-09-09
Resolution : 3.40 Å(reported)

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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:

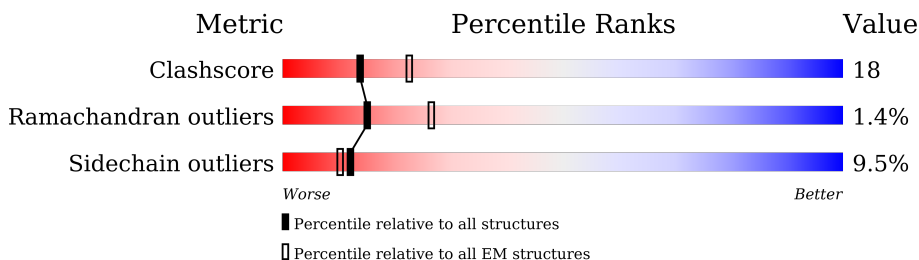
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.









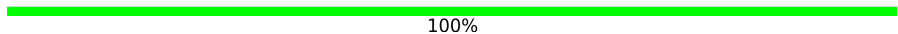



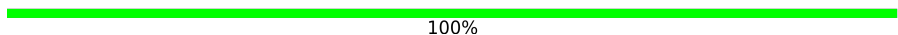




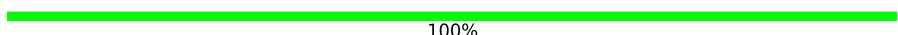


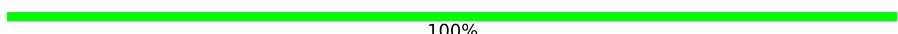


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	55% 19% 22%
1	B	1283	57% 17% 23%
1	C	1283	57% 18% 22%
2	G	219	51% 38%
2	H	219	38% 60% 37%
3	F	215	59% 69% 27% 5%
3	L	215	47% 68% 27% 5%
4	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	E	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	K	2	 50% 50%
4	M	2	 50% 50%
4	N	2	 50% 50%
4	O	2	 100%
4	P	2	 50% 50%
4	Q	2	 50% 50%
4	R	2	 100%
4	S	2	 100%
4	T	2	 50% 50%
4	U	2	 50% 100%
4	V	2	 50% 50%
4	W	2	 50% 50%
4	X	2	 100%
4	Y	2	 50% 50%
4	Z	2	 100%
4	a	2	 100%
4	b	2	 50% 50%
4	c	2	 50% 50%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30966 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
			Total	C	N	O	S		
1	A	1006	7863	5019	1308	1500	36	0	0
1	B	982	7696	4920	1279	1462	35	0	0
1	C	1004	7853	5014	1307	1496	36	0	0

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

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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 a protein called Heavy chain of P5A-3A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	219	Total	C	N	O	S	0	0
			1640	1036	271	327	6		
2	G	219	Total	C	N	O	S	0	0
			1640	1036	271	327	6		

- Molecule 3 is a protein called Light chain of P5A-3A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	215	Total	C	N	O	S	0	0
			1647	1027	281	334	5		
3	F	215	Total	C	N	O	S	0	0
			1647	1027	281	334	5		

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



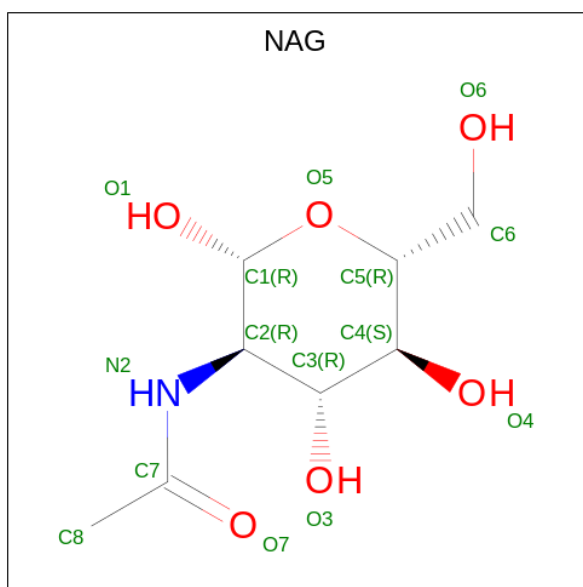
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	I	2	28	16	2	10	0	0
4	J	2	28	16	2	10	0	0
4	K	2	28	16	2	10	0	0
4	M	2	28	16	2	10	0	0
4	N	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16	2	10	0	0
4	U	2	28	16	2	10	0	0
4	V	2	28	16	2	10	0	0
4	W	2	28	16	2	10	0	0
4	X	2	28	16	2	10	0	0
4	Y	2	28	16	2	10	0	0
4	Z	2	28	16	2	10	0	0
4	a	2	28	16	2	10	0	0
4	b	2	28	16	2	10	0	0
4	c	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	A	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0
5	B	1	126	72	9	45	0

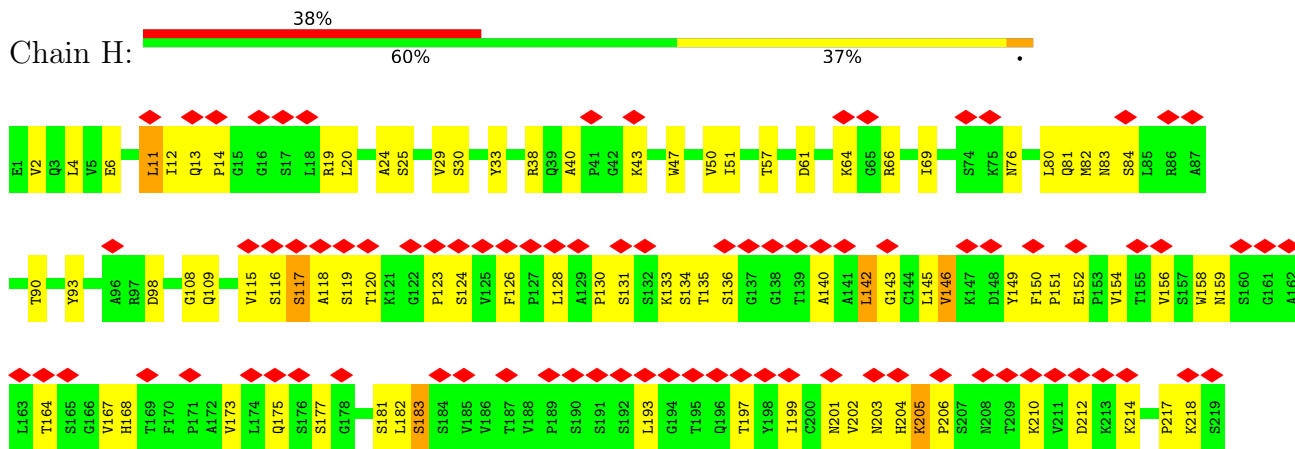
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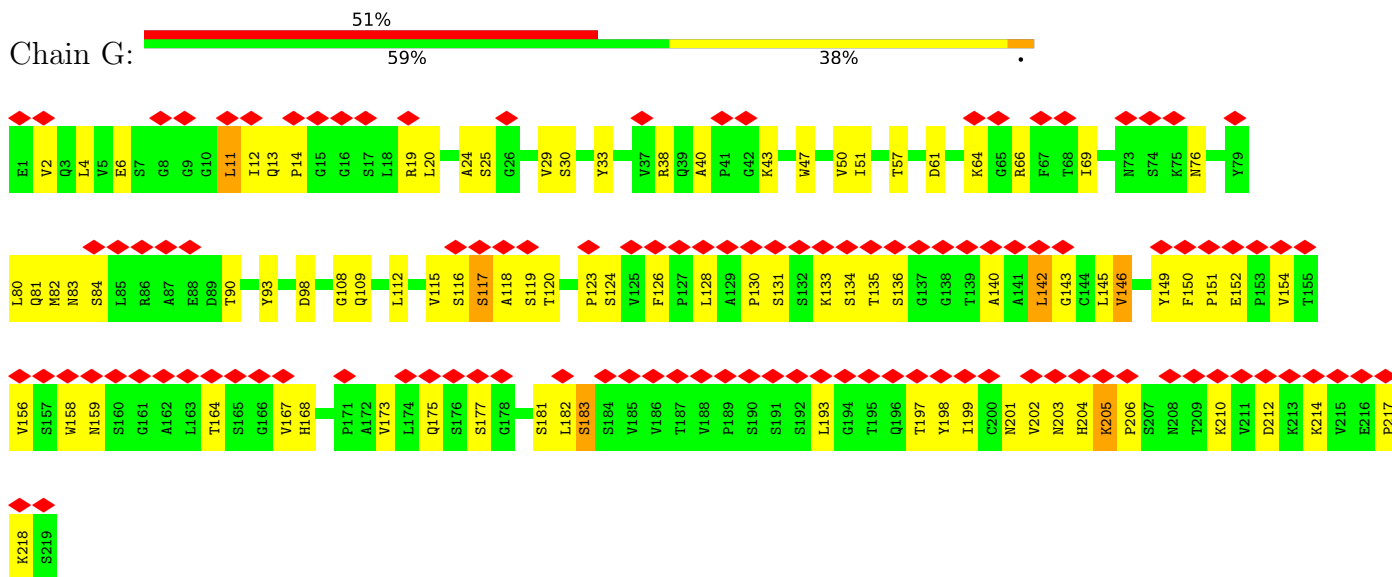
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	Total 126	C 72	N 9	O 45	0
5	B	1	Total 126	C 72	N 9	O 45	0
5	B	1	Total 126	C 72	N 9	O 45	0
5	B	1	Total 126	C 72	N 9	O 45	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0

SER	CYS	GLY	SER	CYS	CYS	LYS	PHE	ASP	GLU	ASP	SER	GLU	PRO	VAL	LEU	LYS	GLY	VAL	LYS	LEU	HIS	THR	LEU	GLU	ASP	LYS	THR	LYS	ASP	ASP	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

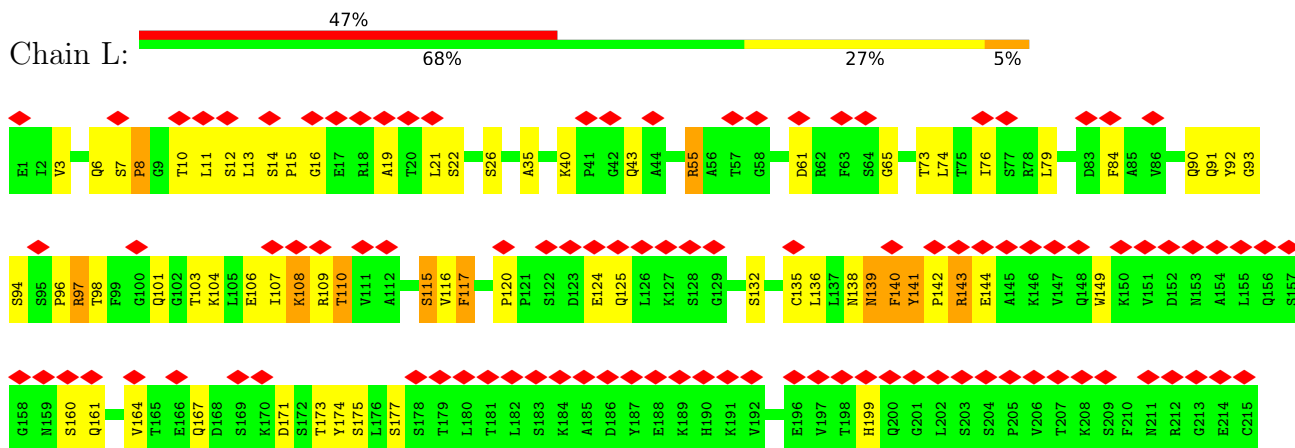
• Molecule 2: Heavy chain of P5A-3A1



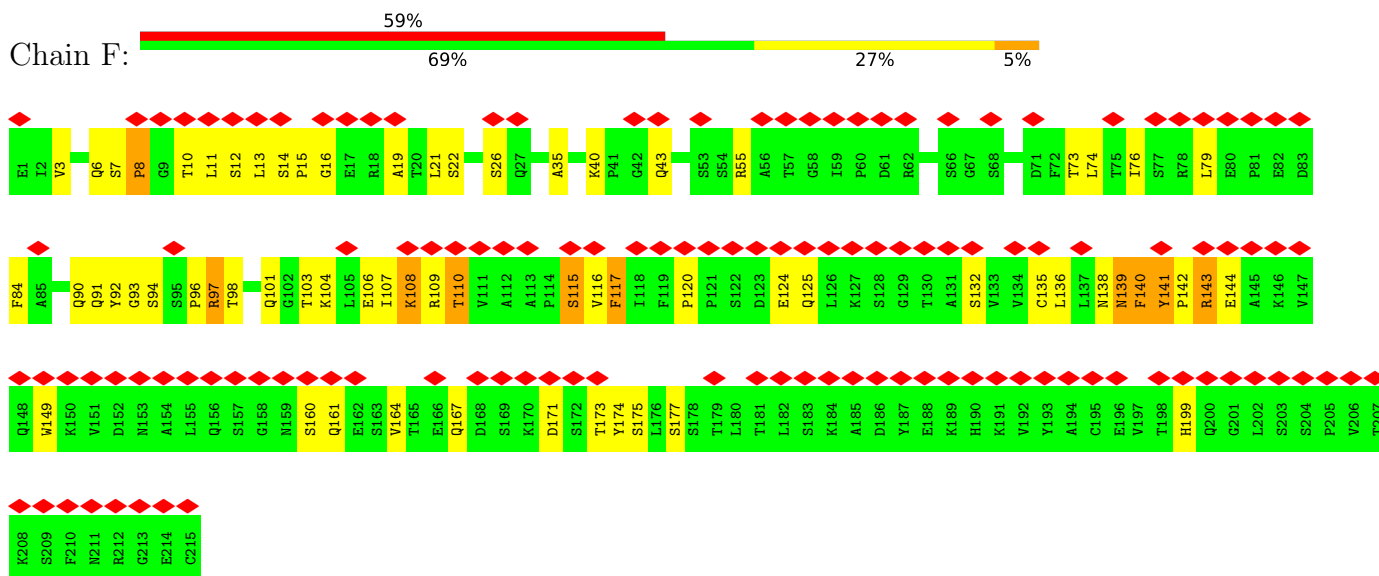
• Molecule 2: Heavy chain of P5A-3A1



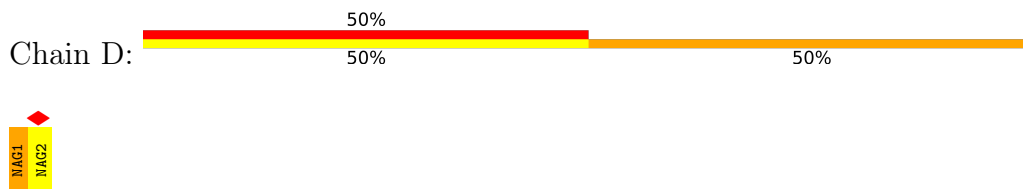
• Molecule 3: Light chain of P5A-3A1



- Molecule 3: Light chain of P5A-3A1



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



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



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



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



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

Chain K:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 100%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain X:  100%

MAG1
MAG2

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

Chain Y:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  50% 50%

MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (\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 (\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	0.50	0/8039	0.55	0/10936
1	B	0.49	0/7864	0.55	0/10691
1	C	0.50	0/8028	0.55	0/10919
2	G	0.34	0/1680	0.55	0/2288
2	H	0.34	0/1680	0.55	0/2288
3	F	0.42	0/1682	0.57	0/2282
3	L	0.42	0/1682	0.57	0/2282
All	All	0.47	0/30655	0.55	0/41686

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7863	0	7659	299	0
1	B	7696	0	7514	163	0
1	C	7853	0	7654	247	0
2	G	1640	0	1594	94	0
2	H	1640	0	1594	94	0
3	F	1647	0	1602	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1647	0	1602	109	0
4	D	28	0	25	6	0
4	E	28	0	25	0	0
4	I	28	0	25	1	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	2	0
4	V	28	0	25	1	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	2	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
5	A	126	0	117	5	0
5	B	126	0	117	6	0
5	C	112	0	104	2	0
All	All	30966	0	30107	1074	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 18.

All (1074) 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:F:15:PRO:HD3	3:F:107:ILE:CD1	1.39	1.52
3:L:15:PRO:HD3	3:L:107:ILE:CD1	1.39	1.51
1:C:391:CYS:SG	1:C:525:CYS:SG	1.47	1.45
3:L:108:LYS:HB3	3:L:141:TYR:OH	1.28	1.32
2:G:14:PRO:CD	2:G:116:SER:HB3	1.60	1.30
2:H:14:PRO:CD	2:H:116:SER:HB3	1.60	1.29
3:F:108:LYS:HB3	3:F:141:TYR:OH	1.28	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:GLN:HA	2:G:116:SER:CB	1.62	1.29
3:F:12:SER:O	3:F:108:LYS:HE3	1.31	1.28
2:H:13:GLN:HA	2:H:116:SER:CB	1.62	1.26
2:H:13:GLN:CA	2:H:116:SER:HB2	1.67	1.24
1:A:342:PHE:CD1	4:D:1:NAG:H81	1.73	1.24
3:L:12:SER:O	3:L:108:LYS:HE3	1.31	1.23
2:G:13:GLN:CA	2:G:116:SER:HB2	1.67	1.23
1:C:361:CYS:N	1:C:524:VAL:HG21	1.51	1.22
1:A:228:ASP:O	1:A:229:LEU:HD22	1.38	1.20
1:B:116:SER:HA	1:B:233:ILE:HD11	1.19	1.17
2:H:14:PRO:HD3	2:H:116:SER:HB3	1.24	1.17
1:C:392:PHE:O	1:C:523:THR:HG22	1.42	1.16
3:F:108:LYS:HB3	3:F:141:TYR:CZ	1.82	1.15
3:L:15:PRO:HD3	3:L:107:ILE:HD11	1.23	1.14
2:G:14:PRO:HD3	2:G:116:SER:HB3	1.24	1.14
1:A:336:CYS:SG	1:A:361:CYS:CB	2.37	1.13
3:L:108:LYS:HB3	3:L:141:TYR:CZ	1.82	1.13
1:A:115:GLN:O	1:A:233:ILE:HD11	1.49	1.12
1:C:332:ILE:CG2	1:C:362:VAL:HG21	1.79	1.13
3:L:15:PRO:CD	3:L:107:ILE:CD1	2.30	1.09
1:C:361:CYS:H	1:C:524:VAL:CG2	1.65	1.09
1:C:391:CYS:HB3	1:C:523:THR:CB	1.83	1.09
3:F:15:PRO:CD	3:F:107:ILE:CD1	2.30	1.09
2:H:11:LEU:HG	2:H:150:PHE:HE2	1.18	1.08
3:F:115:SER:HB2	3:F:117:PHE:CZ	1.89	1.08
1:C:332:ILE:HG22	1:C:362:VAL:HG21	1.12	1.08
3:L:7:SER:HB2	3:L:8:PRO:HD3	1.36	1.08
2:G:14:PRO:HD2	2:G:116:SER:HB3	1.36	1.07
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.36	1.07
1:A:200:TYR:CZ	1:C:521:PRO:HG2	1.90	1.07
3:L:115:SER:HB2	3:L:117:PHE:CZ	1.89	1.06
3:F:15:PRO:HD3	3:F:107:ILE:HD11	1.23	1.06
1:A:230:PRO:HB3	1:C:522:ALA:HB3	1.33	1.06
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.06	1.06
3:L:15:PRO:HD3	3:L:107:ILE:HD12	1.10	1.06
1:A:332:ILE:HD11	1:A:335:LEU:HD11	1.33	1.05
1:C:332:ILE:HG22	1:C:362:VAL:CG2	1.86	1.05
3:L:15:PRO:CD	3:L:107:ILE:HD12	1.85	1.05
1:B:116:SER:HA	1:B:233:ILE:CD1	1.87	1.05
1:A:535:LYS:HE2	1:A:554:GLU:CD	1.76	1.04
3:F:15:PRO:HD3	3:F:107:ILE:HD12	1.10	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:LEU:HG	2:G:150:PHE:HE2	1.18	1.03
3:F:15:PRO:CD	3:F:107:ILE:HD12	1.85	1.03
3:F:7:SER:HB2	3:F:8:PRO:CD	1.89	1.03
3:L:7:SER:HB2	3:L:8:PRO:CD	1.89	1.02
3:F:13:LEU:O	3:F:107:ILE:HG13	1.59	1.02
1:C:335:LEU:H	1:C:335:LEU:HD22	1.16	1.02
1:C:342:PHE:CE2	1:C:368:LEU:HD21	1.93	1.02
3:L:13:LEU:O	3:L:107:ILE:HG13	1.59	1.02
3:L:106:GLU:HB2	3:L:167:GLN:OE1	1.60	1.02
1:A:342:PHE:CE2	1:A:368:LEU:CD2	2.42	1.02
1:C:342:PHE:CE2	1:C:368:LEU:CD2	2.42	1.02
1:A:342:PHE:CE2	1:A:368:LEU:HD21	1.93	1.01
3:F:106:GLU:HB2	3:F:167:GLN:OE1	1.60	1.01
1:B:130:VAL:HG21	1:B:231:ILE:CD1	1.91	1.01
1:B:422:ASN:HD21	1:B:455:LEU:H	1.09	1.00
2:H:14:PRO:HD2	2:H:116:SER:HB3	1.36	1.00
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.01	1.00
1:A:332:ILE:HD11	1:A:335:LEU:CD1	1.92	1.00
2:H:11:LEU:CG	2:H:150:PHE:HE2	1.74	0.99
1:A:342:PHE:HE2	1:A:368:LEU:HD21	1.24	0.99
2:G:11:LEU:CG	2:G:150:PHE:HE2	1.74	0.99
1:A:230:PRO:CB	1:C:522:ALA:HB3	1.90	0.99
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.99
1:C:391:CYS:HB3	1:C:523:THR:OG1	1.63	0.98
1:C:676:THR:HA	1:C:690:GLN:HB3	1.45	0.98
1:A:334:ASN:HB3	1:A:362:VAL:HG23	1.45	0.97
1:C:361:CYS:H	1:C:524:VAL:HG21	0.85	0.97
1:C:675:GLN:HE21	1:C:675:GLN:HA	1.26	0.97
1:C:332:ILE:HD12	1:C:333:THR:H	1.29	0.96
1:C:342:PHE:HE2	1:C:368:LEU:HD21	1.24	0.96
1:A:200:TYR:CE2	1:C:521:PRO:HG2	1.99	0.95
1:A:535:LYS:HE2	1:A:554:GLU:OE2	1.63	0.95
1:A:227:VAL:HG12	1:A:228:ASP:H	1.33	0.94
1:B:577:ARG:HH11	1:B:582:LEU:HD13	1.32	0.93
1:A:230:PRO:CG	1:C:522:ALA:HB3	1.99	0.92
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.92
1:A:115:GLN:HB2	1:A:233:ILE:HD13	1.51	0.92
1:C:342:PHE:CZ	1:C:368:LEU:HD22	2.05	0.91
3:L:143:ARG:HE	3:L:164:VAL:HG11	1.35	0.91
1:C:332:ILE:HD13	1:C:335:LEU:HD13	1.51	0.91
2:H:11:LEU:HD11	2:H:150:PHE:CD2	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PHE:CZ	1:A:368:LEU:HD22	2.05	0.91
3:F:143:ARG:HE	3:F:164:VAL:HG11	1.35	0.91
2:G:11:LEU:HD11	2:G:150:PHE:CD2	2.06	0.90
1:C:332:ILE:HD12	1:C:333:THR:N	1.86	0.90
2:H:14:PRO:CD	2:H:116:SER:CB	2.50	0.90
2:G:14:PRO:CD	2:G:116:SER:CB	2.50	0.90
1:A:230:PRO:HB3	1:C:522:ALA:CB	2.02	0.88
1:A:168:PHE:CZ	1:A:229:LEU:HG	2.07	0.88
3:F:115:SER:HB2	3:F:117:PHE:HZ	1.38	0.88
1:A:332:ILE:HG23	1:A:333:THR:H	1.39	0.88
1:A:336:CYS:HG	1:A:361:CYS:HG	0.93	0.87
1:B:231:ILE:HG21	1:B:233:ILE:HG22	1.56	0.87
1:A:535:LYS:HE2	1:A:554:GLU:OE1	1.73	0.86
1:B:130:VAL:CG2	1:B:231:ILE:HD12	2.00	0.86
1:C:342:PHE:CZ	1:C:368:LEU:CD2	2.59	0.86
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.56	0.86
2:H:11:LEU:CG	2:H:150:PHE:CE2	2.58	0.86
3:L:141:TYR:CD2	3:L:142:PRO:HD3	2.11	0.86
3:F:141:TYR:CD2	3:F:142:PRO:HD3	2.11	0.86
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.86
3:L:115:SER:HB2	3:L:117:PHE:HZ	1.38	0.85
2:G:11:LEU:CG	2:G:150:PHE:CE2	2.58	0.85
1:A:392:PHE:CE2	1:A:517:LEU:HD21	2.11	0.85
1:B:577:ARG:HD3	1:B:582:LEU:CD1	2.07	0.85
1:C:332:ILE:CB	1:C:362:VAL:HG21	2.06	0.84
1:A:342:PHE:CZ	1:A:368:LEU:CD2	2.59	0.84
2:H:11:LEU:HD21	2:H:150:PHE:CE2	2.12	0.84
1:A:168:PHE:CE2	1:A:229:LEU:HG	2.12	0.84
1:C:127:VAL:HG21	5:C:1402:NAG:H5	1.59	0.83
2:G:11:LEU:HD21	2:G:150:PHE:CE2	2.12	0.83
2:H:11:LEU:HG	2:H:150:PHE:CE2	2.10	0.83
3:F:108:LYS:CB	3:F:141:TYR:OH	2.22	0.83
1:A:233:ILE:O	1:A:234:ASN:O	1.96	0.83
3:F:140:PHE:CD1	3:F:174:TYR:O	2.32	0.83
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.83
1:C:532:ASN:OD1	1:C:533:LEU:N	2.12	0.83
3:L:140:PHE:CD1	3:L:174:TYR:O	2.32	0.82
3:L:108:LYS:HA	3:L:141:TYR:CE1	2.14	0.82
3:L:108:LYS:CB	3:L:141:TYR:OH	2.22	0.82
3:F:108:LYS:HA	3:F:141:TYR:CE1	2.14	0.82
1:A:130:VAL:HG21	1:A:231:ILE:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HB3	1:C:523:THR:HB	1.62	0.81
1:A:357:ARG:HB2	1:A:357:ARG:NH2	1.94	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:B:452:LEU:HG	1:B:492:LEU:HD22	1.63	0.81
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.60	0.81
2:G:14:PRO:HD2	2:G:116:SER:CB	2.10	0.81
2:H:14:PRO:HD2	2:H:116:SER:CB	2.10	0.81
1:B:231:ILE:CG2	1:B:233:ILE:HG22	2.10	0.81
3:F:141:TYR:HB3	3:F:142:PRO:HD3	1.63	0.81
1:A:115:GLN:O	1:A:233:ILE:CD1	2.28	0.80
2:G:11:LEU:HG	2:G:150:PHE:CE2	2.10	0.80
1:B:214:ARG:H	1:B:214:ARG:HH21	1.30	0.80
1:A:336:CYS:SG	1:A:361:CYS:HB2	2.21	0.80
3:L:141:TYR:HB3	3:L:142:PRO:HD3	1.63	0.79
2:H:11:LEU:HD21	2:H:150:PHE:CD2	2.18	0.79
1:A:332:ILE:CD1	1:A:335:LEU:HD11	2.13	0.79
1:C:676:THR:C	1:C:690:GLN:HE21	1.86	0.79
1:C:360:ASN:O	1:C:361:CYS:HB3	1.81	0.79
3:L:140:PHE:HD1	3:L:174:TYR:O	1.65	0.79
3:F:140:PHE:CE2	3:F:143:ARG:HA	2.18	0.79
3:F:7:SER:CB	3:F:8:PRO:HD3	2.14	0.78
2:G:11:LEU:HD21	2:G:150:PHE:CD2	2.18	0.77
3:L:140:PHE:CE2	3:L:143:ARG:HA	2.18	0.77
1:B:116:SER:CA	1:B:233:ILE:CD1	2.62	0.77
1:C:391:CYS:SG	1:C:525:CYS:CB	2.73	0.77
1:B:117:LEU:N	1:B:233:ILE:HD12	2.00	0.76
3:F:7:SER:CB	3:F:8:PRO:CD	2.64	0.76
3:F:140:PHE:HD1	3:F:174:TYR:O	1.65	0.76
3:L:138:ASN:O	3:L:139:ASN:O	2.04	0.76
1:C:363:ALA:HB1	1:C:365:TYR:CE2	2.21	0.76
3:L:7:SER:CB	3:L:8:PRO:HD3	2.13	0.76
1:A:392:PHE:C	1:A:524:VAL:CG2	2.54	0.76
3:F:138:ASN:O	3:F:139:ASN:O	2.04	0.76
1:A:336:CYS:SG	1:A:361:CYS:HB3	2.23	0.76
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.76
1:C:675:GLN:HA	1:C:675:GLN:NE2	1.99	0.76
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.75
1:A:334:ASN:CG	1:A:361:CYS:HA	2.07	0.75
1:A:336:CYS:HG	1:A:361:CYS:CB	1.88	0.75
2:H:11:LEU:CD2	2:H:150:PHE:CE2	2.69	0.75
2:G:11:LEU:CD2	2:G:150:PHE:CE2	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ALA:HB1	1:A:365:TYR:CE2	2.21	0.75
2:G:14:PRO:HD3	2:G:116:SER:CB	2.14	0.75
3:L:15:PRO:CD	3:L:107:ILE:HD11	2.09	0.74
1:C:332:ILE:HG22	1:C:362:VAL:HG11	1.68	0.74
1:A:531:THR:OG1	1:A:532:ASN:N	2.21	0.74
3:L:6:GLN:HB2	3:L:101:GLN:NE2	2.03	0.73
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.73
3:F:6:GLN:HB2	3:F:101:GLN:NE2	2.03	0.73
3:F:15:PRO:CD	3:F:107:ILE:HD11	2.10	0.73
1:A:227:VAL:HG12	1:A:228:ASP:N	2.02	0.73
1:B:231:ILE:HG21	1:B:233:ILE:CG2	2.19	0.73
1:A:535:LYS:CE	1:A:554:GLU:OE2	2.37	0.73
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.73
1:B:577:ARG:HH11	1:B:582:LEU:CD1	2.02	0.73
1:B:164:ASN:ND2	5:B:1403:NAG:O6	2.22	0.73
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.73
1:A:357:ARG:HB2	1:A:357:ARG:CZ	2.19	0.72
1:A:527:PRO:O	1:A:528:LYS:HG2	1.89	0.72
1:A:534:VAL:HG23	1:A:535:LYS:N	2.04	0.72
1:A:360:ASN:O	1:A:361:CYS:HB3	1.88	0.72
1:C:345:THR:O	1:C:509:ARG:NH2	2.23	0.72
3:F:141:TYR:CG	3:F:142:PRO:HD3	2.25	0.72
1:B:117:LEU:N	1:B:233:ILE:CD1	2.53	0.71
2:H:11:LEU:HD11	2:H:150:PHE:HD2	1.50	0.71
3:L:141:TYR:CG	3:L:142:PRO:HD3	2.25	0.71
1:A:230:PRO:HG3	1:C:522:ALA:HB3	1.70	0.71
1:B:124:THR:OG1	5:B:1402:NAG:N2	2.22	0.71
2:G:11:LEU:HD11	2:G:150:PHE:HD2	1.50	0.71
3:F:141:TYR:CB	3:F:142:PRO:HD3	2.20	0.71
1:A:334:ASN:C	1:A:335:LEU:HD22	2.11	0.71
1:C:530:SER:OG	1:C:531:THR:N	2.23	0.71
1:C:535:LYS:HE3	1:C:554:GLU:CD	2.10	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
3:L:141:TYR:CB	3:L:142:PRO:HD3	2.20	0.71
1:A:392:PHE:C	1:A:524:VAL:HG22	2.11	0.71
3:F:108:LYS:CB	3:F:141:TYR:CZ	2.71	0.70
1:A:124:THR:HG21	5:A:1402:NAG:HN2	1.56	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
1:B:391:CYS:HA	1:B:525:CYS:HB2	1.73	0.70
1:A:200:TYR:OH	1:C:521:PRO:HG2	1.91	0.69
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:THR:C	1:C:690:GLN:NE2	2.45	0.69
1:C:357:ARG:HB3	1:C:357:ARG:NH2	2.07	0.69
1:B:577:ARG:NH1	1:B:582:LEU:HD13	2.07	0.69
3:F:84:PHE:CE2	3:F:107:ILE:HB	2.28	0.69
1:C:332:ILE:HD13	1:C:335:LEU:CD1	2.21	0.69
1:C:342:PHE:HE2	1:C:368:LEU:CD2	1.93	0.69
1:A:345:THR:O	1:A:509:ARG:NH2	2.23	0.69
1:C:534:VAL:HG23	1:C:535:LYS:N	2.07	0.69
1:C:391:CYS:O	1:C:523:THR:HG21	1.92	0.69
1:C:569:ILE:H	1:C:569:ILE:HD12	1.56	0.69
1:B:233:ILE:O	1:B:235:ILE:HG13	1.93	0.68
3:L:140:PHE:H	3:L:173:THR:HB	1.57	0.68
1:B:117:LEU:H	1:B:233:ILE:CD1	2.06	0.68
1:C:233:ILE:HG12	1:C:234:ASN:H	1.58	0.68
1:C:535:LYS:C	1:C:536:ASN:HD22	1.96	0.68
3:F:140:PHE:H	3:F:173:THR:HB	1.57	0.68
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.74	0.68
1:A:229:LEU:HD12	1:A:230:PRO:HD2	1.74	0.68
1:B:406:GLU:HG3	1:B:418:ILE:HG13	1.74	0.68
3:L:84:PHE:CE2	3:L:107:ILE:HB	2.28	0.68
1:B:403:ARG:NH2	1:B:405:ASP:OD2	2.27	0.68
1:C:528:LYS:O	1:C:529:LYS:CB	2.42	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:C:332:ILE:CG2	1:C:362:VAL:HG11	2.24	0.67
3:L:108:LYS:CB	3:L:141:TYR:CZ	2.71	0.67
1:A:332:ILE:HG23	1:A:333:THR:N	2.08	0.67
2:G:13:GLN:HA	2:G:116:SER:HB2	0.75	0.67
1:A:310:LYS:NZ	1:A:663:ASP:OD1	2.27	0.67
2:H:13:GLN:HG2	2:H:116:SER:OG	1.95	0.67
2:G:13:GLN:HG2	2:G:116:SER:OG	1.95	0.67
1:B:97:LYS:HD3	1:B:97:LYS:H	1.60	0.66
1:C:530:SER:O	1:C:531:THR:HG23	1.95	0.66
2:G:11:LEU:HD11	2:G:150:PHE:CE2	2.30	0.66
1:B:116:SER:C	1:B:233:ILE:HD12	2.15	0.66
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.66
3:L:140:PHE:CE1	3:L:174:TYR:C	2.68	0.66
2:H:11:LEU:HD11	2:H:150:PHE:CE2	2.30	0.66
3:F:84:PHE:HE2	3:F:107:ILE:HB	1.60	0.66
3:F:140:PHE:CE1	3:F:174:TYR:C	2.68	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.66
1:A:233:ILE:O	1:A:234:ASN:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PRO:HA	1:C:237:ARG:HA	1.78	0.66
3:L:13:LEU:O	3:L:107:ILE:HA	1.96	0.66
3:F:13:LEU:O	3:F:107:ILE:HA	1.96	0.66
1:A:392:PHE:HB2	1:A:524:VAL:CG2	2.25	0.66
1:A:527:PRO:C	1:A:528:LYS:HG2	2.16	0.66
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.59	0.66
1:B:577:ARG:NH1	1:B:582:LEU:CD1	2.58	0.66
1:C:480:CYS:HG	1:C:488:CYS:HG	0.71	0.66
3:F:10:THR:HB	3:F:104:LYS:HE2	1.78	0.66
2:H:14:PRO:HD3	2:H:116:SER:CB	2.14	0.66
1:A:392:PHE:HB2	1:A:524:VAL:HG21	1.78	0.66
1:A:392:PHE:O	1:A:524:VAL:HG22	1.96	0.66
1:B:116:SER:CA	1:B:233:ILE:HD11	2.11	0.66
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.28	0.66
3:L:140:PHE:HE2	3:L:143:ARG:HA	1.61	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.65
3:L:115:SER:CB	3:L:117:PHE:CZ	2.75	0.65
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.78	0.65
1:C:332:ILE:HG22	1:C:362:VAL:CG1	2.25	0.65
2:H:126:PHE:CE2	3:L:125:GLN:HG3	2.31	0.65
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.78	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:B:358:ILE:HB	1:B:395:VAL:HB	1.78	0.65
2:G:126:PHE:CE2	3:F:125:GLN:HG3	2.31	0.65
3:F:10:THR:C	3:F:11:LEU:HD12	2.17	0.65
3:F:109:ARG:HD2	3:F:171:ASP:O	1.96	0.65
1:A:705:VAL:HB	1:B:883:THR:HG21	1.78	0.65
1:C:335:LEU:HD22	1:C:335:LEU:N	2.01	0.65
3:L:10:THR:HB	3:L:104:LYS:HE2	1.78	0.65
3:L:12:SER:OG	3:L:108:LYS:HG3	1.96	0.65
3:F:140:PHE:HE2	3:F:143:ARG:HA	1.61	0.65
1:A:529:LYS:HB2	1:A:529:LYS:HZ2	1.61	0.65
3:L:109:ARG:HD2	3:L:171:ASP:O	1.96	0.65
3:F:12:SER:OG	3:F:108:LYS:HG3	1.96	0.65
1:C:335:LEU:H	1:C:335:LEU:CD2	1.96	0.64
1:B:108:THR:HA	1:B:236:THR:HG22	1.79	0.64
1:B:472:ILE:HD13	1:B:474:GLN:HB3	1.79	0.64
1:B:350:VAL:HG22	1:B:453:TYR:HB2	1.79	0.64
1:B:455:LEU:HD21	1:B:457:ARG:HG3	1.78	0.64
1:A:392:PHE:O	1:A:524:VAL:CG2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:GLN:HG2	3:F:103:THR:HG23	1.80	0.64
1:A:342:PHE:HD1	4:D:1:NAG:H81	1.54	0.64
1:C:676:THR:HA	1:C:690:GLN:CB	2.25	0.64
3:L:84:PHE:HE2	3:L:107:ILE:HB	1.60	0.64
3:F:117:PHE:CD2	3:F:136:LEU:HD23	2.33	0.64
2:H:203:ASN:HB3	2:H:210:LYS:HE2	1.79	0.64
3:L:10:THR:C	3:L:11:LEU:HD12	2.17	0.64
3:L:117:PHE:CD2	3:L:136:LEU:HD23	2.33	0.64
2:H:173:VAL:HG22	3:L:161:GLN:OE1	1.98	0.64
2:G:13:GLN:CG	2:G:116:SER:OG	2.46	0.64
1:B:607:GLN:O	1:B:608:VAL:HG23	1.98	0.63
1:A:342:PHE:CD1	4:D:1:NAG:C8	2.67	0.63
2:G:203:ASN:HB3	2:G:210:LYS:HE2	1.79	0.63
1:A:168:PHE:HZ	1:A:229:LEU:HG	1.62	0.63
2:G:173:VAL:HG22	3:F:161:GLN:OE1	1.98	0.63
2:H:13:GLN:HA	2:H:116:SER:HB2	0.75	0.63
2:H:13:GLN:CG	2:H:116:SER:OG	2.46	0.63
3:F:141:TYR:HB3	3:F:142:PRO:CD	2.27	0.63
1:C:196:ASN:ND2	1:C:200:TYR:O	2.32	0.63
3:L:141:TYR:HB3	3:L:142:PRO:CD	2.27	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.63	0.63
3:F:115:SER:CB	3:F:117:PHE:CZ	2.75	0.63
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
1:B:111:ASP:OD1	1:B:112:SER:N	2.31	0.62
1:C:332:ILE:HG22	1:C:362:VAL:CB	2.29	0.62
2:H:156:VAL:HG22	2:H:202:VAL:HG22	1.81	0.62
3:L:15:PRO:CG	3:L:107:ILE:HD12	2.29	0.62
1:A:392:PHE:CA	1:A:524:VAL:HG23	2.29	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:C:394:ASN:H	1:C:516:GLU:HB3	1.64	0.62
1:C:391:CYS:C	1:C:523:THR:HG21	2.18	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
2:H:116:SER:O	2:H:117:SER:HB2	1.98	0.62
2:G:116:SER:O	2:G:117:SER:HB2	1.98	0.62
2:G:128:LEU:HD11	2:G:145:LEU:HB2	1.81	0.62
3:L:6:GLN:H	3:L:101:GLN:HE22	1.47	0.62
2:H:173:VAL:CG2	3:L:161:GLN:OE1	2.47	0.62
3:L:6:GLN:HG2	3:L:103:THR:HG23	1.80	0.62
1:B:454:ARG:HH21	1:B:493:GLN:HG3	1.63	0.62
1:B:391:CYS:CA	1:B:525:CYS:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:173:VAL:CG2	3:F:161:GLN:OE1	2.47	0.61
1:A:115:GLN:CB	1:A:233:ILE:HD13	2.28	0.61
1:B:560:LEU:H	1:B:563:GLN:HE21	1.45	0.61
3:F:15:PRO:CG	3:F:107:ILE:HD12	2.29	0.61
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:C:389:ASP:OD1	1:C:389:ASP:N	2.33	0.61
2:H:128:LEU:HD11	2:H:145:LEU:HB2	1.81	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
2:H:11:LEU:CD1	2:H:150:PHE:CE2	2.84	0.61
3:L:117:PHE:HE2	3:L:138:ASN:HB2	1.65	0.61
1:A:392:PHE:N	1:A:524:VAL:HG23	2.15	0.61
2:G:11:LEU:CD1	2:G:150:PHE:CE2	2.84	0.61
1:A:363:ALA:HB1	1:A:365:TYR:CZ	2.35	0.61
1:A:353:TRP:O	1:A:466:ARG:NH1	2.34	0.60
2:G:156:VAL:HG22	2:G:202:VAL:HG22	1.81	0.60
3:F:6:GLN:H	3:F:101:GLN:HE22	1.47	0.60
1:C:112:SER:HB2	1:C:113:LYS:HD3	1.83	0.60
1:C:363:ALA:HB1	1:C:365:TYR:CZ	2.35	0.60
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.82	0.60
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.60
3:F:108:LYS:CA	3:F:141:TYR:CE1	2.85	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.60
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.84	0.60
1:B:409:GLN:NE2	1:B:416:GLY:HA3	2.16	0.60
1:A:480:CYS:HG	1:A:488:CYS:HG	0.66	0.60
1:C:353:TRP:O	1:C:466:ARG:NH1	2.34	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
2:H:13:GLN:CG	2:H:116:SER:CB	2.80	0.60
3:L:143:ARG:NE	3:L:164:VAL:HG11	2.13	0.60
1:B:116:SER:CA	1:B:233:ILE:HD12	2.31	0.59
1:B:206:LYS:HD2	1:B:207:HIS:H	1.67	0.59
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.84	0.59
1:C:529:LYS:O	1:C:529:LYS:HG2	2.02	0.59
3:L:14:SER:HA	3:L:107:ILE:CD1	2.31	0.59
1:A:342:PHE:CE2	1:A:368:LEU:HD22	2.27	0.59
1:C:95:THR:HG22	1:C:96:GLU:H	1.66	0.59
1:C:455:LEU:HD22	1:C:493:GLN:HB2	1.84	0.59
3:F:141:TYR:CB	3:F:142:PRO:CD	2.80	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
3:L:91:GLN:HE21	3:L:98:THR:H	1.50	0.59
3:L:141:TYR:CB	3:L:142:PRO:CD	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:14:SER:HA	3:F:107:ILE:CD1	2.31	0.59
1:A:115:GLN:C	1:A:233:ILE:HD11	2.21	0.59
1:A:389:ASP:N	1:A:389:ASP:OD1	2.33	0.59
3:L:108:LYS:CA	3:L:141:TYR:CE1	2.85	0.59
2:G:13:GLN:CG	2:G:116:SER:CB	2.80	0.59
3:F:117:PHE:HE2	3:F:138:ASN:HB2	1.65	0.59
1:C:363:ALA:CB	1:C:365:TYR:CE2	2.86	0.59
1:C:392:PHE:C	1:C:523:THR:HG22	2.20	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.67	0.59
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.59
1:A:529:LYS:HB2	1:A:529:LYS:NZ	2.18	0.59
1:A:228:ASP:O	1:A:229:LEU:CD2	2.33	0.59
1:A:455:LEU:HD22	1:A:493:GLN:HB2	1.85	0.59
1:C:599:THR:HG22	1:C:601:GLY:H	1.67	0.58
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.58
1:A:392:PHE:H	1:A:524:VAL:HG23	1.67	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:A:363:ALA:CB	1:A:365:TYR:CE2	2.86	0.58
1:A:392:PHE:HE2	1:A:517:LEU:HD21	1.67	0.58
1:B:452:LEU:HD21	1:B:492:LEU:HD13	1.85	0.58
4:Y:2:NAG:H3	4:Y:2:NAG:H83	1.86	0.58
1:A:334:ASN:OD1	1:A:361:CYS:HA	2.03	0.58
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.58
2:H:81:GLN:NE2	2:H:83:ASN:OD1	2.37	0.58
3:F:108:LYS:HB3	3:F:141:TYR:CE1	2.37	0.58
1:B:214:ARG:HD3	1:B:214:ARG:N	2.18	0.57
1:A:200:TYR:CE2	1:C:521:PRO:CG	2.84	0.57
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.86	0.57
5:A:1405:NAG:H3	5:A:1405:NAG:H83	1.86	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
3:F:143:ARG:NE	3:F:164:VAL:HG11	2.13	0.57
3:F:7:SER:HB2	3:F:8:PRO:HD2	1.84	0.57
3:F:91:GLN:HE21	3:F:98:THR:H	1.50	0.57
1:A:480:CYS:SG	1:A:488:CYS:CB	2.92	0.57
3:L:116:VAL:O	3:L:117:PHE:CD1	2.58	0.57
1:A:229:LEU:HD12	1:A:230:PRO:CD	2.34	0.57
2:G:81:GLN:NE2	2:G:83:ASN:OD1	2.37	0.57
5:B:1405:NAG:H83	5:B:1405:NAG:H3	1.87	0.57
1:C:480:CYS:SG	1:C:488:CYS:CB	2.92	0.57
1:A:535:LYS:CD	1:A:554:GLU:OE2	2.53	0.57
1:C:528:LYS:O	1:C:529:LYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PHE:C	1:A:524:VAL:HG23	2.25	0.56
2:H:13:GLN:CG	2:H:116:SER:HB2	2.35	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:444:LYS:NZ	1:A:445:VAL:O	2.37	0.56
2:H:33:TYR:HB2	2:H:98:ASP:HB3	1.88	0.56
1:A:537:LYS:O	1:A:538:CYS:C	2.43	0.56
1:B:105:ILE:HG13	1:B:110:LEU:HD11	1.87	0.56
1:B:213:VAL:HB	1:B:214:ARG:HD3	1.87	0.56
1:B:408:ARG:O	1:B:414:GLN:NE2	2.32	0.56
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.56
2:H:13:GLN:HG2	2:H:116:SER:CB	2.36	0.56
3:L:19:ALA:HB3	3:L:76:ILE:HB	1.87	0.56
2:G:13:GLN:CG	2:G:116:SER:HB2	2.35	0.56
4:Z:2:NAG:H3	4:Z:2:NAG:H83	1.87	0.56
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.33	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
2:G:13:GLN:HG2	2:G:116:SER:CB	2.36	0.56
1:A:393:THR:HA	1:A:523:THR:H	1.69	0.56
1:B:187:LYS:NZ	1:B:213:VAL:HG13	2.21	0.56
1:A:233:ILE:O	1:A:233:ILE:HG23	2.05	0.56
1:A:533:LEU:O	1:A:533:LEU:HD23	2.06	0.56
5:C:1405:NAG:H3	5:C:1405:NAG:H83	1.88	0.56
3:F:19:ALA:HB3	3:F:76:ILE:HB	1.87	0.56
3:F:116:VAL:O	3:F:117:PHE:CD1	2.58	0.56
2:G:33:TYR:HB2	2:G:98:ASP:HB3	1.87	0.56
2:H:123:PRO:HB2	2:H:146:VAL:HG23	1.88	0.56
4:J:2:NAG:H83	4:J:2:NAG:H3	1.87	0.56
1:C:129:LYS:HZ3	1:C:169:GLU:HG2	1.70	0.55
3:L:108:LYS:HB3	3:L:141:TYR:CE1	2.37	0.55
2:G:203:ASN:HD22	2:G:205:LYS:HE3	1.71	0.55
1:C:336:CYS:SG	1:C:337:PRO:HD2	2.47	0.55
1:A:342:PHE:HE2	1:A:368:LEU:CD2	1.93	0.55
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
2:G:123:PRO:HB2	2:G:146:VAL:HG23	1.88	0.55
1:C:113:LYS:HD2	1:C:164:ASN:HD21	1.71	0.55
1:C:444:LYS:NZ	1:C:445:VAL:O	2.37	0.55
3:L:91:GLN:NE2	3:L:94:SER:OG	2.40	0.55
2:G:51:ILE:HG13	2:G:57:THR:HG22	1.89	0.55
1:A:332:ILE:HD11	1:A:335:LEU:HD13	1.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:CD	1:B:582:LEU:HD13	2.35	0.55
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.89	0.55
1:A:332:ILE:O	1:A:334:ASN:N	2.39	0.55
1:B:661:GLU:OE2	1:B:698:SER:OG	2.25	0.55
3:L:91:GLN:NE2	3:L:96:PRO:O	2.40	0.55
3:F:91:GLN:NE2	3:F:96:PRO:O	2.40	0.55
1:C:129:LYS:HD3	1:C:131:CYS:SG	2.46	0.55
4:D:1:NAG:H61	4:D:2:NAG:HN2	1.72	0.55
4:U:1:NAG:H61	4:U:2:NAG:HN2	1.71	0.55
1:A:402:ILE:HD12	1:A:406:GLU:HG3	1.88	0.54
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:B:352:ALA:HB2	1:B:468:ILE:HD12	1.88	0.54
2:H:130:PRO:HG3	2:H:142:LEU:HD23	1.89	0.54
2:H:203:ASN:HD22	2:H:205:LYS:HE3	1.72	0.54
3:L:117:PHE:HD2	3:L:136:LEU:HD23	1.72	0.54
1:C:340:GLU:HG3	1:C:341:VAL:HG23	1.89	0.54
3:L:7:SER:HB2	3:L:8:PRO:HD2	1.84	0.54
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.90	0.54
1:C:391:CYS:CB	1:C:523:THR:HB	2.34	0.54
1:C:357:ARG:HG3	1:C:396:TYR:OH	2.07	0.54
1:A:551:VAL:HB	1:A:588:THR:HG23	1.88	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.54
2:H:38:ARG:NH2	2:H:93:TYR:OH	2.41	0.54
3:F:142:PRO:O	3:F:199:HIS:NE2	2.40	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:B:166:CYS:SG	1:B:167:THR:N	2.81	0.54
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.89	0.54
2:G:130:PRO:HG3	2:G:142:LEU:HD23	1.89	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
2:H:152:GLU:CD	2:H:152:GLU:H	2.11	0.54
1:B:165:ASN:OD1	5:B:1403:NAG:N2	2.40	0.54
1:B:333:THR:OG1	1:B:334:ASN:N	2.41	0.53
3:F:40:LYS:HB2	3:F:43:GLN:HB2	1.89	0.53
3:L:40:LYS:HB2	3:L:43:GLN:HB2	1.89	0.53
1:C:97:LYS:HB3	1:C:187:LYS:HA	1.89	0.53
1:C:360:ASN:O	1:C:361:CYS:CB	2.52	0.53
2:G:117:SER:O	2:G:118:ALA:HB3	2.08	0.53
1:C:458:LYS:NZ	2:G:30:SER:OG	2.41	0.53
3:L:142:PRO:O	3:L:199:HIS:NE2	2.40	0.53
1:A:392:PHE:CB	1:A:524:VAL:CG2	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:O	1:B:234:ASN:C	2.46	0.53
4:I:2:NAG:H3	4:I:2:NAG:H83	1.90	0.53
1:A:227:VAL:CG1	1:A:228:ASP:H	2.12	0.53
1:A:534:VAL:O	1:A:535:LYS:HG3	2.09	0.53
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.53
1:C:402:ILE:HD12	1:C:406:GLU:HG3	1.88	0.53
1:A:340:GLU:HG3	1:A:341:VAL:HG23	1.89	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:C:342:PHE:CE2	1:C:368:LEU:HD22	2.27	0.53
1:C:357:ARG:CZ	1:C:357:ARG:CB	2.86	0.53
2:G:40:ALA:HB3	2:G:43:LYS:HB2	1.89	0.53
2:G:47:TRP:HE1	2:G:50:VAL:HG13	1.73	0.53
1:A:115:GLN:C	1:A:233:ILE:CD1	2.76	0.53
1:A:458:LYS:NZ	2:H:30:SER:OG	2.41	0.53
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.53
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.91	0.53
2:G:152:GLU:H	2:G:152:GLU:CD	2.11	0.53
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.53
1:B:402:ILE:O	1:B:507:PRO:HA	2.09	0.53
2:G:38:ARG:NH2	2:G:93:TYR:OH	2.40	0.53
2:G:143:GLY:HA2	2:G:158:TRP:HZ2	1.73	0.53
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.72	0.52
2:H:47:TRP:HE1	2:H:50:VAL:HG13	1.73	0.52
2:H:12:ILE:O	2:H:116:SER:N	2.43	0.52
2:H:117:SER:O	2:H:118:ALA:HB3	2.08	0.52
2:H:143:GLY:HA2	2:H:158:TRP:HZ2	1.73	0.52
1:B:112:SER:O	1:B:113:LYS:HB2	2.10	0.52
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.52
2:G:12:ILE:O	2:G:116:SER:N	2.43	0.52
3:F:141:TYR:CG	3:F:142:PRO:CD	2.93	0.52
1:C:193:VAL:HG23	1:C:223:LEU:HD23	1.91	0.52
1:C:391:CYS:CB	1:C:523:THR:OG1	2.47	0.52
1:A:334:ASN:CB	1:A:362:VAL:HG23	2.27	0.52
1:B:424:LYS:HB3	1:B:463:PRO:HA	1.92	0.52
1:B:457:ARG:NH2	1:B:469:SER:O	2.43	0.52
1:C:457:ARG:NH1	1:C:460:ASN:O	2.43	0.52
3:L:109:ARG:NH1	3:L:110:THR:OG1	2.43	0.52
1:C:113:LYS:HD3	1:C:113:LYS:N	2.25	0.52
2:H:13:GLN:CB	2:H:116:SER:HB2	2.39	0.52
1:A:130:VAL:CG2	1:A:231:ILE:HG23	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HA	1:B:495:TYR:OH	2.10	0.52
1:C:332:ILE:C	1:C:334:ASN:H	2.14	0.52
1:C:1101:HIS:CD2	4:Z:1:NAG:H5	2.45	0.52
3:L:141:TYR:CG	3:L:142:PRO:CD	2.93	0.52
1:A:457:ARG:NH1	1:A:460:ASN:O	2.43	0.51
1:B:555:SER:OG	1:B:584:ILE:O	2.28	0.51
1:A:480:CYS:HG	1:A:488:CYS:CB	2.21	0.51
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.46	0.51
1:B:380:TYR:O	1:B:430:THR:HA	2.11	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.51
1:A:392:PHE:CE2	1:A:517:LEU:CD2	2.88	0.51
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:B:560:LEU:H	1:B:563:GLN:NE2	2.08	0.51
3:L:6:GLN:CG	3:L:103:THR:HG23	2.40	0.51
3:L:90:GLN:NE2	3:L:91:GLN:O	2.43	0.51
1:A:529:LYS:NZ	1:A:529:LYS:CB	2.73	0.51
3:L:140:PHE:CE1	3:L:174:TYR:HB2	2.46	0.51
3:F:140:PHE:CE1	3:F:174:TYR:HB2	2.46	0.51
1:C:83:VAL:HG22	1:C:237:ARG:HD2	1.92	0.51
3:L:6:GLN:H	3:L:101:GLN:NE2	2.09	0.51
2:G:133:LYS:NZ	3:F:120:PRO:HG3	2.26	0.51
3:F:90:GLN:NE2	3:F:91:GLN:O	2.43	0.51
1:C:97:LYS:HD3	1:C:187:LYS:HA	1.92	0.51
2:H:133:LYS:NZ	3:L:120:PRO:HG3	2.26	0.51
3:F:109:ARG:NH1	3:F:110:THR:OG1	2.43	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
3:F:135:CYS:HB2	3:F:149:TRP:CH2	2.45	0.51
1:A:230:PRO:HD3	1:C:522:ALA:CB	2.40	0.51
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.45	0.51
1:C:533:LEU:HG	1:C:533:LEU:O	2.11	0.51
1:C:535:LYS:HB3	1:C:536:ASN:HD22	1.76	0.51
1:A:529:LYS:HE3	1:A:529:LYS:HA	1.91	0.51
1:C:113:LYS:H	1:C:132:GLU:HB3	1.76	0.51
3:L:140:PHE:CD1	3:L:174:TYR:C	2.84	0.51
3:F:115:SER:CB	3:F:117:PHE:HZ	2.16	0.51
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.76	0.50
3:L:141:TYR:CD2	3:L:142:PRO:CD	2.91	0.50
3:F:6:GLN:CG	3:F:103:THR:HG23	2.40	0.50
1:A:230:PRO:CG	1:C:522:ALA:CB	2.82	0.50
1:C:357:ARG:HB3	1:C:357:ARG:HH21	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:LYS:O	1:C:536:ASN:HB2	2.10	0.50
3:F:91:GLN:NE2	3:F:94:SER:OG	2.40	0.50
3:F:140:PHE:CD1	3:F:174:TYR:C	2.84	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
3:L:135:CYS:HB2	3:L:149:TRP:CH2	2.46	0.50
3:F:117:PHE:HD2	3:F:136:LEU:HD23	1.73	0.50
1:A:964:LYS:HE3	1:C:570:ALA:HA	1.93	0.50
1:A:518:LEU:CD1	1:A:518:LEU:N	2.75	0.50
2:G:2:VAL:O	2:G:25:SER:OG	2.25	0.50
4:R:1:NAG:H62	4:R:2:NAG:H2	1.93	0.50
1:B:616:ASN:HB3	1:B:618:THR:HG22	1.94	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
3:L:12:SER:OG	3:L:108:LYS:CG	2.59	0.50
2:G:90:THR:HG22	2:G:115:VAL:HG12	1.94	0.50
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.50
1:A:342:PHE:CE1	4:D:1:NAG:H81	2.41	0.50
1:B:31:SER:O	1:B:59:PHE:HA	2.10	0.50
1:B:675:GLN:HA	1:B:690:GLN:HG3	1.93	0.50
1:A:392:PHE:O	1:A:522:ALA:HB1	2.12	0.49
1:A:534:VAL:HG23	1:A:535:LYS:H	1.73	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:B:350:VAL:HG23	1:B:422:ASN:HD22	1.77	0.49
2:H:90:THR:HG22	2:H:115:VAL:HG12	1.94	0.49
2:H:159:ASN:ND2	2:H:197:THR:O	2.45	0.49
3:F:6:GLN:H	3:F:101:GLN:NE2	2.09	0.49
3:F:141:TYR:CD2	3:F:142:PRO:CD	2.91	0.49
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.49
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.12	0.49
1:B:112:SER:N	1:B:133:PHE:O	2.45	0.49
1:C:357:ARG:NH2	1:C:357:ARG:CB	2.73	0.49
3:F:12:SER:OG	3:F:108:LYS:CG	2.59	0.49
3:F:140:PHE:CE1	3:F:174:TYR:CB	2.95	0.49
3:L:115:SER:CB	3:L:117:PHE:HZ	2.16	0.49
1:B:231:ILE:HG22	1:B:233:ILE:H	1.76	0.49
1:B:331:ASN:HD22	4:N:1:NAG:H83	1.78	0.49
1:C:117:LEU:HB2	1:C:130:VAL:HG22	1.94	0.49
1:C:550:GLY:CA	1:C:590:CYS:SG	2.90	0.49
2:H:120:THR:OG1	2:H:151:PRO:HG2	2.12	0.49
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.49
2:H:123:PRO:HD3	2:H:204:HIS:HD1	1.78	0.49
3:L:139:ASN:O	3:L:140:PHE:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:PRO:HD3	2:G:204:HIS:HD1	1.78	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
1:A:364:ASP:N	1:A:364:ASP:OD1	2.45	0.49
1:A:432:CYS:H	1:A:513:LEU:HB2	1.77	0.49
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.13	0.49
1:C:363:ALA:CB	1:C:365:TYR:CZ	2.96	0.49
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.48
1:B:396:TYR:HB2	1:B:514:SER:HB2	1.95	0.48
1:B:457:ARG:NH1	1:B:467:ASP:HB3	2.28	0.48
1:C:332:ILE:CA	1:C:362:VAL:HG21	2.42	0.48
1:C:424:LYS:HB2	1:C:461:LEU:HB2	1.95	0.48
1:C:432:CYS:H	1:C:513:LEU:HB2	1.77	0.48
2:G:13:GLN:CB	2:G:116:SER:HB2	2.39	0.48
3:F:139:ASN:O	3:F:140:PHE:HB3	2.13	0.48
1:A:334:ASN:OD1	1:A:361:CYS:CB	2.62	0.48
2:G:120:THR:OG1	2:G:151:PRO:HG2	2.13	0.48
1:C:480:CYS:CB	1:C:488:CYS:HG	2.22	0.48
1:A:424:LYS:HB2	1:A:461:LEU:HB2	1.95	0.48
1:B:281:GLU:OE2	5:B:1405:NAG:H81	2.14	0.48
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.96	0.48
1:C:364:ASP:N	1:C:364:ASP:OD1	2.45	0.48
1:C:394:ASN:O	1:C:516:GLU:N	2.47	0.48
1:C:473:TYR:N	1:C:489:TYR:O	2.42	0.48
2:H:154:VAL:HG22	2:H:204:HIS:CD2	2.49	0.48
3:L:140:PHE:CE1	3:L:174:TYR:CB	2.95	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.76	0.48
1:A:363:ALA:CB	1:A:365:TYR:CZ	2.96	0.48
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.94	0.48
1:C:384:PRO:HA	1:C:387:LEU:HB2	1.96	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
1:A:340:GLU:HG3	1:A:341:VAL:N	2.28	0.48
1:B:576:VAL:O	1:B:584:ILE:HA	2.13	0.48
1:A:529:LYS:HA	1:A:529:LYS:CE	2.43	0.48
1:C:118:LEU:O	1:C:128:ILE:HA	2.14	0.48
1:C:197:ILE:HG22	1:C:198:ASP:H	1.78	0.48
1:C:675:GLN:NE2	1:C:675:GLN:CA	2.73	0.48
2:H:13:GLN:HG3	2:H:116:SER:OG	2.13	0.48
3:L:35:ALA:N	3:L:90:GLN:O	2.43	0.48
1:A:230:PRO:CB	1:C:522:ALA:CB	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PRO:HA	1:A:387:LEU:HB2	1.96	0.47
1:A:474:GLN:HG3	1:A:476:GLY:H	1.79	0.47
2:G:159:ASN:ND2	2:G:197:THR:O	2.45	0.47
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.47
1:C:340:GLU:HG3	1:C:341:VAL:N	2.28	0.47
2:H:151:PRO:HB2	2:H:204:HIS:NE2	2.29	0.47
2:G:154:VAL:HG22	2:G:204:HIS:CD2	2.49	0.47
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:C:366:SER:H	1:C:388:ASN:HD21	1.62	0.47
2:H:20:LEU:HG	2:H:82:MET:HE1	1.97	0.47
1:A:45:SER:O	1:A:47:VAL:HG22	2.14	0.47
1:A:366:SER:H	1:A:388:ASN:HD21	1.62	0.47
1:B:557:LYS:NZ	1:B:575:ALA:HB2	2.29	0.47
3:L:21:LEU:O	3:L:74:LEU:N	2.43	0.47
1:C:140:PHE:CE2	1:C:244:LEU:HB2	2.49	0.47
2:G:175:GLN:OE1	2:G:181:SER:OG	2.31	0.47
1:A:230:PRO:HD3	1:C:522:ALA:HB1	1.96	0.47
3:L:109:ARG:O	3:L:110:THR:C	2.53	0.47
2:G:13:GLN:HG3	2:G:116:SER:OG	2.13	0.47
1:A:340:GLU:HG3	1:A:341:VAL:CG2	2.44	0.47
1:A:521:PRO:HG3	1:B:199:GLY:O	2.15	0.47
1:B:577:ARG:HD3	1:B:582:LEU:HD11	1.92	0.47
1:C:66:HIS:CE1	1:C:214:ARG:HH22	2.32	0.47
1:C:278:LYS:HB2	1:C:306:PHE:CZ	2.50	0.47
1:C:394:ASN:N	1:C:516:GLU:HB3	2.29	0.47
1:C:474:GLN:HG3	1:C:476:GLY:H	1.79	0.47
1:C:605:SER:OG	1:C:606:ASN:N	2.47	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.96	0.47
2:H:135:THR:HG23	2:H:140:ALA:HB2	1.96	0.47
2:G:151:PRO:HB2	2:G:204:HIS:NE2	2.29	0.47
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.38	0.47
1:A:394:ASN:O	1:A:516:GLU:N	2.47	0.47
1:B:403:ARG:NH2	1:B:504:GLY:O	2.47	0.47
1:C:340:GLU:HG3	1:C:341:VAL:CG2	2.44	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.47
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.97	0.47
1:A:227:VAL:O	1:A:228:ASP:HB2	2.15	0.47
1:C:332:ILE:CD1	1:C:335:LEU:CD1	2.93	0.47
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.47
2:G:20:LEU:HG	2:G:82:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:135:THR:HG23	2:G:140:ALA:HB2	1.96	0.47
1:A:334:ASN:OD1	1:A:361:CYS:HB2	2.15	0.46
1:C:66:HIS:HE1	1:C:214:ARG:HH22	1.62	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:C:357:ARG:CZ	1:C:357:ARG:HB2	2.44	0.46
2:H:4:LEU:HB3	2:H:108:GLY:HA2	1.97	0.46
2:H:119:SER:O	2:H:150:PHE:CD2	2.69	0.46
1:A:985:ASP:OD1	1:A:985:ASP:N	2.46	0.46
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.46
2:G:6:GLU:HG3	2:G:109:GLN:H	1.79	0.46
2:G:119:SER:O	2:G:150:PHE:CD2	2.69	0.46
2:G:131:SER:HB3	2:G:133:LYS:HG2	1.98	0.46
1:A:115:GLN:O	1:A:233:ILE:CG1	2.63	0.46
1:B:603:ASN:OD1	5:B:1407:NAG:N2	2.49	0.46
1:C:480:CYS:HG	1:C:488:CYS:CB	2.21	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
2:H:6:GLU:HG3	2:H:109:GLN:H	1.79	0.46
2:G:19:ARG:HA	2:G:81:GLN:HA	1.98	0.46
3:F:19:ALA:O	3:F:76:ILE:N	2.41	0.46
3:F:109:ARG:O	3:F:110:THR:C	2.53	0.46
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:A:229:LEU:HB3	1:A:230:PRO:HD2	1.97	0.46
1:A:332:ILE:CG2	1:A:333:THR:H	2.18	0.46
1:A:334:ASN:O	1:A:335:LEU:HD22	2.15	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:C:396:TYR:N	1:C:514:SER:O	2.48	0.46
1:A:127:VAL:HG11	5:A:1402:NAG:H61	1.98	0.46
1:A:230:PRO:CD	1:C:522:ALA:CB	2.93	0.46
1:B:205:SER:OG	1:B:226:LEU:HD22	2.16	0.46
1:B:532:ASN:ND2	1:B:533:LEU:H	2.14	0.46
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.51	0.46
1:C:480:CYS:SG	1:C:488:CYS:HB3	2.56	0.46
1:A:392:PHE:HB2	1:A:524:VAL:HG23	1.98	0.46
1:C:349:SER:OG	1:C:350:VAL:N	2.49	0.46
2:H:204:HIS:CD2	2:H:206:PRO:HD2	2.51	0.46
1:A:357:ARG:NH2	1:A:357:ARG:CB	2.74	0.46
1:A:394:ASN:H	1:A:516:GLU:HB3	1.81	0.46
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.46
1:C:534:VAL:CG2	1:C:535:LYS:N	2.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:SER:HB3	2:H:133:LYS:HG2	1.98	0.46
1:A:168:PHE:HE2	1:A:229:LEU:HG	1.72	0.46
1:A:349:SER:OG	1:A:350:VAL:N	2.49	0.46
1:A:396:TYR:N	1:A:514:SER:O	2.48	0.46
1:B:437:ASN:HD21	1:B:506:GLN:HE21	1.64	0.46
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.46
1:B:424:LYS:HG3	1:B:461:LEU:O	2.17	0.45
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.84	0.45
2:H:19:ARG:HA	2:H:81:GLN:HA	1.98	0.45
3:L:19:ALA:O	3:L:76:ILE:N	2.41	0.45
2:G:4:LEU:H	2:G:24:ALA:HA	1.81	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:B:567:ARG:HE	1:B:567:ARG:HB3	1.47	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.99	0.45
2:H:149:TYR:OH	2:H:182:LEU:HD23	2.17	0.45
2:G:4:LEU:HB3	2:G:108:GLY:HA2	1.97	0.45
3:F:143:ARG:HH21	3:F:164:VAL:HB	1.81	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:C:363:ALA:H	1:C:526:GLY:HA2	1.81	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:B:230:PRO:C	1:B:231:ILE:HG12	2.37	0.45
3:L:3:VAL:N	3:L:26:SER:OG	2.48	0.45
1:C:37:TYR:HA	1:C:223:LEU:H	1.81	0.45
1:C:314:GLN:HE21	1:C:314:GLN:HB2	1.56	0.45
1:C:357:ARG:HA	1:C:394:ASN:HD21	1.82	0.45
1:A:360:ASN:O	1:A:361:CYS:CB	2.58	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:472:ILE:H	1:B:472:ILE:HG13	1.56	0.45
1:C:676:THR:CA	1:C:690:GLN:HE21	2.29	0.45
3:L:15:PRO:HA	3:L:79:LEU:HB3	1.99	0.45
2:G:204:HIS:CD2	2:G:206:PRO:HD2	2.51	0.45
1:A:357:ARG:HA	1:A:394:ASN:HD21	1.82	0.45
1:B:364:ASP:OD1	1:B:364:ASP:N	2.50	0.45
1:B:521:PRO:HG3	1:B:564:GLN:HE21	1.81	0.45
2:H:2:VAL:O	2:H:25:SER:OG	2.25	0.45
2:H:4:LEU:H	2:H:24:ALA:HA	1.81	0.45
2:H:115:VAL:HG22	2:H:116:SER:N	2.31	0.45
3:L:106:GLU:CB	3:L:167:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
1:A:519:HIS:O	1:A:520:ALA:HB3	2.17	0.45
1:A:676:THR:HB	1:A:693:ILE:HG21	1.98	0.45
1:B:521:PRO:HG3	1:B:564:GLN:NE2	2.32	0.45
3:L:140:PHE:HE1	3:L:174:TYR:C	2.21	0.45
3:F:15:PRO:HA	3:F:79:LEU:HB3	1.99	0.45
1:A:480:CYS:SG	1:A:488:CYS:HB3	2.56	0.44
1:B:437:ASN:OD1	1:B:438:SER:N	2.51	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:B:350:VAL:HG11	1:B:402:ILE:HG23	2.00	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.44
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:A:166:CYS:O	1:C:357:ARG:NE	2.50	0.44
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.44
1:B:453:TYR:HD1	1:B:453:TYR:H	1.64	0.44
2:H:61:ASP:HA	2:H:64:LYS:HG2	2.00	0.44
2:G:149:TYR:OH	2:G:182:LEU:HD23	2.17	0.44
1:B:233:ILE:O	1:B:233:ILE:HG23	2.18	0.44
1:B:376:THR:CG2	1:B:378:LYS:HG3	2.48	0.44
3:L:12:SER:C	3:L:108:LYS:HE3	2.23	0.44
3:L:143:ARG:HH21	3:L:164:VAL:HB	1.81	0.44
1:A:166:CYS:O	1:C:357:ARG:CD	2.66	0.44
1:A:388:ASN:O	1:A:527:PRO:HD2	2.17	0.44
1:B:454:ARG:NH2	1:B:456:PHE:HZ	2.16	0.44
1:C:142:GLY:H	1:C:243:ALA:HA	1.83	0.44
2:H:158:TRP:HD1	2:H:167:VAL:HG13	1.83	0.44
2:G:66:ARG:NH2	2:G:84:SER:O	2.50	0.44
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.44
1:C:338:PHE:CD1	1:C:342:PHE:HD2	2.36	0.44
1:C:505:TYR:OH	3:F:93:GLY:O	2.36	0.44
3:L:22:SER:HA	3:L:73:THR:HA	2.00	0.44
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.51	0.44
5:A:1404:NAG:HO3	5:A:1404:NAG:C7	2.30	0.44
1:B:231:ILE:HG22	1:B:233:ILE:HG22	1.96	0.44
2:G:81:GLN:NE2	2:G:82:MET:O	2.51	0.44
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.44
1:A:392:PHE:CA	1:A:524:VAL:CG2	2.93	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.44
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.44
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ARG:NH2	2:H:84:SER:O	2.50	0.44
3:L:11:LEU:N	3:L:104:LYS:O	2.41	0.44
2:G:158:TRP:HD1	2:G:167:VAL:HG13	1.83	0.44
1:A:338:PHE:CD1	1:A:342:PHE:HD2	2.36	0.43
1:C:84:LEU:HD13	1:C:238:PHE:CE1	2.52	0.43
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.43
3:L:94:SER:OG	3:L:96:PRO:O	2.36	0.43
2:G:115:VAL:HG22	2:G:116:SER:N	2.32	0.43
3:F:12:SER:O	3:F:108:LYS:CE	2.28	0.43
3:F:94:SER:OG	3:F:96:PRO:O	2.36	0.43
1:A:529:LYS:CE	1:A:529:LYS:CA	2.94	0.43
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.00	0.43
1:B:439:ASN:HB3	1:B:506:GLN:HB2	1.99	0.43
3:F:12:SER:C	3:F:108:LYS:HE3	2.23	0.43
3:F:21:LEU:O	3:F:74:LEU:N	2.43	0.43
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.85	0.43
1:C:331:ASN:O	1:C:332:ILE:HG23	2.18	0.43
2:G:199:ILE:HG23	2:G:214:LYS:HD2	2.00	0.43
1:A:379:CYS:N	1:A:432:CYS:SG	2.92	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.18	0.43
1:B:121:ASN:O	1:B:121:ASN:ND2	2.49	0.43
1:B:167:THR:HG22	1:B:168:PHE:H	1.82	0.43
1:C:119:ILE:HG13	1:C:128:ILE:HG23	2.01	0.43
2:H:64:LYS:HD3	2:H:64:LYS:HA	1.82	0.43
3:F:22:SER:HA	3:F:73:THR:HA	2.00	0.43
3:F:35:ALA:N	3:F:90:GLN:O	2.43	0.43
1:A:353:TRP:N	1:A:466:ARG:HH12	2.17	0.43
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.43
4:D:1:NAG:H61	4:D:2:NAG:N2	2.33	0.43
1:A:440:ASN:OD1	1:A:440:ASN:N	2.51	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:C:396:TYR:HB2	1:C:514:SER:HB3	2.01	0.43
1:B:559:PHE:O	1:B:560:LEU:HD13	2.18	0.43
2:G:159:ASN:OD1	2:G:199:ILE:HG13	2.19	0.43
3:F:92:TYR:HA	3:F:97:ARG:HG3	2.01	0.43
4:U:1:NAG:H61	4:U:2:NAG:N2	2.33	0.43
1:A:366:SER:H	1:A:388:ASN:ND2	2.17	0.43
1:A:392:PHE:CD2	1:A:517:LEU:CD2	3.02	0.43
1:C:366:SER:H	1:C:388:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:146:VAL:HG13	2:G:182:LEU:HG	2.00	0.43
2:G:151:PRO:HD2	2:G:204:HIS:CE1	2.54	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:A:334:ASN:OD1	1:A:361:CYS:CA	2.66	0.43
1:A:396:TYR:HB2	1:A:514:SER:HB3	2.01	0.43
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.43
1:B:230:PRO:O	1:B:231:ILE:HD13	2.18	0.43
1:B:462:LYS:H	1:B:462:LYS:HD3	1.84	0.43
1:C:353:TRP:N	1:C:466:ARG:HH12	2.17	0.43
1:C:530:SER:HB2	1:C:580:GLN:HE22	1.84	0.43
3:L:14:SER:HA	3:L:107:ILE:HD11	1.99	0.43
2:G:64:LYS:HD3	2:G:64:LYS:HA	1.82	0.43
2:G:69:ILE:HG22	2:G:80:LEU:HD13	2.01	0.43
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.43
1:A:226:LEU:HB3	1:A:227:VAL:H	1.57	0.43
1:A:233:ILE:C	1:A:234:ASN:O	2.54	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:A:505:TYR:OH	3:L:93:GLY:O	2.36	0.43
1:A:517:LEU:HD13	1:A:517:LEU:HA	1.83	0.43
1:B:472:ILE:CD1	1:B:474:GLN:HB3	2.47	0.43
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.00	0.43
1:C:342:PHE:HZ	1:C:368:LEU:HD22	1.76	0.43
2:H:159:ASN:OD1	2:H:199:ILE:HG13	2.19	0.43
2:G:29:VAL:HG21	2:G:76:ASN:HA	2.01	0.43
2:G:134:SER:HA	3:F:117:PHE:HB3	2.00	0.43
3:F:140:PHE:HE1	3:F:174:TYR:C	2.21	0.43
1:B:91:TYR:OH	1:B:191:GLU:HG2	2.18	0.42
1:B:459:SER:C	1:B:461:LEU:H	2.23	0.42
1:C:379:CYS:N	1:C:432:CYS:SG	2.92	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.42
2:H:134:SER:HA	3:L:117:PHE:HB3	2.00	0.42
2:G:61:ASP:HA	2:G:64:LYS:HG2	2.00	0.42
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.42
1:A:127:VAL:HG21	5:A:1402:NAG:H5	2.01	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
1:B:748:GLU:CD	1:B:981:LEU:HD21	2.39	0.42
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.42
2:H:81:GLN:NE2	2:H:82:MET:O	2.51	0.42
2:H:120:THR:O	2:H:120:THR:HG23	2.19	0.42
2:G:126:PHE:HD1	3:F:124:GLU:OE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:C	1:C:154:GLU:HA	2.39	0.42
2:H:175:GLN:OE1	2:H:181:SER:OG	2.31	0.42
2:H:199:ILE:HG23	2:H:214:LYS:HD2	2.00	0.42
3:L:12:SER:O	3:L:108:LYS:CE	2.28	0.42
3:F:3:VAL:N	3:F:26:SER:OG	2.48	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:359:SER:OG	1:A:360:ASN:N	2.52	0.42
1:B:231:ILE:HG22	1:B:233:ILE:N	2.34	0.42
2:H:119:SER:O	2:H:150:PHE:CG	2.72	0.42
2:H:120:THR:OG1	2:H:151:PRO:CG	2.67	0.42
3:L:7:SER:CB	3:L:8:PRO:CD	2.64	0.42
2:G:120:THR:OG1	2:G:151:PRO:CG	2.67	0.42
2:G:133:LYS:HZ1	3:F:120:PRO:HG3	1.83	0.42
1:A:405:ASP:OD1	1:A:405:ASP:N	2.53	0.42
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.42
1:B:29:THR:OG1	1:B:30:ASN:N	2.50	0.42
1:C:556:ASN:HD22	1:C:556:ASN:HA	1.53	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:B:567:ARG:HG2	1:C:42:VAL:HG11	2.02	0.42
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.42
2:H:126:PHE:HD1	3:L:124:GLU:OE1	2.01	0.42
2:H:146:VAL:HG13	2:H:182:LEU:HG	2.01	0.42
2:H:203:ASN:HB3	2:H:210:LYS:CE	2.49	0.42
3:L:116:VAL:C	3:L:117:PHE:CG	2.93	0.42
2:G:11:LEU:CD1	2:G:151:PRO:HG3	2.49	0.42
2:G:119:SER:O	2:G:150:PHE:CG	2.72	0.42
3:F:14:SER:HA	3:F:107:ILE:HD11	2.00	0.42
1:A:537:LYS:HE2	1:A:537:LYS:HB2	1.71	0.42
1:C:334:ASN:C	1:C:336:CYS:N	2.73	0.42
1:C:334:ASN:O	1:C:336:CYS:N	2.52	0.42
1:C:359:SER:OG	1:C:360:ASN:N	2.52	0.42
1:C:453:TYR:O	1:C:493:GLN:N	2.47	0.42
2:H:182:LEU:HD12	2:H:183:SER:N	2.34	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:C:440:ASN:N	1:C:440:ASN:OD1	2.51	0.42
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
2:G:173:VAL:HG21	3:F:161:GLN:HB3	2.02	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.42
1:B:226:LEU:C	1:B:227:VAL:HG13	2.40	0.42
1:C:233:ILE:HG12	1:C:234:ASN:N	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.42
2:H:193:LEU:HB3	2:H:217:PRO:HG3	2.02	0.42
2:G:193:LEU:HB3	2:G:217:PRO:HG3	2.02	0.42
3:F:73:THR:OG1	3:F:74:LEU:N	2.53	0.42
3:F:104:LYS:HE2	3:F:104:LYS:HB2	1.85	0.42
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.55	0.42
2:H:11:LEU:CD1	2:H:151:PRO:HG3	2.49	0.42
3:L:73:THR:OG1	3:L:74:LEU:N	2.53	0.42
2:G:133:LYS:HE3	3:F:120:PRO:HD3	2.02	0.42
2:G:203:ASN:HB3	2:G:210:LYS:CE	2.49	0.42
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.71	0.41
1:B:341:VAL:HG23	1:B:342:PHE:HD1	1.84	0.41
1:B:495:TYR:CZ	1:B:507:PRO:HG3	2.55	0.41
2:H:151:PRO:HD2	2:H:204:HIS:CE1	2.54	0.41
4:V:1:NAG:H3	4:V:1:NAG:H83	2.02	0.41
1:A:229:LEU:HD13	1:A:229:LEU:HA	1.82	0.41
1:A:529:LYS:HE3	1:A:529:LYS:CA	2.50	0.41
1:A:530:SER:CB	1:A:580:GLN:NE2	2.84	0.41
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.41
3:L:65:GLY:HA2	3:L:74:LEU:HA	2.03	0.41
3:L:104:LYS:HE2	3:L:104:LYS:HB2	1.85	0.41
3:F:116:VAL:C	3:F:117:PHE:CG	2.93	0.41
1:A:231:ILE:HG22	1:A:233:ILE:HG22	2.02	0.41
1:A:392:PHE:O	1:A:524:VAL:HG23	2.17	0.41
1:A:473:TYR:N	1:A:489:TYR:O	2.42	0.41
1:A:516:GLU:OE2	1:A:516:GLU:HA	2.20	0.41
1:C:122:ASN:ND2	1:C:125:ASN:HB2	2.35	0.41
1:C:534:VAL:HG23	1:C:535:LYS:H	1.82	0.41
2:H:133:LYS:HE3	3:L:120:PRO:HD3	2.01	0.41
3:L:92:TYR:HA	3:L:97:ARG:HG3	2.01	0.41
1:B:81:ASN:O	1:B:239:GLN:NE2	2.54	0.41
1:B:376:THR:O	1:B:434:ILE:HA	2.20	0.41
1:C:117:LEU:HD22	1:C:231:ILE:HD12	2.03	0.41
2:G:120:THR:HG23	2:G:120:THR:O	2.19	0.41
2:G:182:LEU:HD12	2:G:183:SER:N	2.34	0.41
1:A:480:CYS:CB	1:A:488:CYS:HG	2.28	0.41
1:B:142:GLY:O	1:B:156:GLU:HG3	2.21	0.41
1:B:187:LYS:HG2	1:B:212:LEU:O	2.21	0.41
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.41
2:H:69:ILE:HG22	2:H:80:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:PHE:HE1	3:L:175:SER:N	2.18	0.41
1:A:115:GLN:C	1:A:233:ILE:HG12	2.40	0.41
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.41
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.41
1:B:541:PHE:O	1:B:547:THR:HA	2.20	0.41
1:C:391:CYS:HB3	1:C:523:THR:HG1	1.76	0.41
1:A:295:PRO:HB2	1:A:608:VAL:HG11	2.02	0.41
1:A:453:TYR:O	1:A:493:GLN:N	2.47	0.41
1:C:391:CYS:SG	1:C:525:CYS:CA	3.09	0.41
2:H:90:THR:CG2	2:H:115:VAL:HG12	2.51	0.41
3:L:11:LEU:HD12	3:L:11:LEU:N	2.35	0.41
3:F:140:PHE:HE1	3:F:175:SER:N	2.18	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.50	0.41
1:C:188:ASN:HB2	1:C:190:ARG:HH11	1.86	0.41
1:A:116:SER:HA	1:A:233:ILE:HG12	2.03	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:230:PRO:HB2	1:C:520:ALA:HB1	2.02	0.41
1:A:232:GLY:C	1:A:233:ILE:HG22	2.41	0.41
1:B:122:ASN:OD1	1:B:122:ASN:N	2.48	0.41
1:B:229:LEU:H	1:B:229:LEU:HG	1.61	0.41
1:B:403:ARG:NE	1:B:505:TYR:HD1	2.19	0.41
1:C:530:SER:HB2	1:C:580:GLN:NE2	2.36	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
2:H:29:VAL:HG21	2:H:76:ASN:HA	2.01	0.41
3:F:11:LEU:HD12	3:F:11:LEU:N	2.35	0.41
3:F:16:GLY:H	3:F:79:LEU:HB3	1.86	0.41
1:A:115:GLN:HB2	1:A:233:ILE:CD1	2.36	0.41
1:A:346:ARG:HD2	1:A:346:ARG:HA	1.88	0.41
1:A:536:ASN:HA	1:A:551:VAL:HG13	2.02	0.41
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.41
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.41
2:H:11:LEU:CD1	2:H:150:PHE:CD2	2.90	0.41
2:G:198:TYR:H	2:G:214:LYS:HE3	1.86	0.41
3:F:19:ALA:N	3:F:76:ILE:O	2.51	0.41
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.40
1:A:392:PHE:CB	1:A:524:VAL:HG23	2.50	0.40
1:A:530:SER:OG	1:A:580:GLN:NE2	2.54	0.40
1:B:416:GLY:O	1:B:420:ASP:N	2.45	0.40
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.40
1:C:332:ILE:HA	1:C:362:VAL:HG21	2.02	0.40
1:C:365:TYR:C	1:C:367:VAL:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.40
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.40
3:F:11:LEU:N	3:F:104:LYS:O	2.41	0.40
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.40
1:A:433:VAL:HG23	1:A:512:VAL:HG12	2.03	0.40
1:A:530:SER:CB	1:A:580:GLN:HE22	2.34	0.40
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.21	0.40
1:C:338:PHE:CE2	1:C:364:ASP:OD2	2.74	0.40
1:C:402:ILE:HD11	1:C:407:VAL:HG12	2.04	0.40
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.40
2:H:173:VAL:HG21	3:L:161:GLN:HB3	2.02	0.40
3:L:55:ARG:NE	3:L:61:ASP:OD1	2.54	0.40
2:G:112:LEU:HD23	2:G:112:LEU:HA	1.94	0.40
1:A:365:TYR:O	1:A:367:VAL:N	2.55	0.40
1:B:132:GLU:HG3	1:B:165:ASN:HB2	2.02	0.40
1:B:135:PHE:HE1	1:B:159:VAL:HG12	1.86	0.40
1:B:458:LYS:HE2	1:B:458:LYS:HB2	1.79	0.40
1:B:646:ARG:O	1:B:646:ARG:HG3	2.22	0.40
1:C:365:TYR:O	1:C:367:VAL:N	2.55	0.40
1:C:433:VAL:HG23	1:C:512:VAL:HG12	2.03	0.40
1:C:524:VAL:HG22	1:C:524:VAL:O	2.21	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.40
2:H:204:HIS:HD2	2:H:206:PRO:HD2	1.86	0.40
3:L:15:PRO:HG3	3:L:107:ILE:HD12	2.03	0.40
3:L:16:GLY:H	3:L:79:LEU:HB3	1.86	0.40
1:A:342:PHE:HB3	1:A:343:ASN:H	1.76	0.40
1:A:504:GLY:N	1:A:506:GLN:OE1	2.54	0.40
1:A:542:ASN:HA	1:A:546:LEU:O	2.21	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:C:309:GLU:O	1:C:313:TYR:OH	2.28	0.40
2:H:133:LYS:HE3	2:H:218:LYS:HE2	2.04	0.40
2:G:133:LYS:HE3	2:G:218:LYS:HE2	2.04	0.40
1:A:230:PRO:CD	1:C:522:ALA:HB3	2.51	0.40
1:A:338:PHE:CE2	1:A:364:ASP:OD2	2.74	0.40
1:B:556:ASN:OD1	1:B:556:ASN:N	2.54	0.40
1:B:984:LEU:HD23	1:B:988:GLU:HB3	2.03	0.40
1:C:504:GLY:N	1:C:506:GLN:OE1	2.54	0.40
1:C:615:VAL:HG12	1:C:616:ASN:O	2.20	0.40
3:L:117:PHE:CE2	3:L:138:ASN:HB2	2.51	0.40
3:F:91:GLN:HE21	3:F:98:THR:HG23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:LYS:CB	3:F:141:TYR:CE1	3.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	988/1283 (77%)	877 (89%)	96 (10%)	15 (2%)	10	36
1	B	958/1283 (75%)	864 (90%)	92 (10%)	2 (0%)	47	78
1	C	986/1283 (77%)	879 (89%)	86 (9%)	21 (2%)	7	30
2	G	217/219 (99%)	198 (91%)	18 (8%)	1 (0%)	29	61
2	H	217/219 (99%)	198 (91%)	18 (8%)	1 (0%)	29	61
3	F	213/215 (99%)	194 (91%)	13 (6%)	6 (3%)	5	24
3	L	213/215 (99%)	194 (91%)	13 (6%)	6 (3%)	5	24
All	All	3792/4717 (80%)	3404 (90%)	336 (9%)	52 (1%)	15	37

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	531	THR
1	C	331	ASN
1	C	529	LYS
1	C	531	THR
1	C	534	VAL
1	C	814	LYS
3	L	139	ASN
3	F	139	ASN
1	A	227	VAL

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Mol	Chain	Res	Type
1	A	228	ASP
1	A	360	ASN
1	A	518	LEU
1	A	534	VAL
1	A	535	LYS
1	B	231	ILE
1	C	332	ILE
1	C	360	ASN
1	C	530	SER
1	C	535	LYS
1	C	591	SER
1	C	810	SER
2	H	117	SER
2	G	117	SER
1	A	233	ILE
1	A	342	PHE
1	A	343	ASN
1	C	342	PHE
1	C	343	ASN
1	C	361	CYS
3	L	8	PRO
3	F	8	PRO
1	A	333	THR
1	C	335	LEU
1	C	338	PHE
1	C	521	PRO
1	C	813	SER
3	L	141	TYR
3	F	141	TYR
1	A	361	CYS
1	B	88	ASP
1	C	812	PRO
3	L	110	THR
3	L	140	PHE
3	L	144	GLU
3	F	110	THR
3	F	140	PHE
3	F	144	GLU
1	A	520	ALA
1	C	811	LYS
1	A	232	GLY
1	C	520	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	881/1122 (78%)	788 (89%)	93 (11%)	6	24
1	B	862/1122 (77%)	758 (88%)	104 (12%)	5	18
1	C	879/1122 (78%)	799 (91%)	80 (9%)	9	32
2	G	184/184 (100%)	172 (94%)	12 (6%)	17	46
2	H	184/184 (100%)	172 (94%)	12 (6%)	17	46
3	F	186/186 (100%)	177 (95%)	9 (5%)	25	56
3	L	186/186 (100%)	177 (95%)	9 (5%)	25	56
All	All	3362/4106 (82%)	3043 (90%)	319 (10%)	12	29

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	226	LEU
1	A	229	LEU
1	A	282	ASN
1	A	296	LEU

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Mol	Chain	Res	Type
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	318	PHE
1	A	324	GLU
1	A	325	SER
1	A	336	CYS
1	A	342	PHE
1	A	365	TYR
1	A	379	CYS
1	A	408	ARG
1	A	517	LEU
1	A	518	LEU
1	A	523	THR
1	A	528	LYS
1	A	529	LYS
1	A	530	SER
1	A	532	ASN
1	A	535	LYS
1	A	537	LYS
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR
1	A	590	CYS
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	698	SER
1	A	703	ASN
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER

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Mol	Chain	Res	Type
1	A	773	GLU
1	A	785	VAL
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	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	982	SER
1	A	994	ASP
1	A	1005	GLN
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	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	45	SER
1	B	48	LEU
1	B	50	SER
1	B	51	THR
1	B	52	GLN
1	B	53	ASP
1	B	60	SER
1	B	87	ASN
1	B	88	ASP
1	B	95	THR
1	B	97	LYS

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Mol	Chain	Res	Type
1	B	99	ASN
1	B	108	THR
1	B	109	THR
1	B	112	SER
1	B	113	LYS
1	B	116	SER
1	B	120	VAL
1	B	127	VAL
1	B	158	ARG
1	B	164	ASN
1	B	205	SER
1	B	207	HIS
1	B	208	THR
1	B	214	ARG
1	B	229	LEU
1	B	233	ILE
1	B	240	THR
1	B	278	LYS
1	B	307	THR
1	B	318	PHE
1	B	328	ARG
1	B	345	THR
1	B	359	SER
1	B	371	SER
1	B	382	VAL
1	B	385	THR
1	B	388	ASN
1	B	402	ILE
1	B	403	ARG
1	B	409	GLN
1	B	417	LYS
1	B	430	THR
1	B	453	TYR
1	B	456	PHE
1	B	462	LYS
1	B	464	PHE
1	B	467	ASP
1	B	473	TYR
1	B	487	ASN
1	B	488	CYS
1	B	490	PHE
1	B	494	SER

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Mol	Chain	Res	Type
1	B	495	TYR
1	B	506	GLN
1	B	514	SER
1	B	525	CYS
1	B	531	THR
1	B	532	ASN
1	B	533	LEU
1	B	534	VAL
1	B	567	ARG
1	B	569	ILE
1	B	576	VAL
1	B	582	LEU
1	B	597	VAL
1	B	606	ASN
1	B	607	GLN
1	B	614	ASP
1	B	615	VAL
1	B	617	CYS
1	B	640	SER
1	B	649	CYS
1	B	676	THR
1	B	704	SER
1	B	710	ASN
1	B	746	SER
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	808	ASP
1	B	854	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	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL

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Mol	Chain	Res	Type
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	29	THR
1	C	50	SER
1	C	51	THR
1	C	60	SER
1	C	63	THR
1	C	84	LEU
1	C	86	PHE
1	C	98	SER
1	C	113	LYS
1	C	114	THR
1	C	117	LEU
1	C	120	VAL
1	C	125	ASN
1	C	143	VAL
1	C	156	GLU
1	C	172	SER
1	C	190	ARG
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	212	LEU
1	C	215	ASP
1	C	221	SER
1	C	234	ASN
1	C	271	GLN
1	C	287	ASP
1	C	301	CYS
1	C	305	SER
1	C	314	GLN
1	C	318	PHE
1	C	335	LEU
1	C	336	CYS
1	C	342	PHE

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Mol	Chain	Res	Type
1	C	357	ARG
1	C	365	TYR
1	C	379	CYS
1	C	408	ARG
1	C	528	LYS
1	C	531	THR
1	C	533	LEU
1	C	535	LYS
1	C	546	LEU
1	C	551	VAL
1	C	555	SER
1	C	556	ASN
1	C	567	ARG
1	C	573	THR
1	C	584	ILE
1	C	586	ASP
1	C	591	SER
1	C	602	THR
1	C	606	ASN
1	C	641	ASN
1	C	658	ASN
1	C	675	GLN
1	C	690	GLN
1	C	697	MET
1	C	703	ASN
1	C	727	LEU
1	C	740	MET
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	859	THR
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL

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Mol	Chain	Res	Type
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	H	11	LEU
2	H	124	SER
2	H	136	SER
2	H	142	LEU
2	H	146	VAL
2	H	164	THR
2	H	168	HIS
2	H	177	SER
2	H	183	SER
2	H	201	ASN
2	H	205	LYS
2	H	212	ASP
3	L	55	ARG
3	L	97	ARG
3	L	108	LYS
3	L	115	SER
3	L	117	PHE
3	L	132	SER
3	L	143	ARG
3	L	160	SER
3	L	177	SER
2	G	11	LEU
2	G	124	SER
2	G	136	SER
2	G	142	LEU
2	G	146	VAL
2	G	164	THR
2	G	168	HIS
2	G	177	SER
2	G	183	SER
2	G	201	ASN
2	G	205	LYS
2	G	212	ASP
3	F	55	ARG
3	F	97	ARG
3	F	108	LYS
3	F	115	SER

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Mol	Chain	Res	Type
3	F	117	PHE
3	F	132	SER
3	F	143	ARG
3	F	160	SER
3	F	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	388	ASN
1	A	540	ASN
1	A	556	ASN
1	A	580	GLN
1	A	644	GLN
1	A	658	ASN
1	A	690	GLN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	856	ASN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	115	GLN
1	B	134	GLN
1	B	164	ASN
1	B	188	ASN
1	B	245	HIS
1	B	354	ASN
1	B	422	ASN
1	B	487	ASN
1	B	506	GLN

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Mol	Chain	Res	Type
1	B	532	ASN
1	B	540	ASN
1	B	563	GLN
1	B	606	ASN
1	B	607	GLN
1	B	655	HIS
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	66	HIS
1	C	188	ASN
1	C	207	HIS
1	C	271	GLN
1	C	314	GLN
1	C	321	GLN
1	C	334	ASN
1	C	388	ASN
1	C	536	ASN
1	C	556	ASN
1	C	606	ASN
1	C	641	ASN
1	C	675	GLN
1	C	690	GLN
1	C	703	ASN
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	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS

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Mol	Chain	Res	Type
1	C	1106	GLN
2	H	81	GLN
3	L	101	GLN
2	G	81	GLN
3	F	101	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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
4	NAG	D	1	4,1	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	0.46	0
4	NAG	E	1	4,1	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	0.46	0
4	NAG	I	1	4,1	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	I	2	4	14,14,15	0.30	0	17,19,21	1.32	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	1.41	3 (17%)
4	NAG	K	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	K	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	M	1	4,1	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
4	NAG	M	2	4	14,14,15	0.15	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	N	1	4,1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	N	2	4	14,14,15	0.15	0	17,19,21	0.47	0
4	NAG	O	1	4,1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	NAG	P	1	4,1	14,14,15	0.34	0	17,19,21	1.12	1 (5%)
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	Q	1	4,1	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
4	NAG	Q	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	R	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	R	2	4	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
4	NAG	S	1	4,1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	S	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	T	1	4,1	14,14,15	0.41	0	17,19,21	0.58	0
4	NAG	T	2	4	14,14,15	0.26	0	17,19,21	0.60	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.55	0	17,19,21	0.56	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	V	1	4,1	14,14,15	0.22	0	17,19,21	1.36	1 (5%)
4	NAG	V	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	W	1	4,1	14,14,15	0.54	0	17,19,21	0.69	1 (5%)
4	NAG	W	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	X	1	4,1	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	X	2	4	14,14,15	0.19	0	17,19,21	0.72	0
4	NAG	Y	1	4,1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	Y	2	4	14,14,15	0.56	0	17,19,21	1.33	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.44	0
4	NAG	Z	2	4	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
4	NAG	a	1	4,1	14,14,15	0.41	0	17,19,21	0.44	0
4	NAG	a	2	4	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	b	1	4,1	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
4	NAG	b	2	4	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	c	1	4,1	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	c	2	4	14,14,15	0.34	0	17,19,21	0.42	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	1/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1	NAG	O5-C1	-2.72	1.39	1.43
4	K	1	NAG	O5-C1	-2.55	1.39	1.43
4	J	1	NAG	O5-C1	-2.35	1.40	1.43
4	Z	1	NAG	O5-C1	-2.19	1.40	1.43
4	D	1	NAG	O5-C1	-2.02	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1	NAG	C2-N2-C7	4.67	129.56	122.90
4	J	2	NAG	C2-N2-C7	4.39	129.16	122.90
4	Y	2	NAG	C2-N2-C7	4.36	129.12	122.90
4	Z	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	I	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	P	1	NAG	C1-O5-C5	3.25	116.60	112.19
4	J	2	NAG	C1-C2-N2	2.42	114.62	110.49
4	R	1	NAG	O4-C4-C3	-2.39	104.83	110.35
4	c	1	NAG	C8-C7-N2	2.31	120.02	116.10
4	b	1	NAG	C8-C7-N2	2.31	120.01	116.10
4	Z	2	NAG	C1-C2-N2	2.25	114.34	110.49
4	Q	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	I	2	NAG	C1-C2-N2	2.24	114.32	110.49
4	W	1	NAG	C1-O5-C5	2.23	115.21	112.19
4	M	1	NAG	C1-O5-C5	2.18	115.14	112.19
4	J	2	NAG	C1-O5-C5	2.12	115.07	112.19
4	E	1	NAG	C1-O5-C5	2.06	114.98	112.19
4	T	2	NAG	C1-O5-C5	2.04	114.96	112.19
4	R	2	NAG	C1-O5-C5	2.03	114.94	112.19
4	b	1	NAG	C2-N2-C7	-2.02	120.02	122.90
4	c	1	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	V	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	S	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
4	U	2	NAG	C1-C2-N2-C7
4	Z	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
4	P	1	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	X	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	V	1	NAG	C1-C2-N2-C7
4	U	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	U	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7

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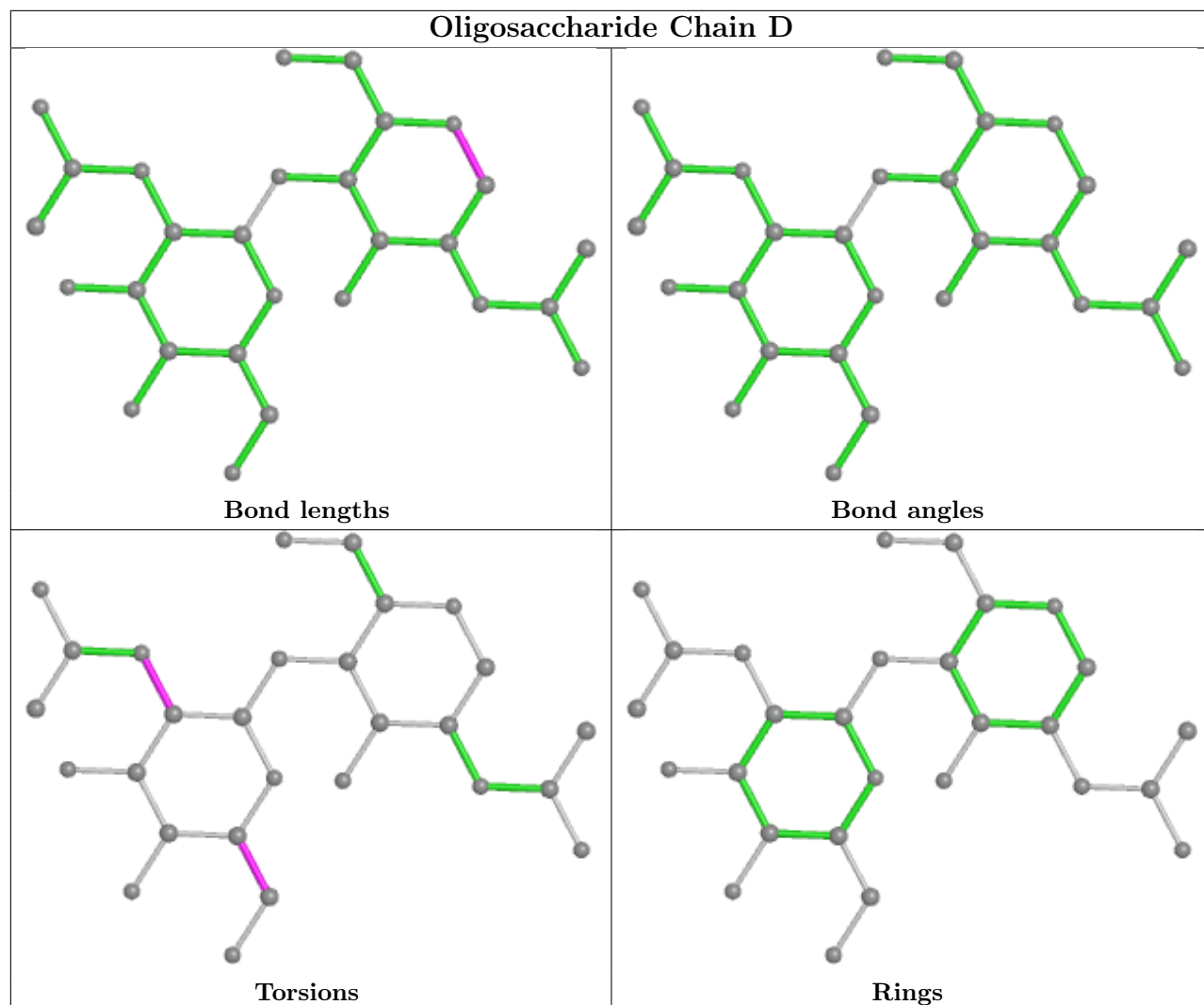
Mol	Chain	Res	Type	Atoms
4	Z	2	NAG	C3-C2-N2-C7
4	D	2	NAG	O5-C5-C6-O6

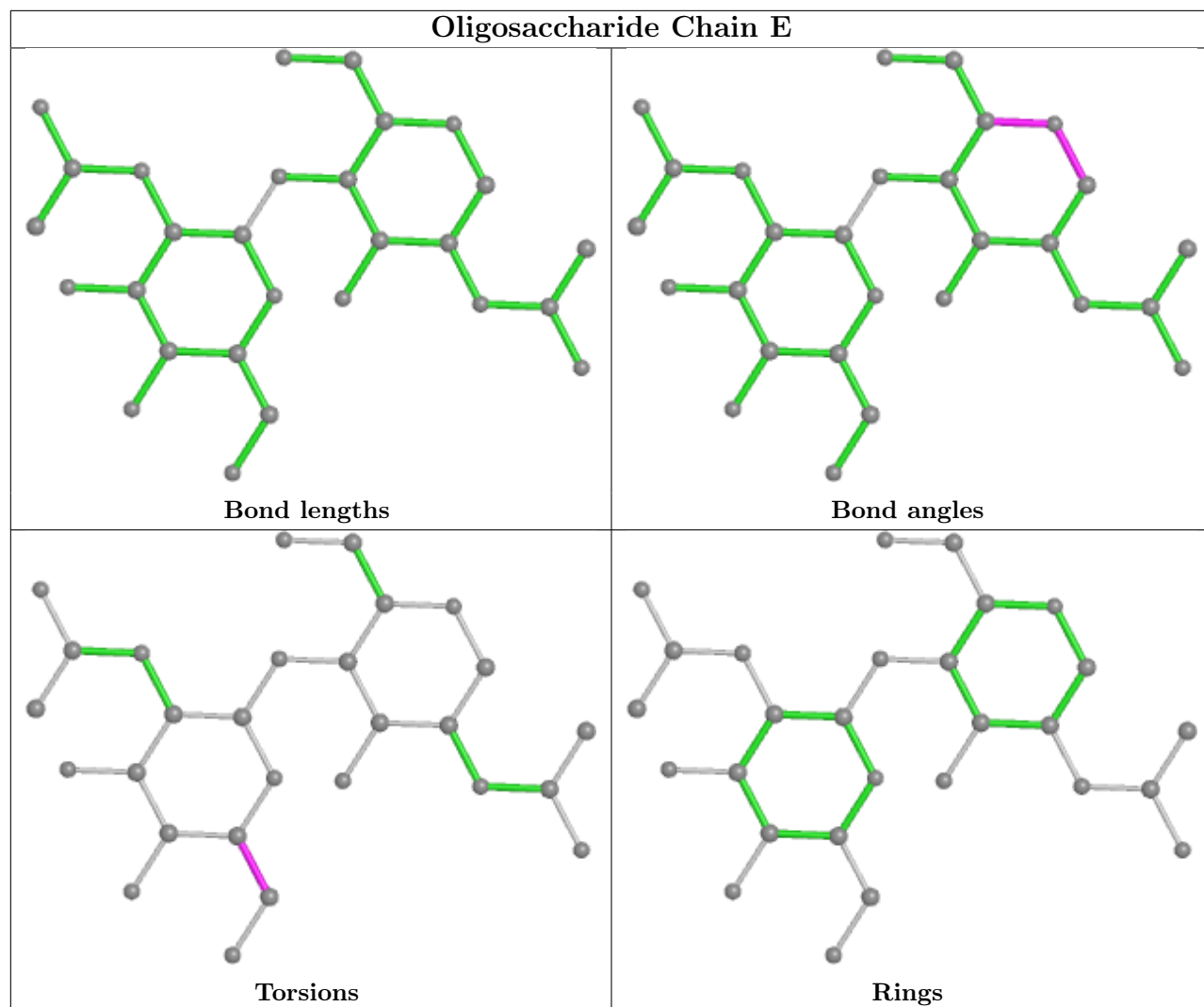
There are no ring outliers.

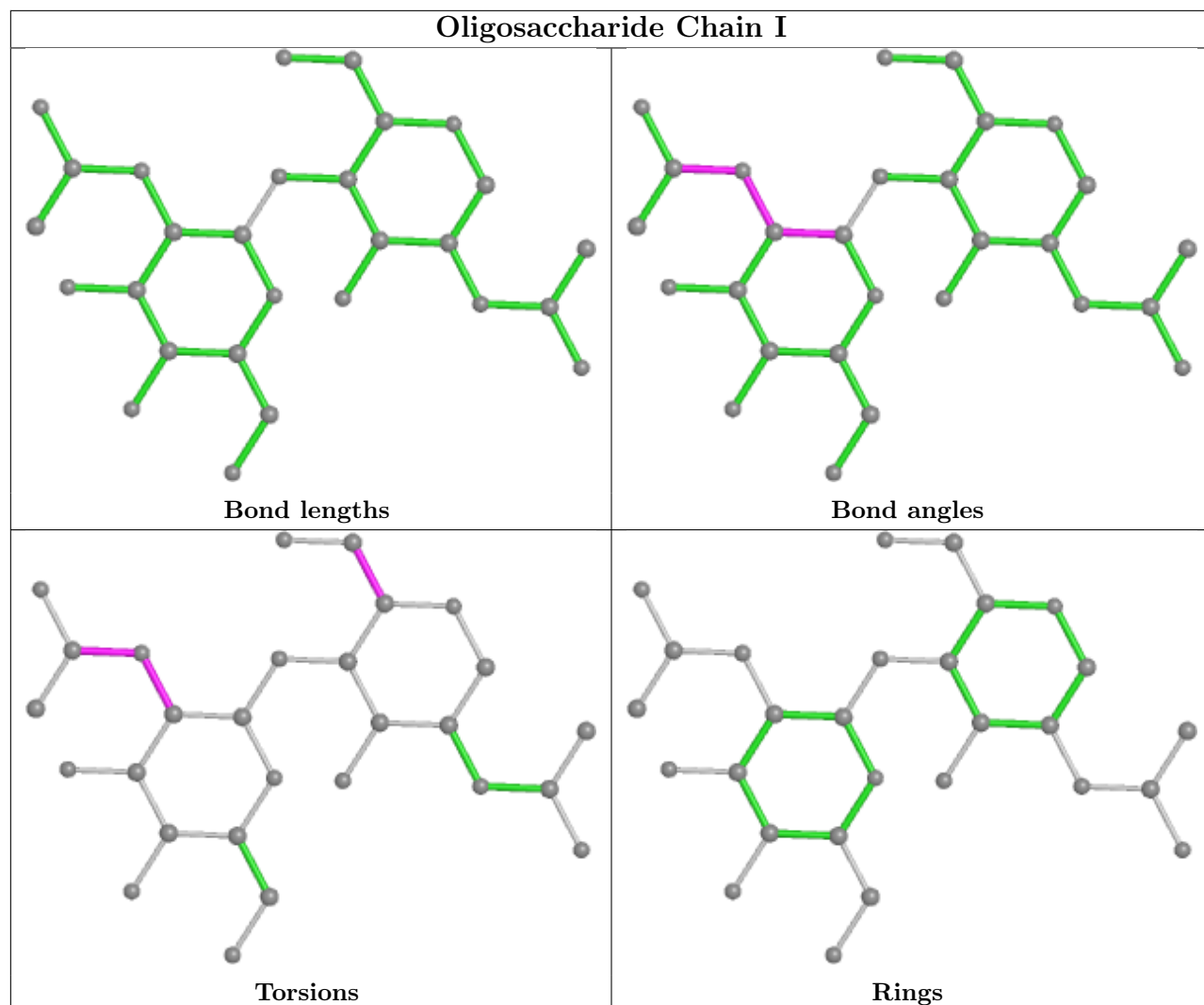
13 monomers are involved in 16 short contacts:

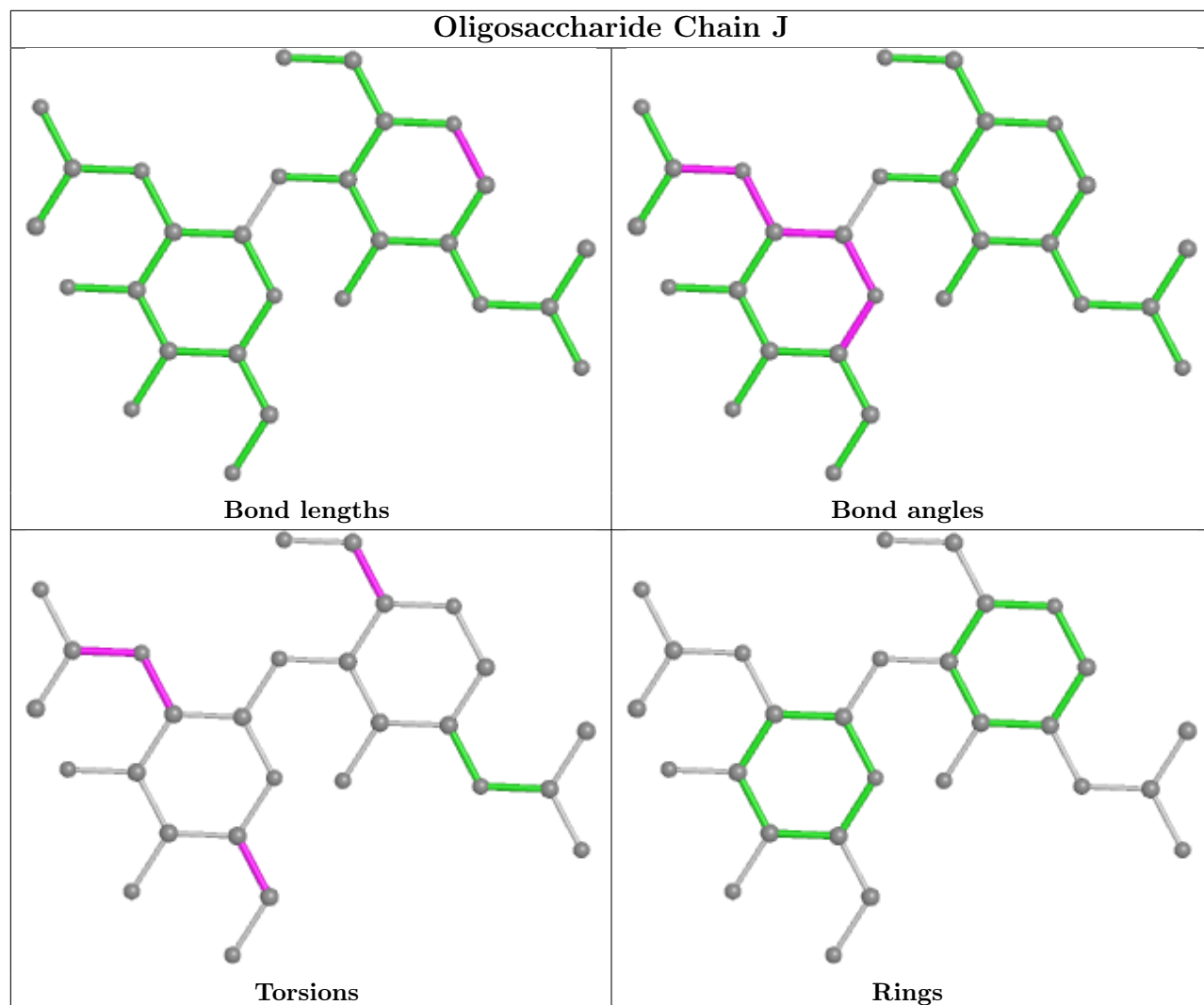
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	2	NAG	1	0
4	U	1	NAG	2	0
4	D	1	NAG	6	0
4	N	1	NAG	1	0
4	J	2	NAG	1	0
4	Y	2	NAG	1	0
4	Z	2	NAG	1	0
4	I	2	NAG	1	0
4	U	2	NAG	2	0
4	V	1	NAG	1	0
4	D	2	NAG	2	0
4	Z	1	NAG	1	0
4	R	1	NAG	1	0

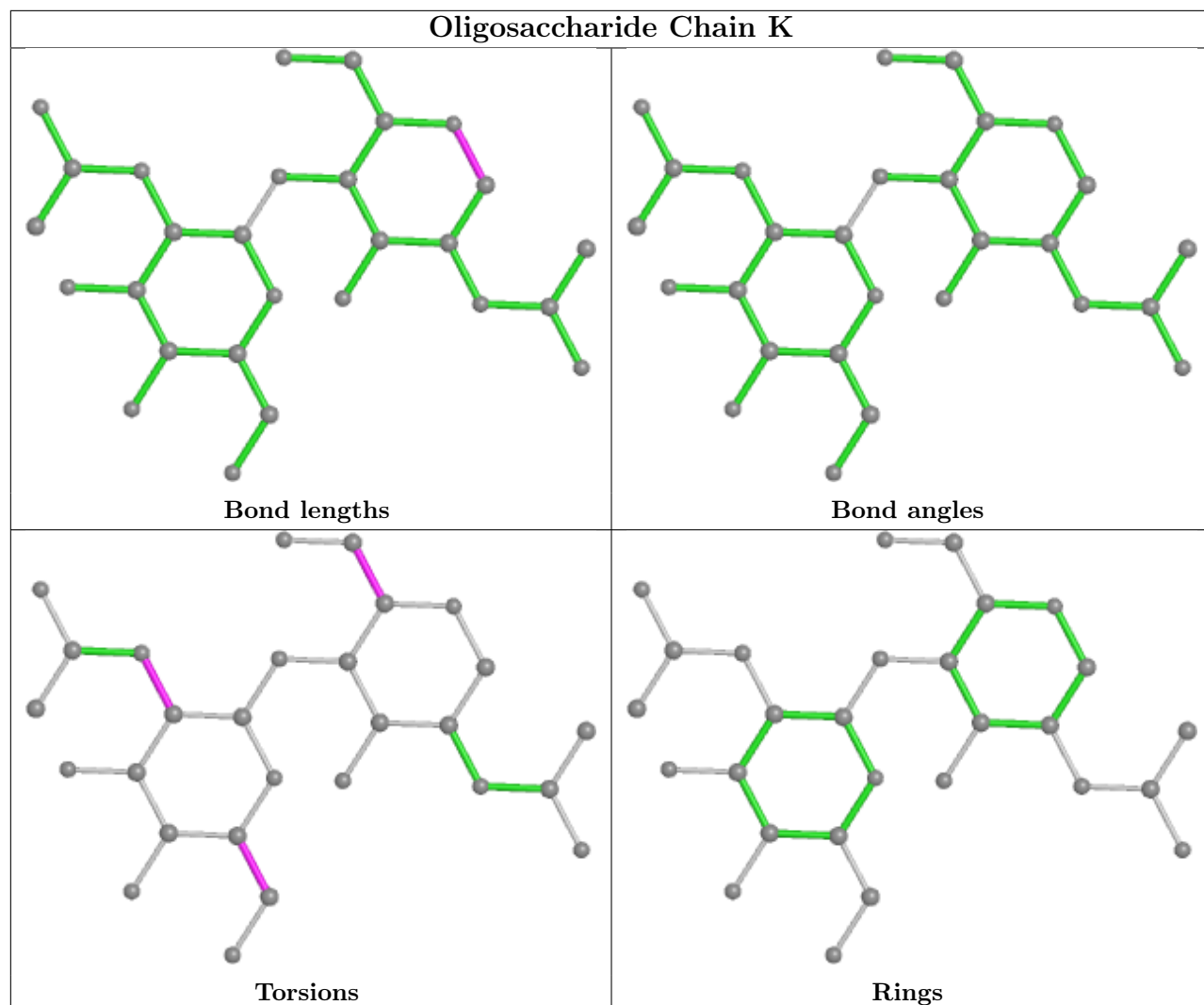
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

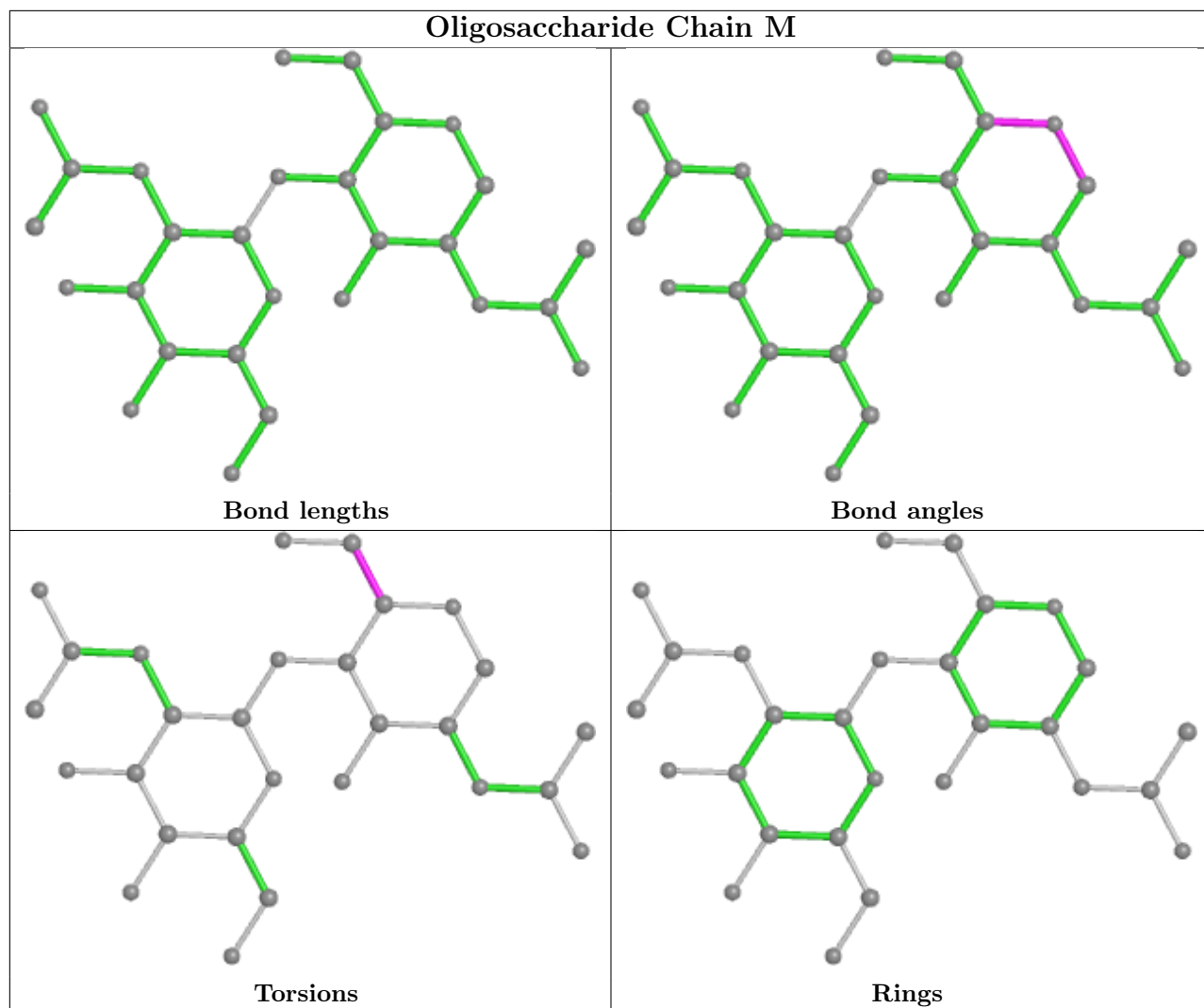


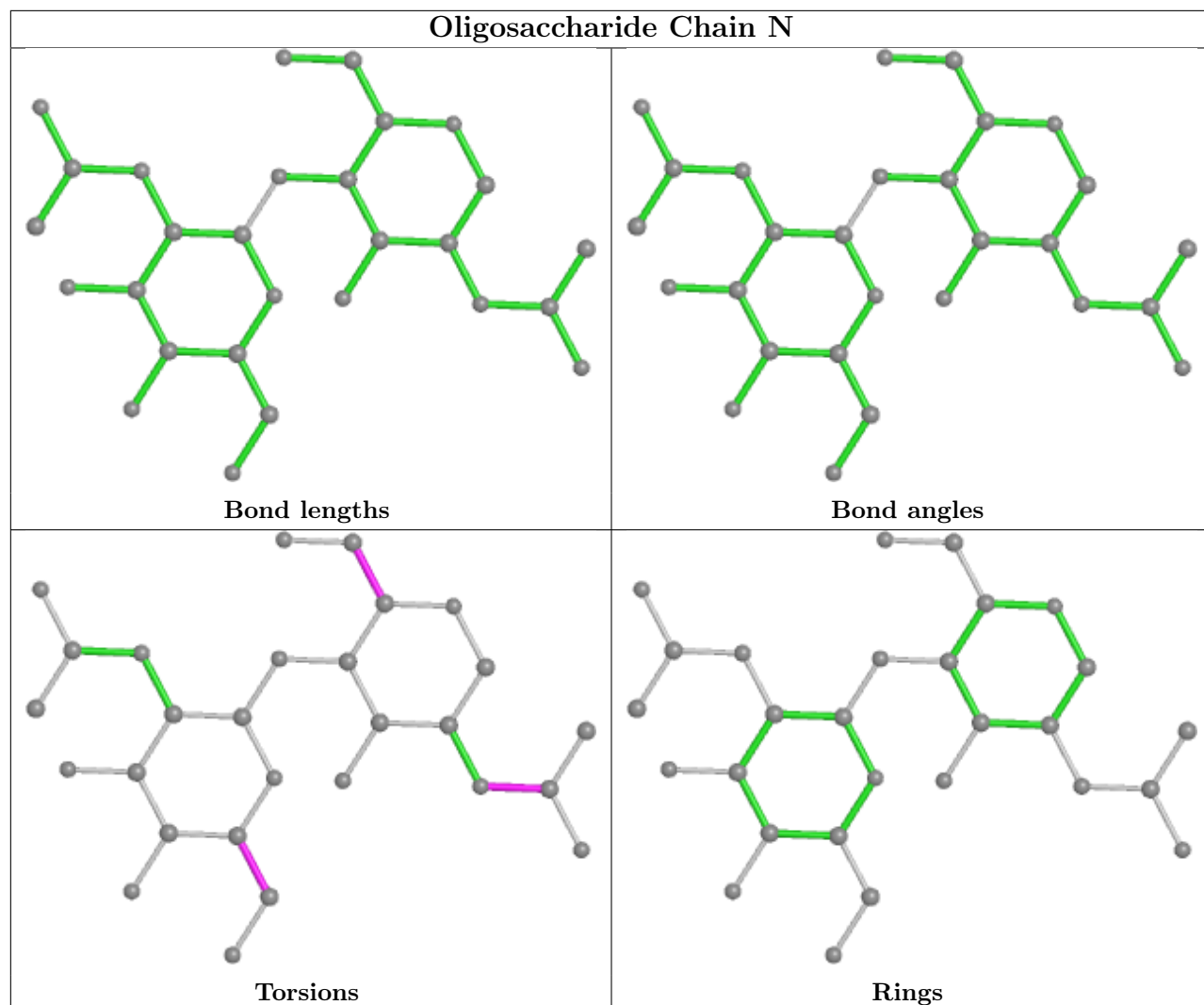


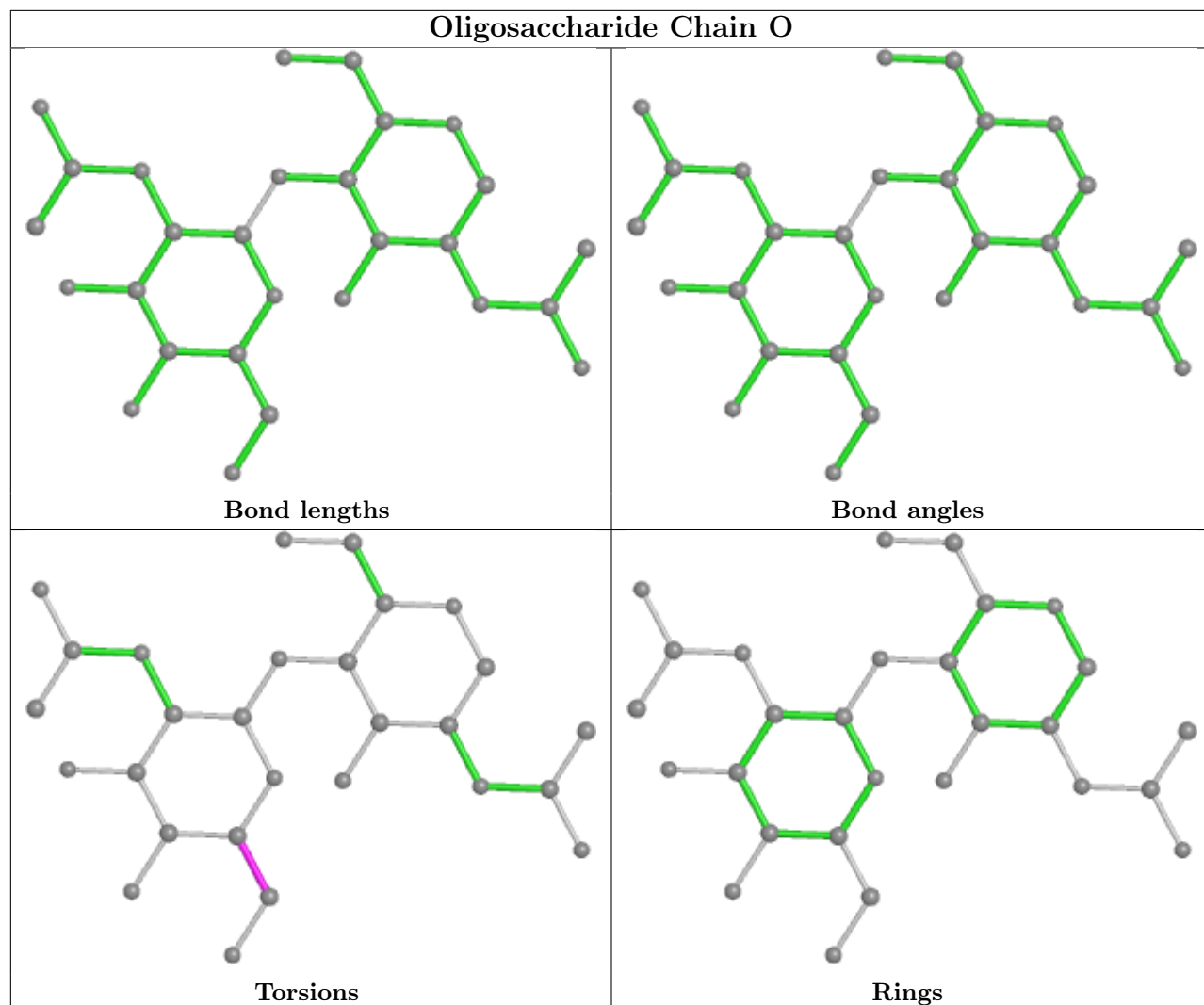


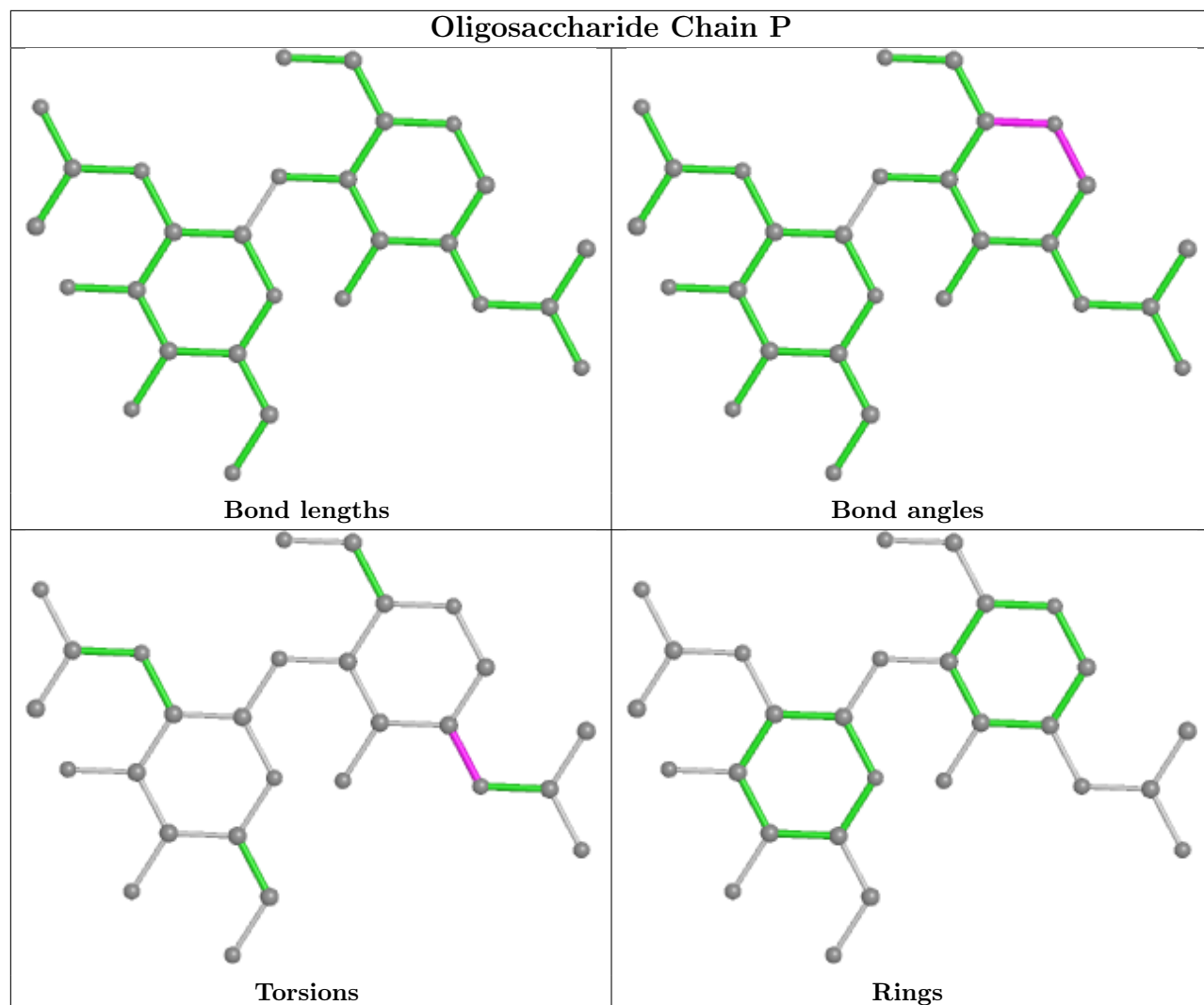


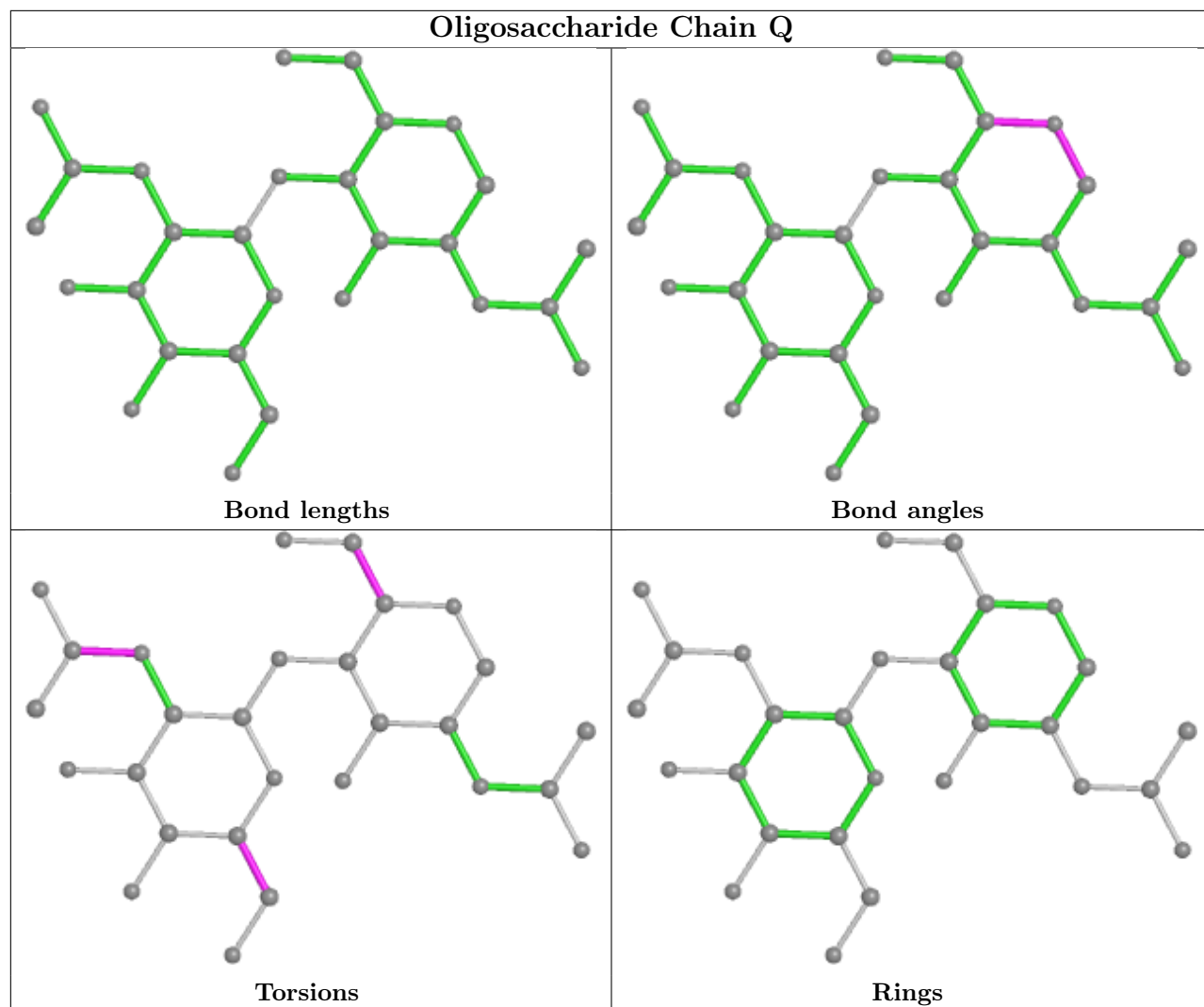


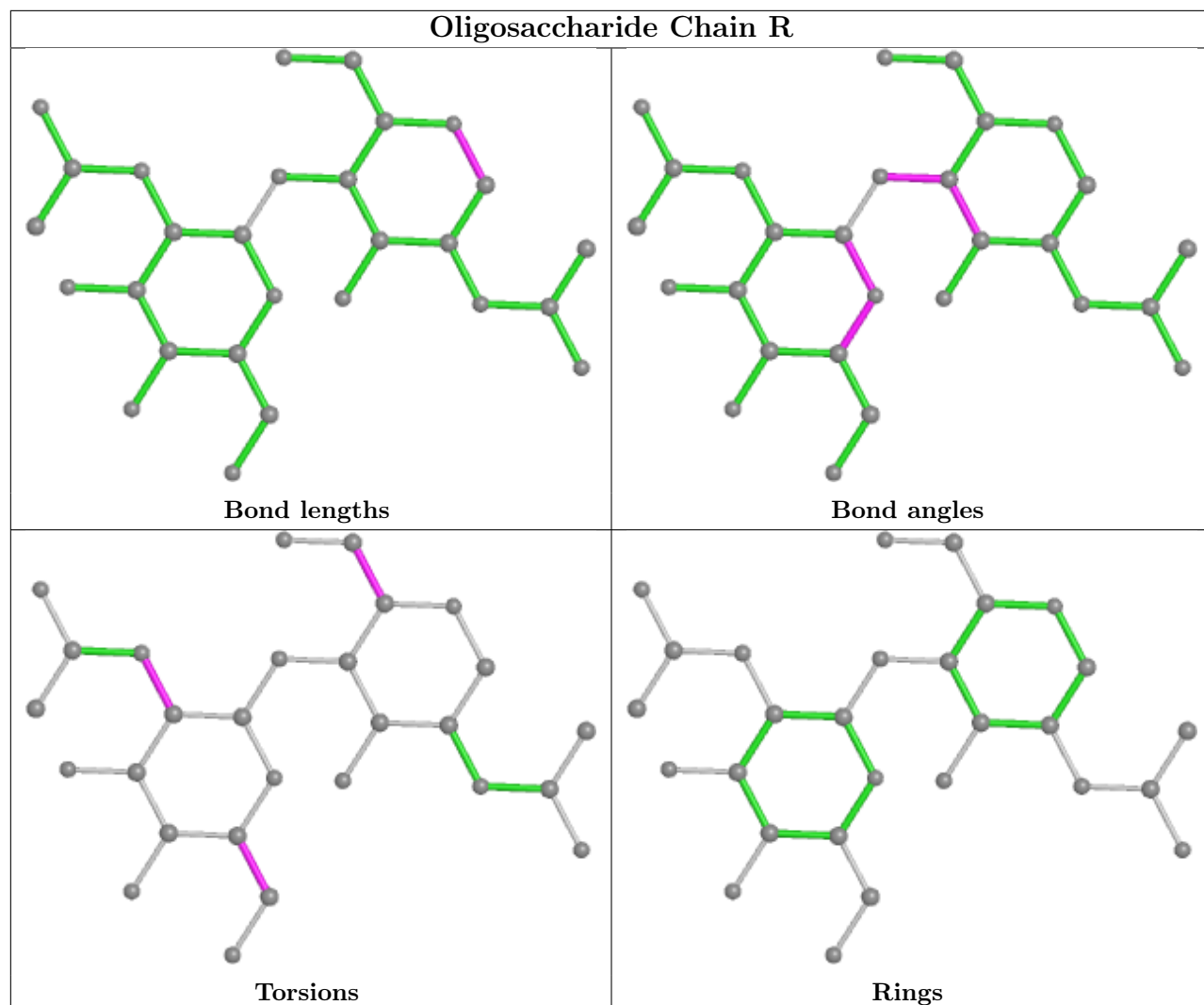


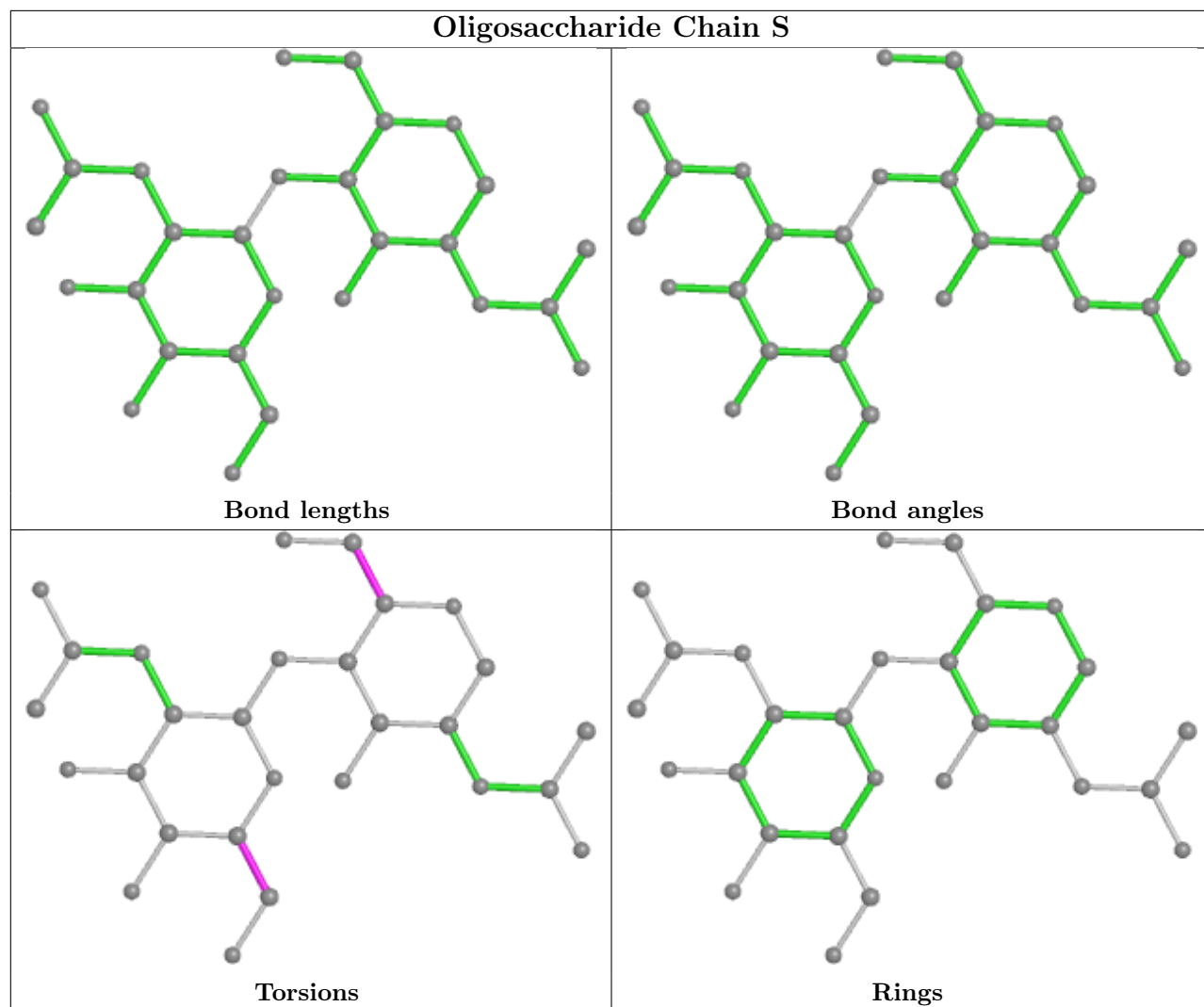


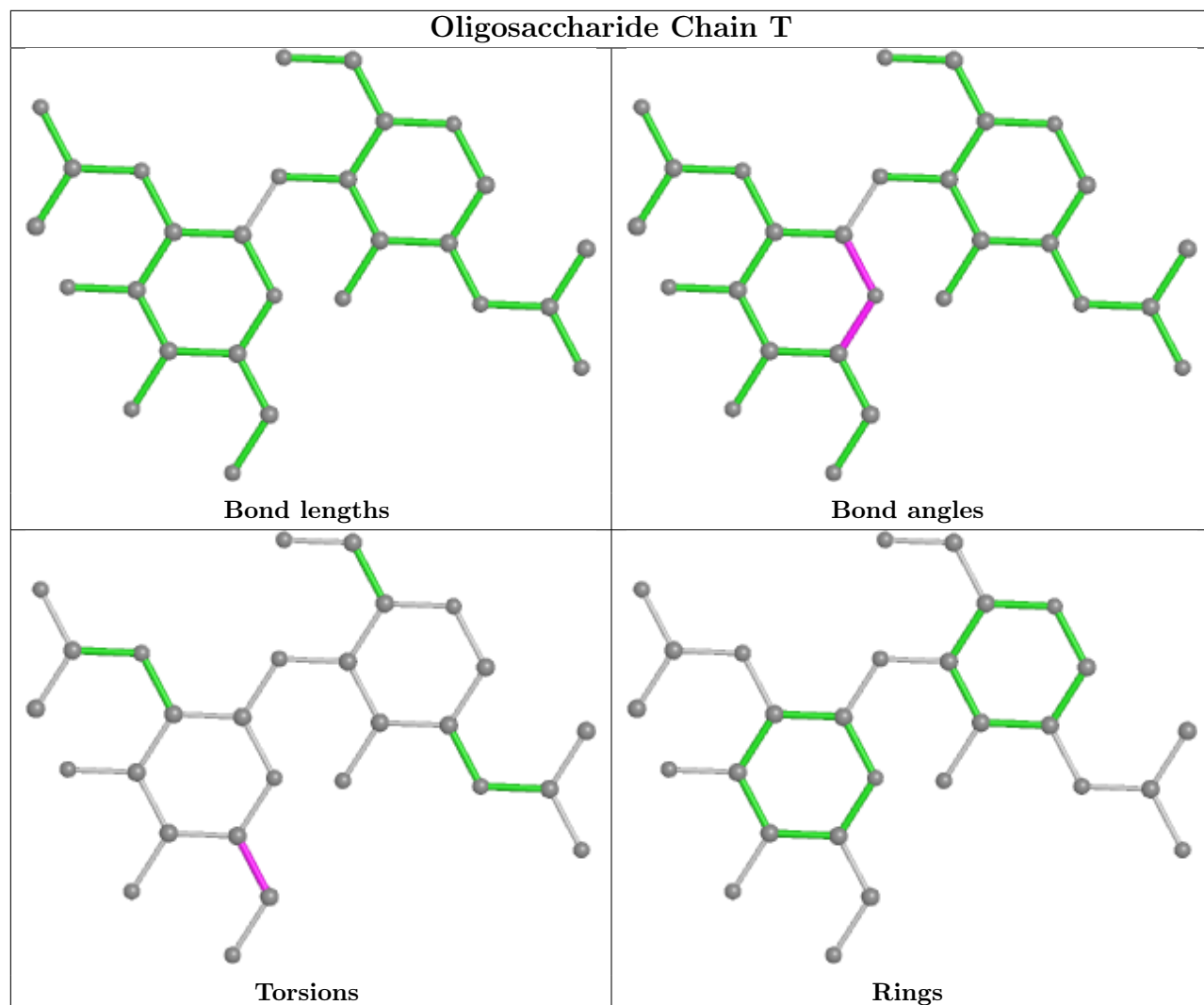


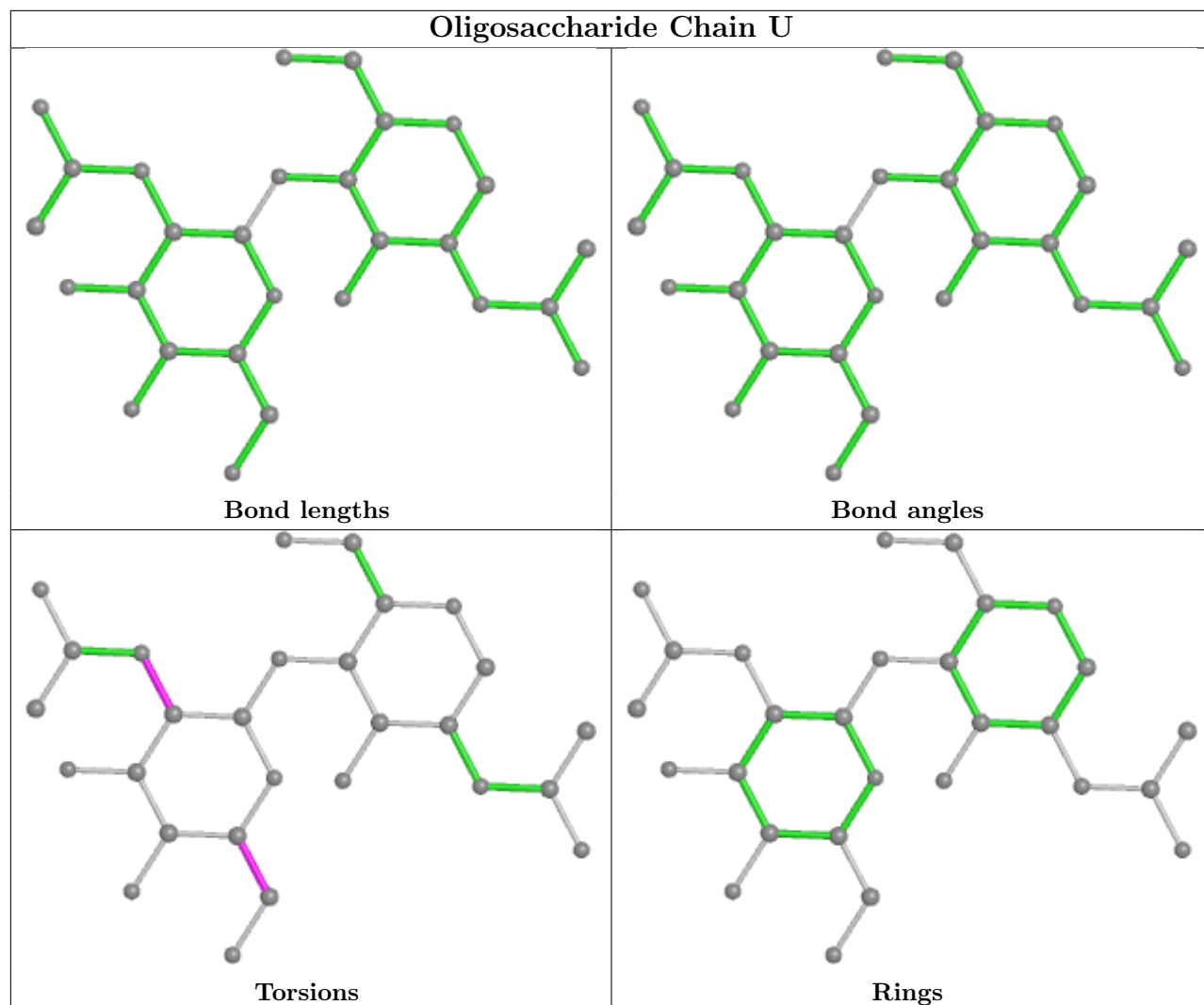


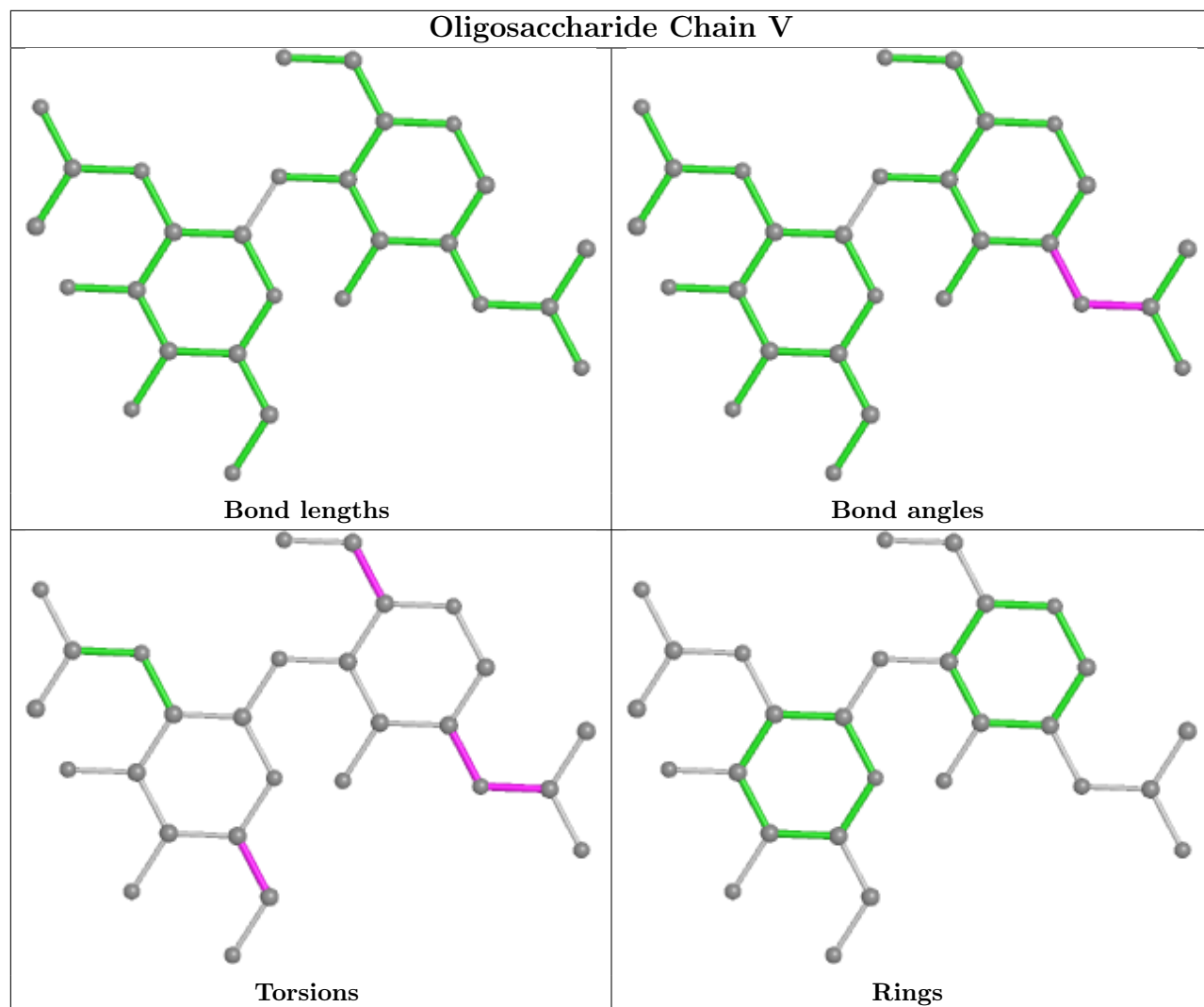


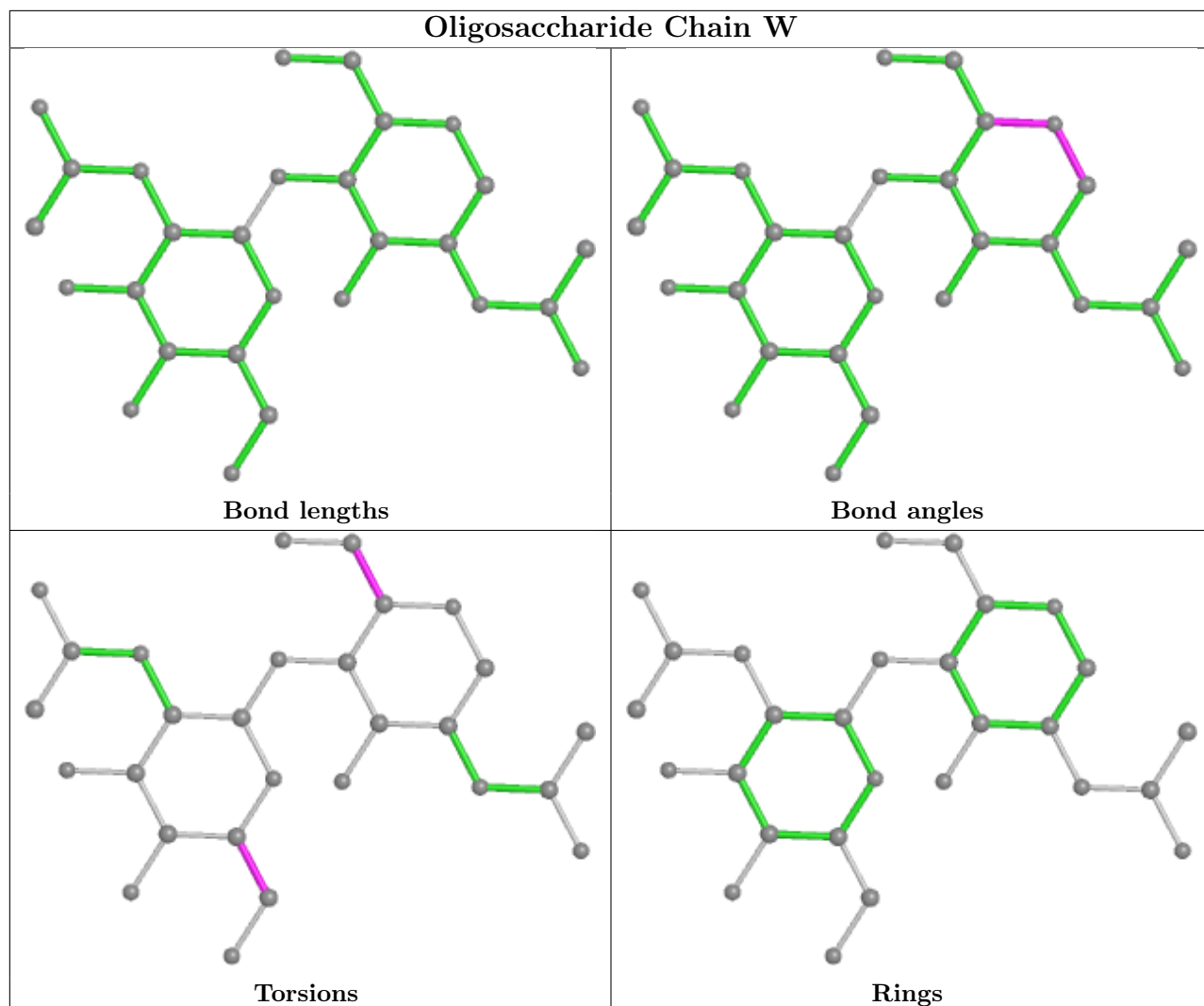


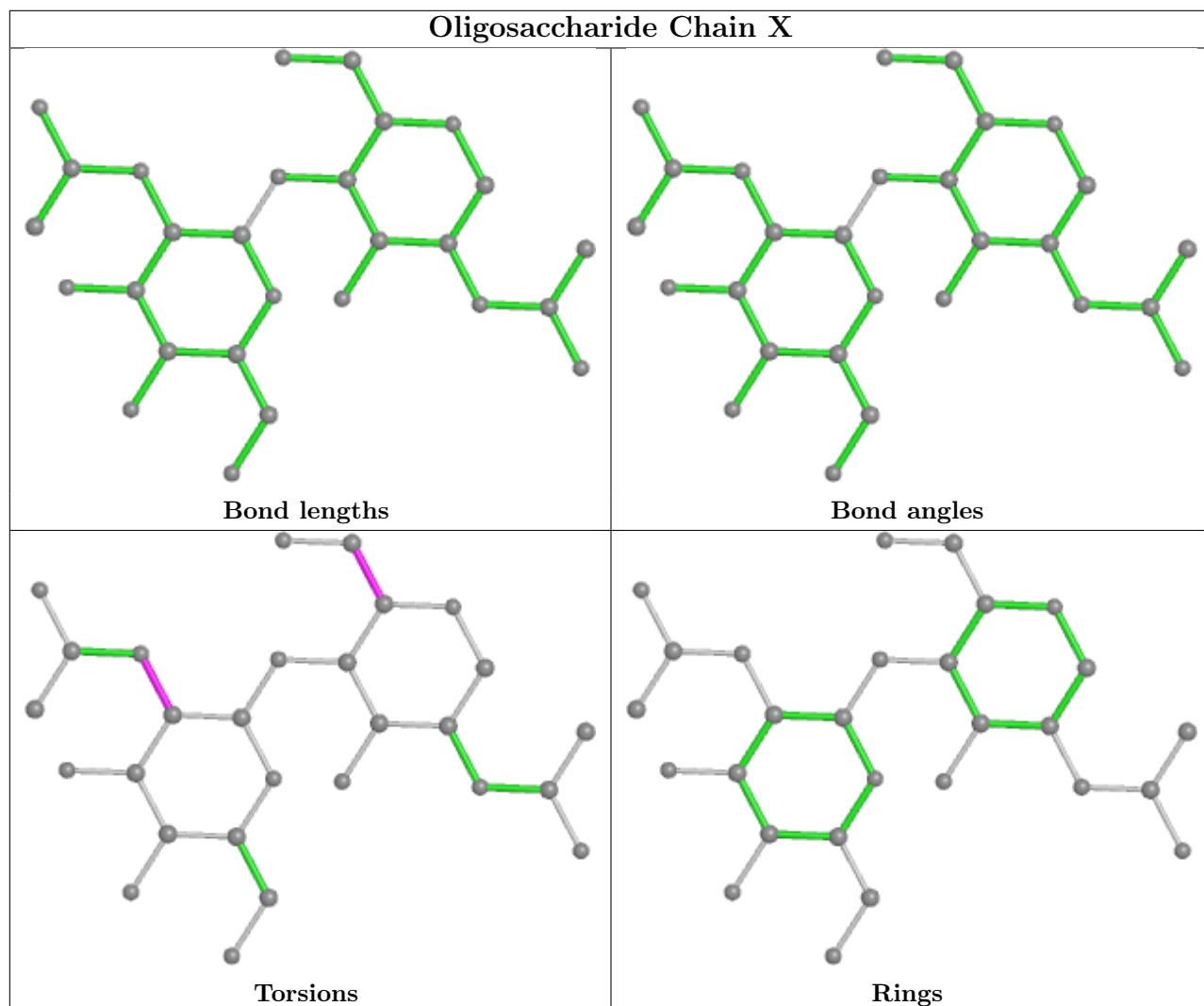


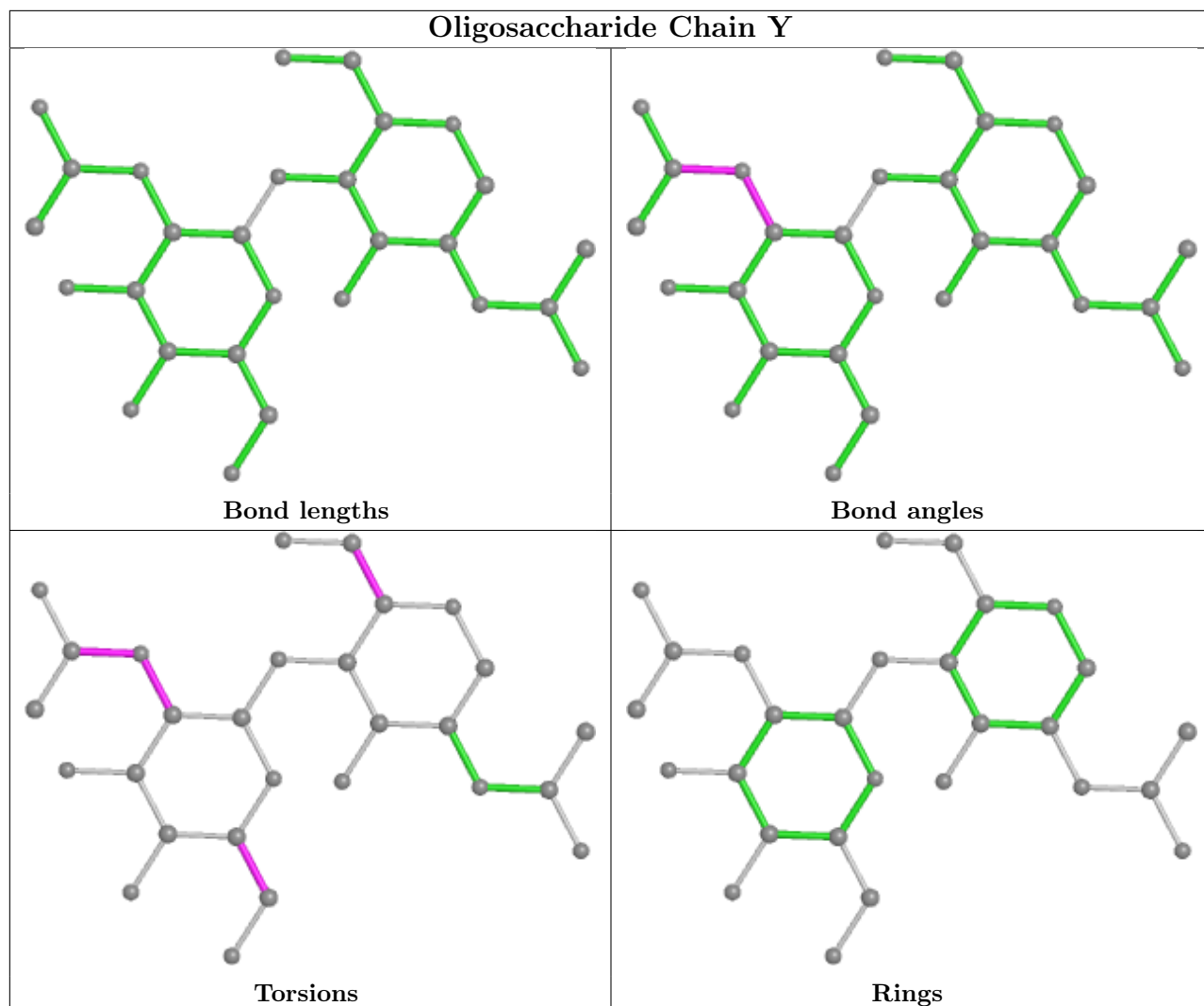


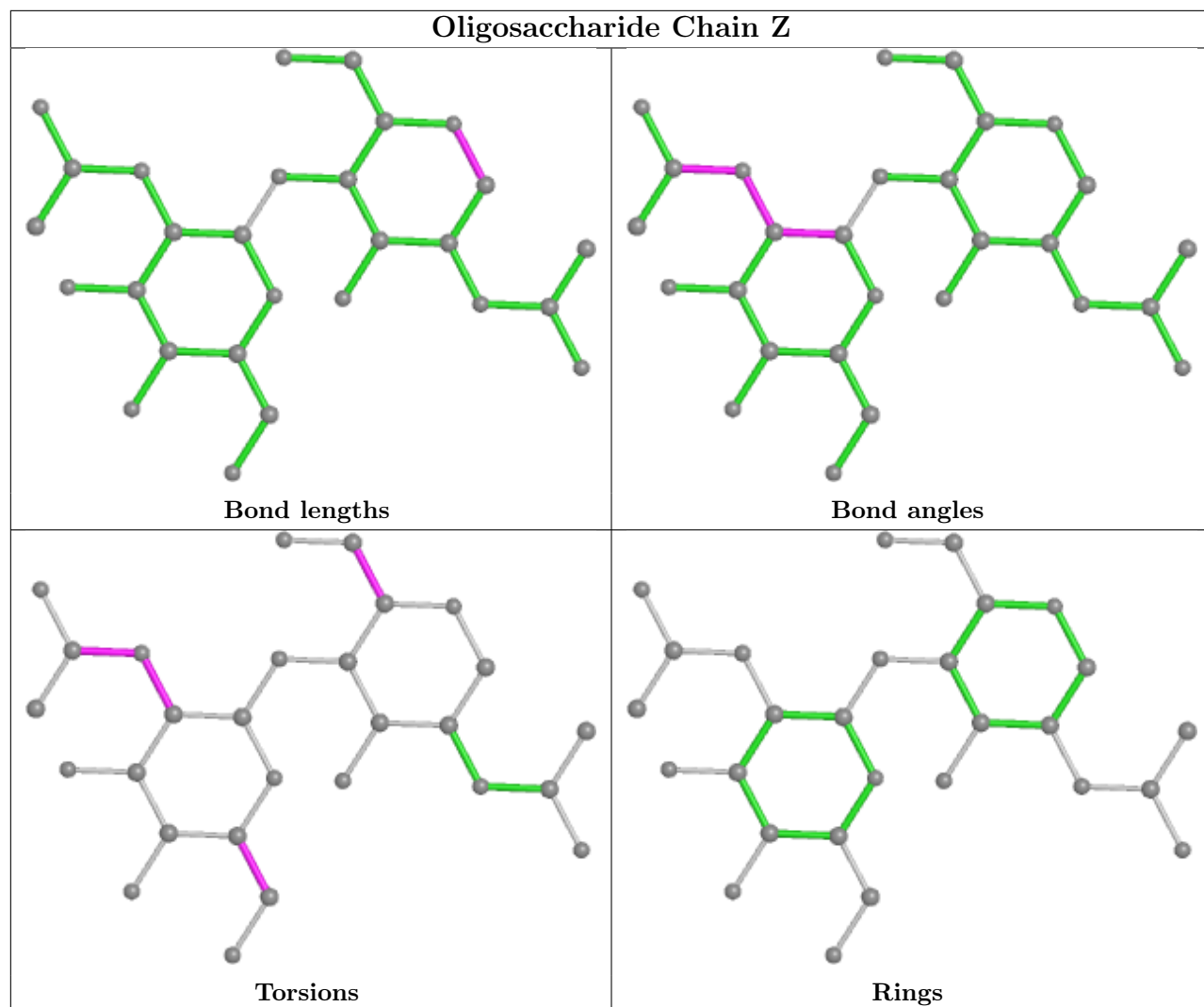


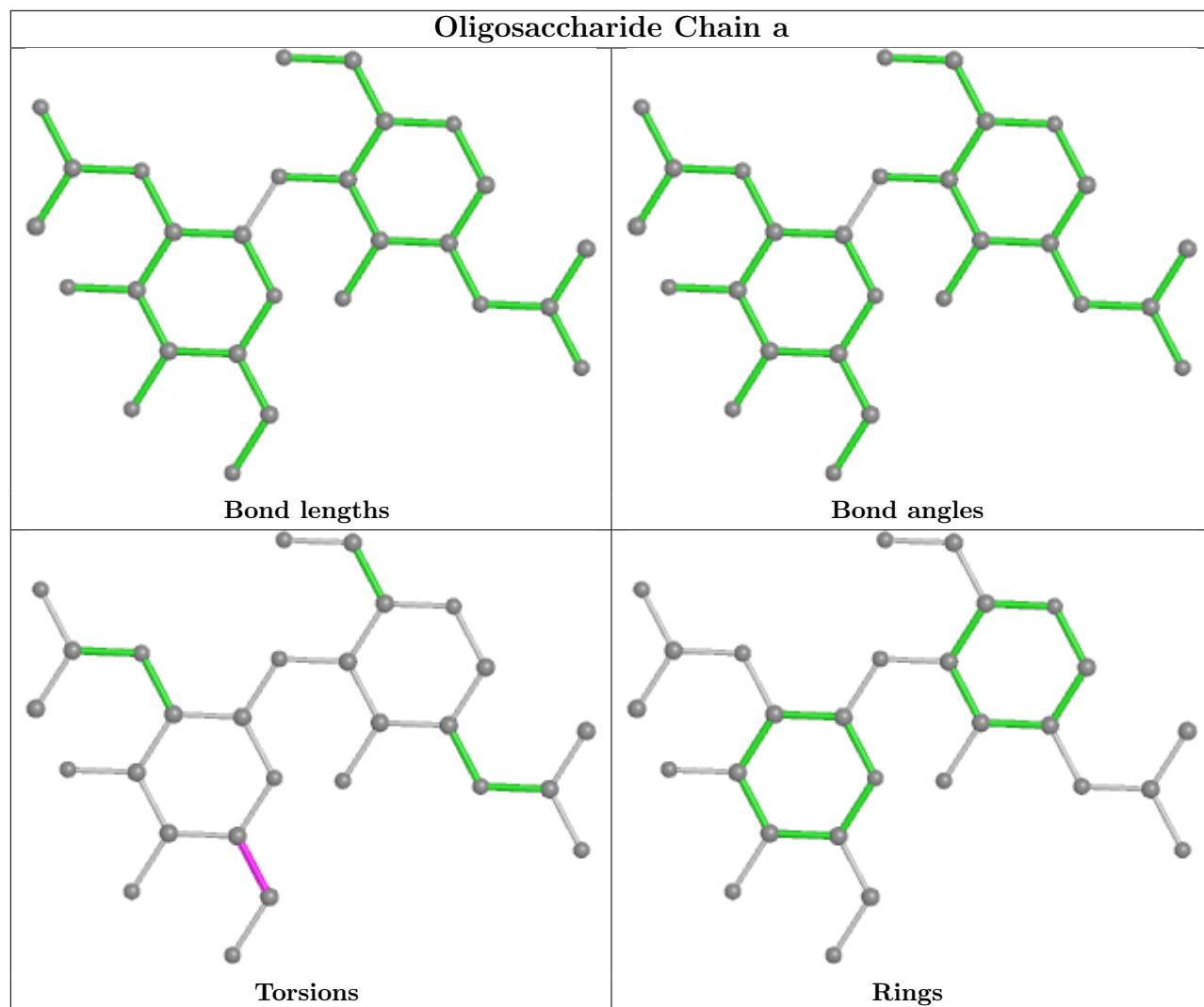


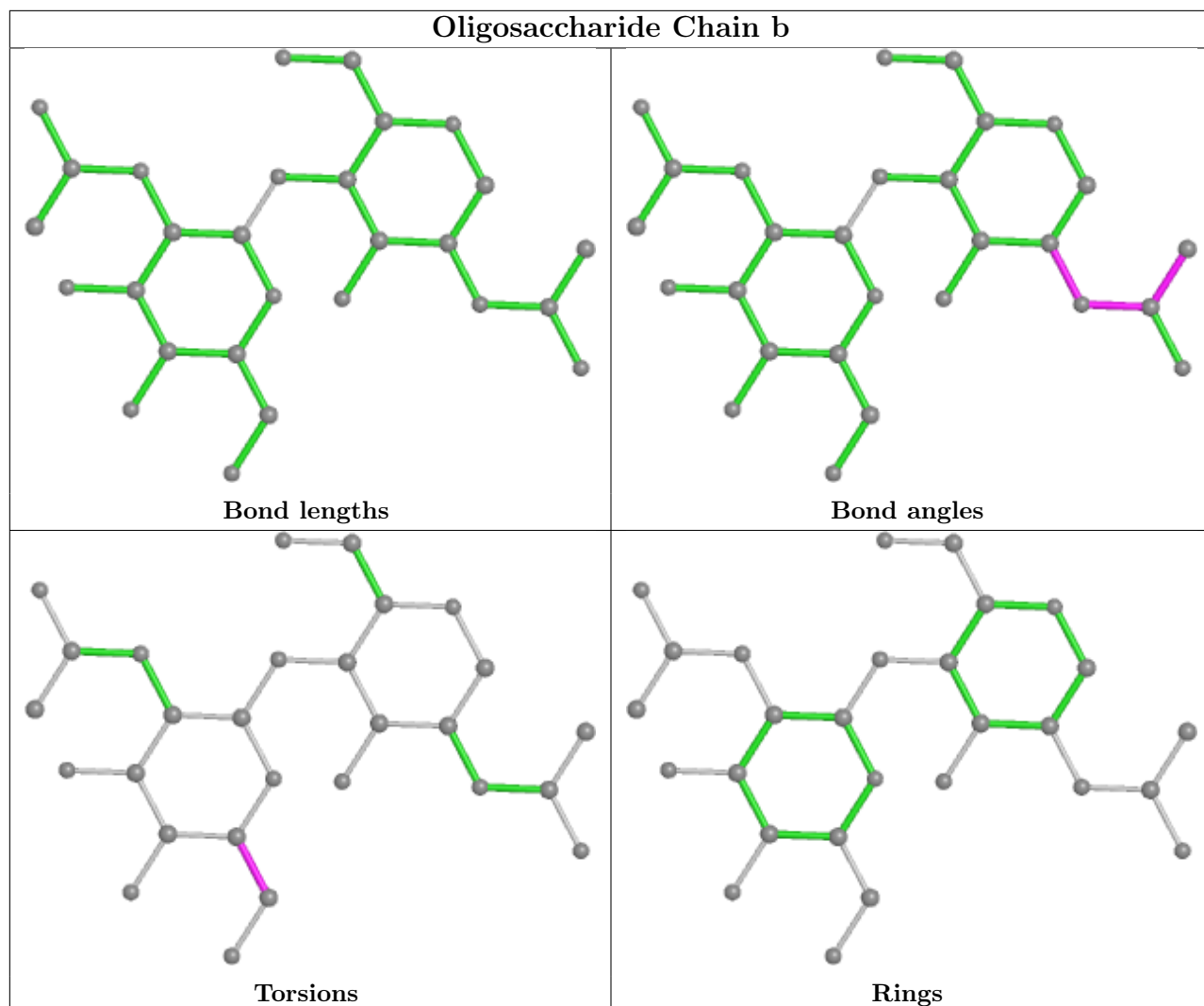


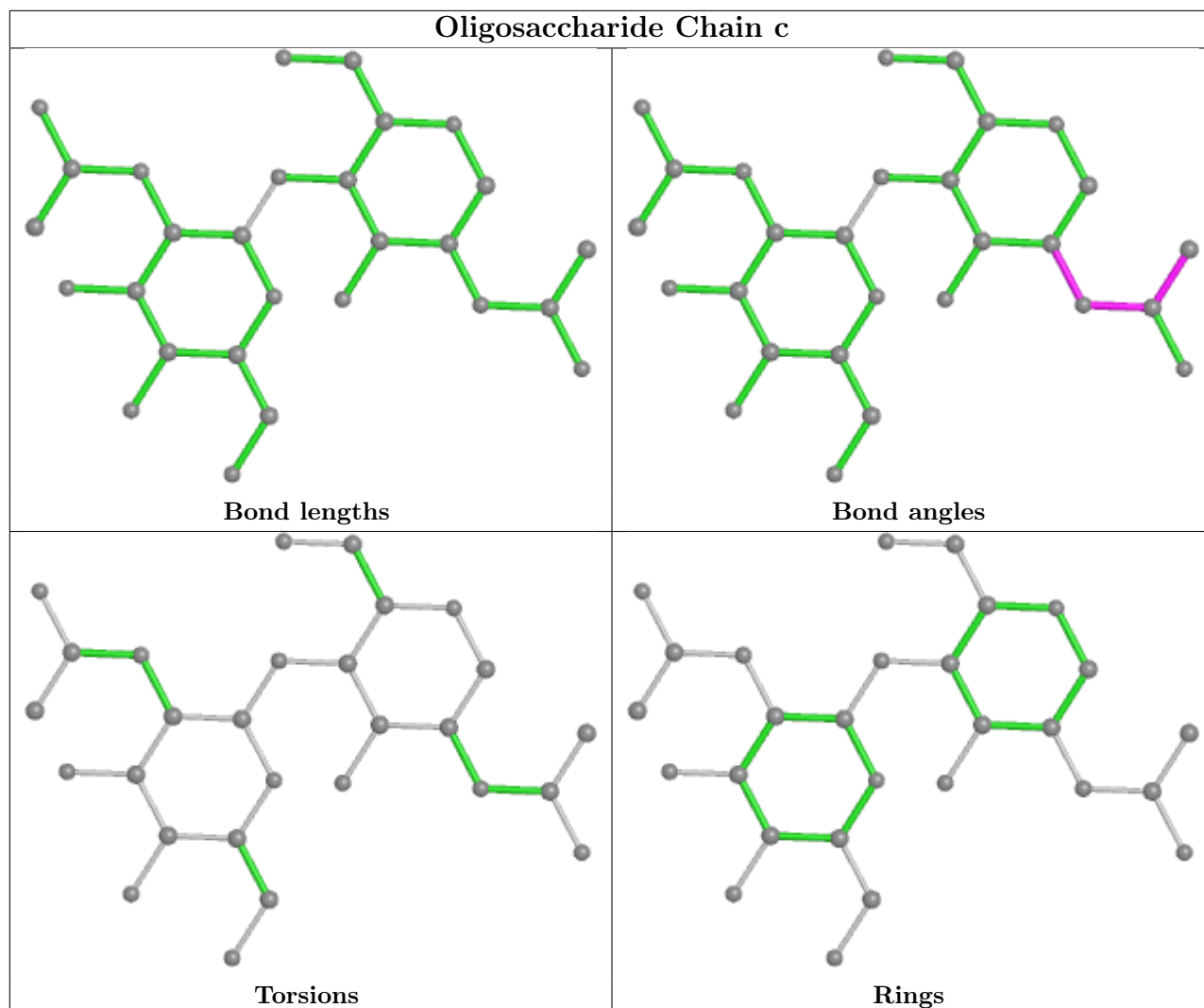












5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
5	NAG	B	1404	1	14,14,15	0.32	0	17,19,21	0.59	0
5	NAG	B	1405	1	14,14,15	0.39	0	17,19,21	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1404	1	14,14,15	0.45	0	17,19,21	0.54	0
5	NAG	A	1409	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1406	1	14,14,15	0.20	0	17,19,21	0.37	0
5	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
5	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
5	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	A	1410	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	C	1407	1	14,14,15	0.36	0	17,19,21	0.64	0
5	NAG	C	1404	1	14,14,15	0.29	0	17,19,21	0.38	0
5	NAG	B	1407	1	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
5	NAG	C	1403	1	14,14,15	0.54	0	17,19,21	0.45	0
5	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.54	0
5	NAG	C	1408	1	14,14,15	0.16	0	17,19,21	0.56	0
5	NAG	B	1406	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
5	NAG	C	1405	1	14,14,15	0.36	0	17,19,21	1.29	2 (11%)
5	NAG	B	1403	1	14,14,15	0.28	0	17,19,21	0.39	0
5	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
5	NAG	B	1402	1	14,14,15	0.33	0	17,19,21	0.65	0
5	NAG	C	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	B	1409	1	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	A	1411	1	14,14,15	0.50	0	17,19,21	0.35	0
5	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.40	0
5	NAG	C	1402	1	14,14,15	0.47	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	0/6/23/26	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(°)
5	A	1405	NAG	C2-N2-C7	4.31	129.04	122.90
5	C	1405	NAG	C2-N2-C7	4.30	129.03	122.90
5	B	1405	NAG	C2-N2-C7	4.12	128.76	122.90
5	C	1401	NAG	C1-O5-C5	2.87	116.08	112.19
5	B	1406	NAG	C1-O5-C5	2.55	115.65	112.19
5	B	1407	NAG	C1-O5-C5	2.40	115.45	112.19
5	C	1405	NAG	C1-C2-N2	2.22	114.28	110.49
5	B	1405	NAG	C1-C2-N2	2.13	114.12	110.49

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1408	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1402	NAG	O5-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	A	1411	NAG	C4-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	A	1410	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1405	NAG	C8-C7-N2-C2
5	A	1405	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	C	1406	NAG	C8-C7-N2-C2
5	C	1406	NAG	O7-C7-N2-C2
5	A	1411	NAG	O5-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	C	1407	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C1-C2-N2-C7
5	A	1410	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6

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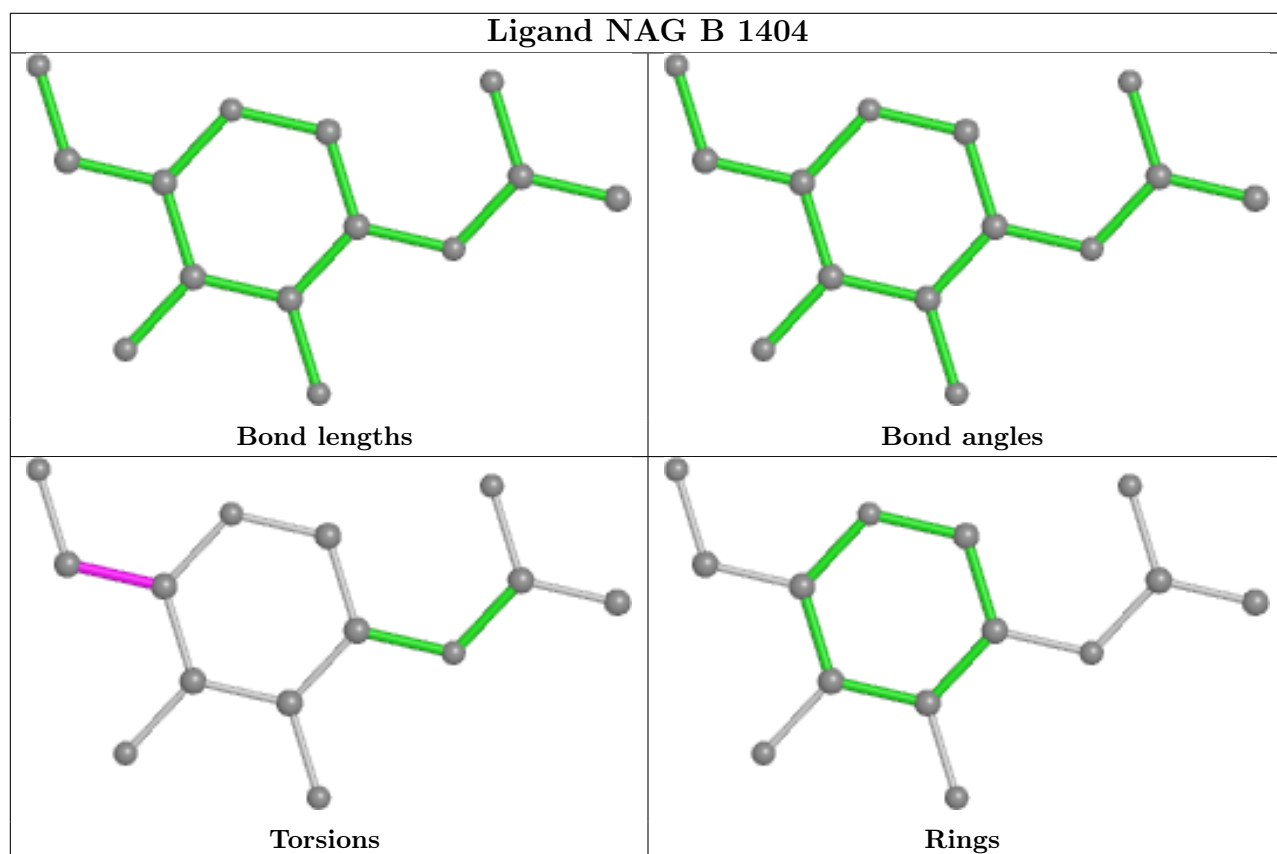
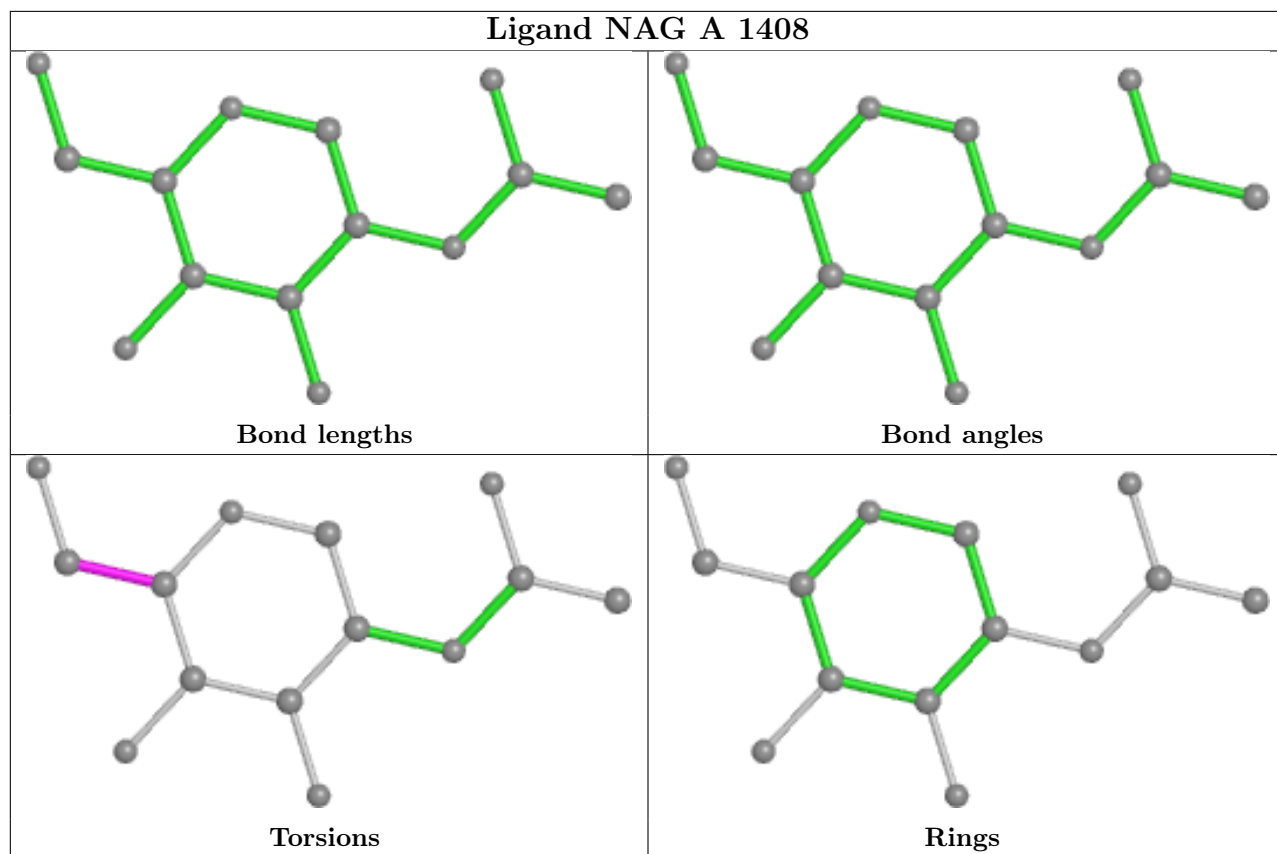
Mol	Chain	Res	Type	Atoms
5	C	1404	NAG	O5-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	B	1406	NAG	C3-C2-N2-C7
5	B	1407	NAG	C3-C2-N2-C7
5	C	1407	NAG	C3-C2-N2-C7
5	A	1409	NAG	C1-C2-N2-C7
5	A	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7
5	C	1403	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7

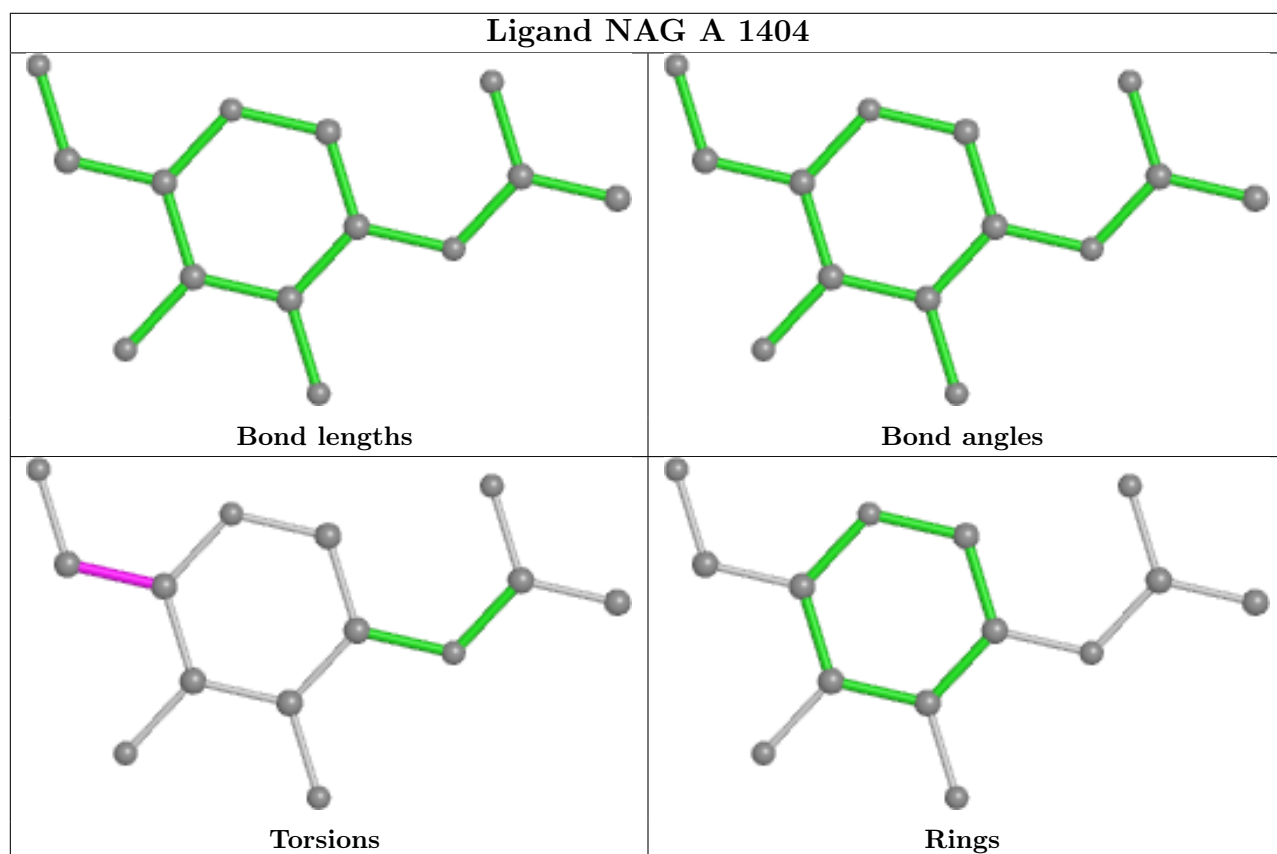
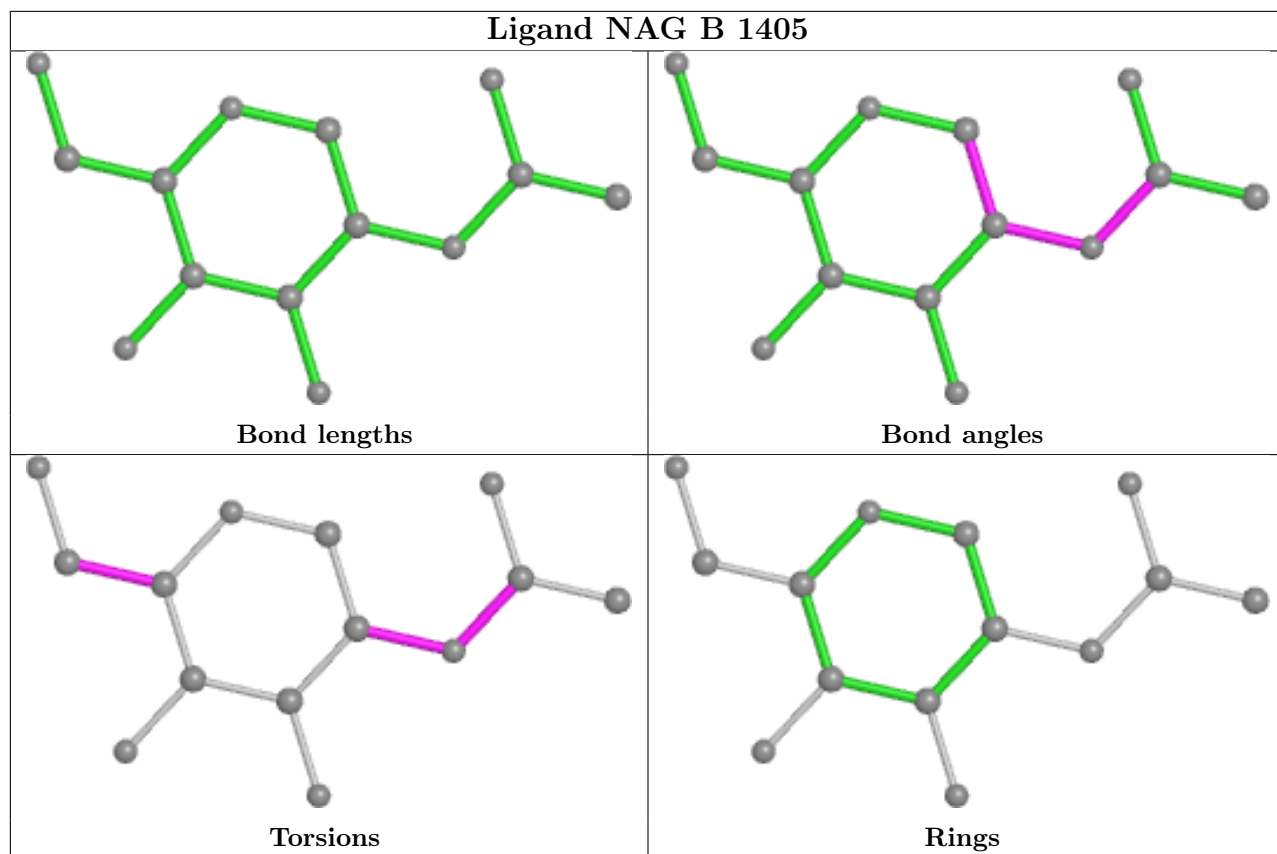
There are no ring outliers.

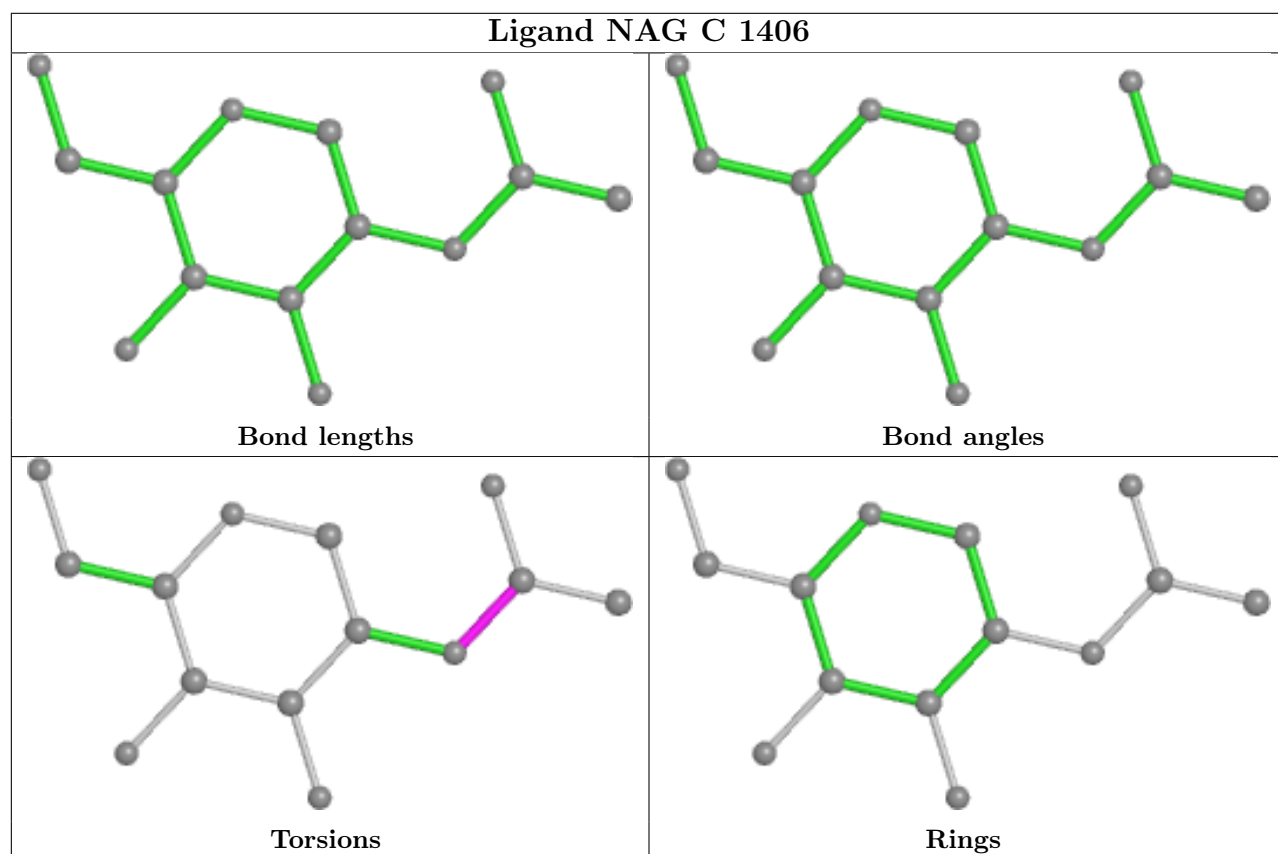
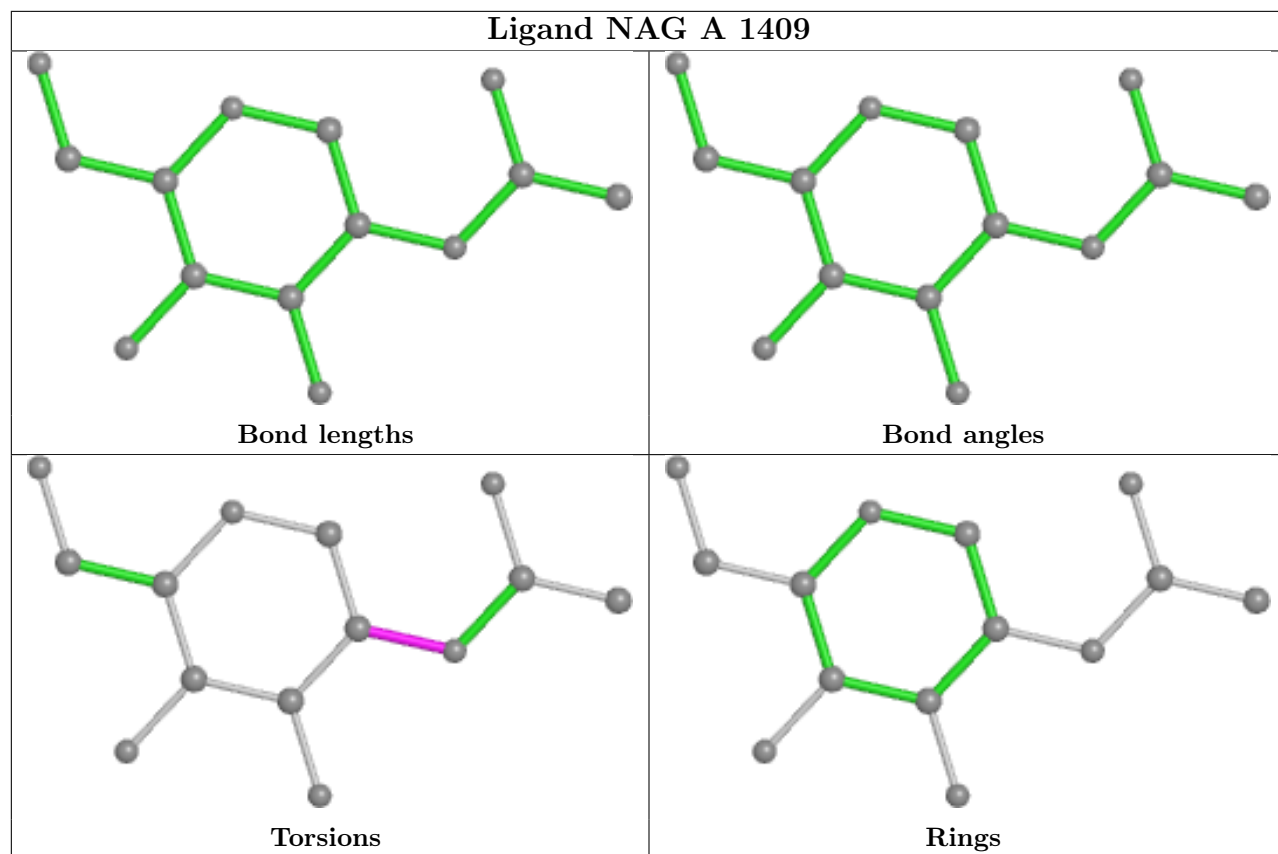
9 monomers are involved in 13 short contacts:

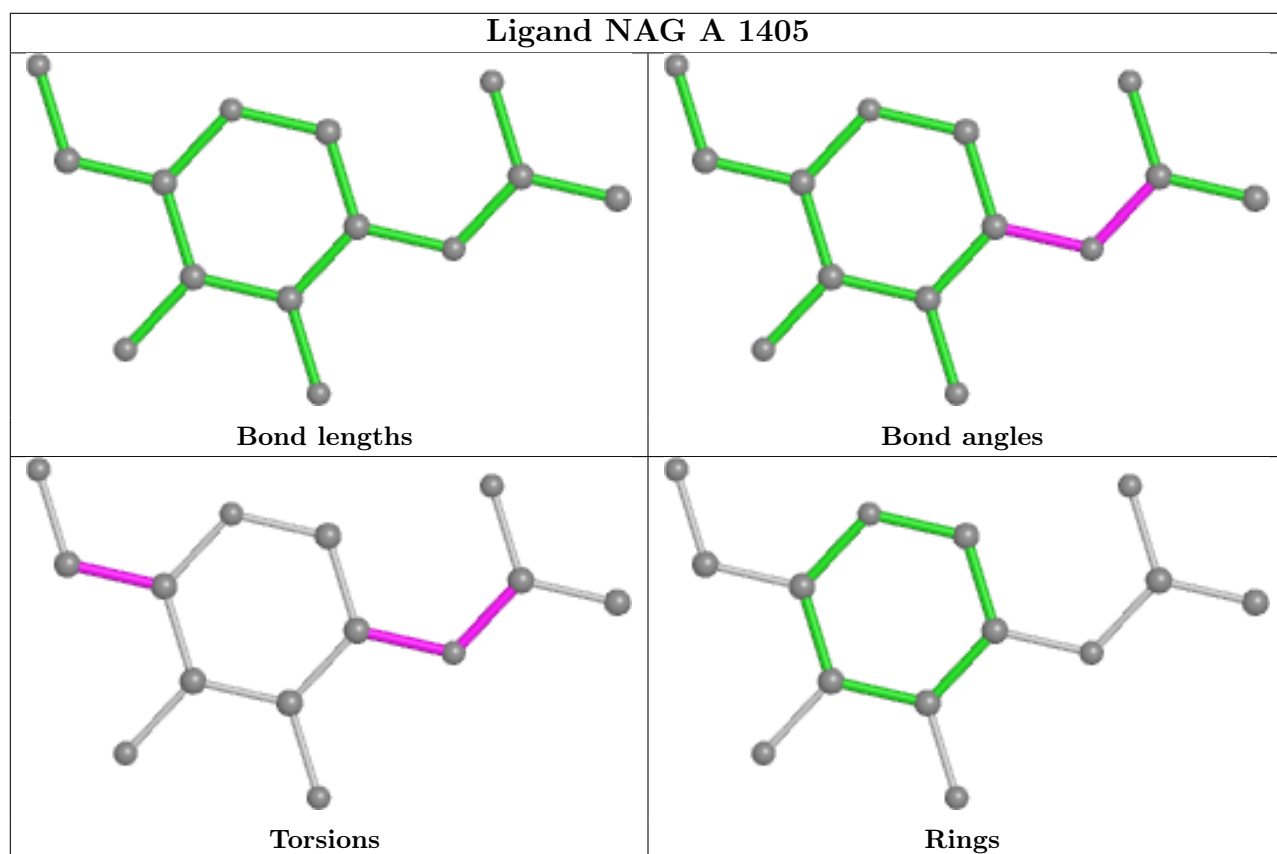
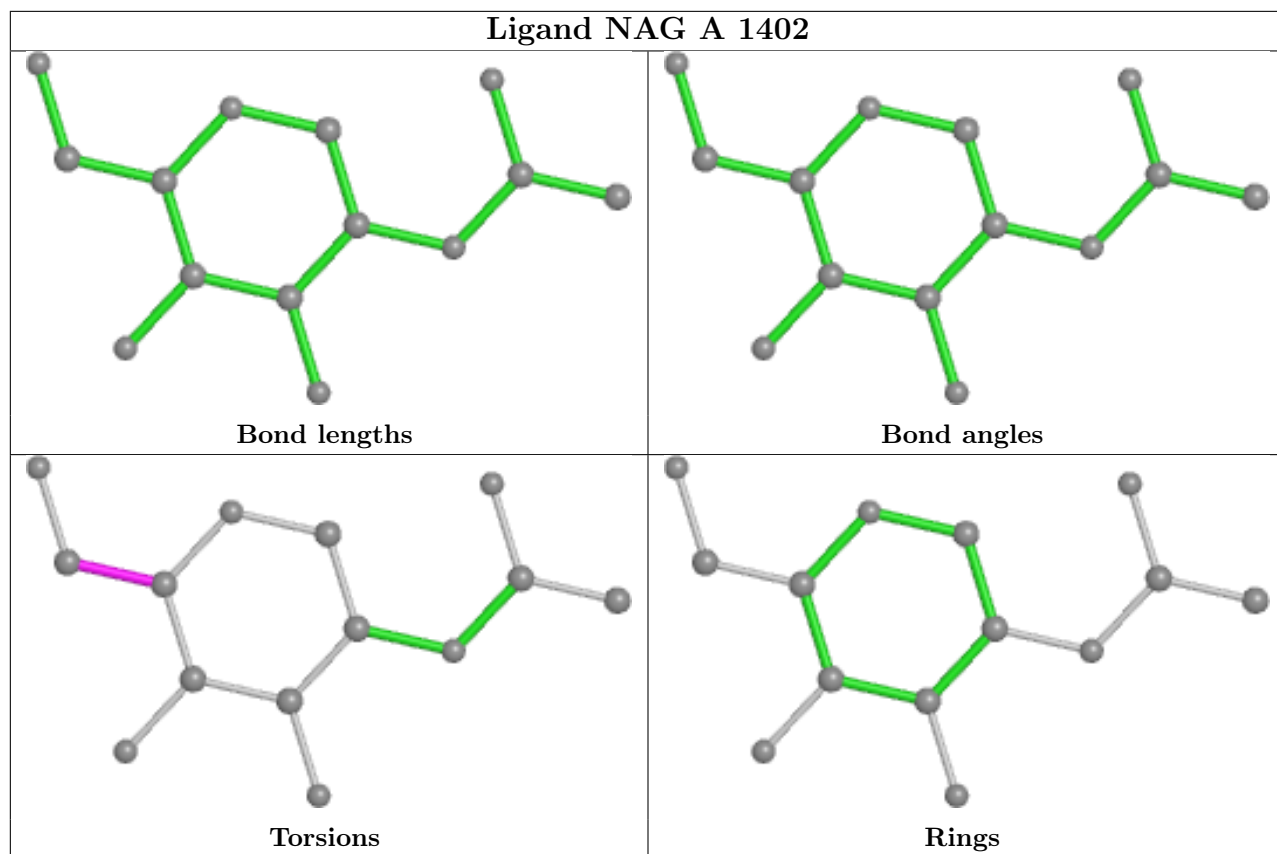
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1405	NAG	2	0
5	A	1404	NAG	1	0
5	A	1402	NAG	3	0
5	A	1405	NAG	1	0
5	B	1407	NAG	1	0
5	C	1405	NAG	1	0
5	B	1403	NAG	2	0
5	B	1402	NAG	1	0
5	C	1402	NAG	1	0

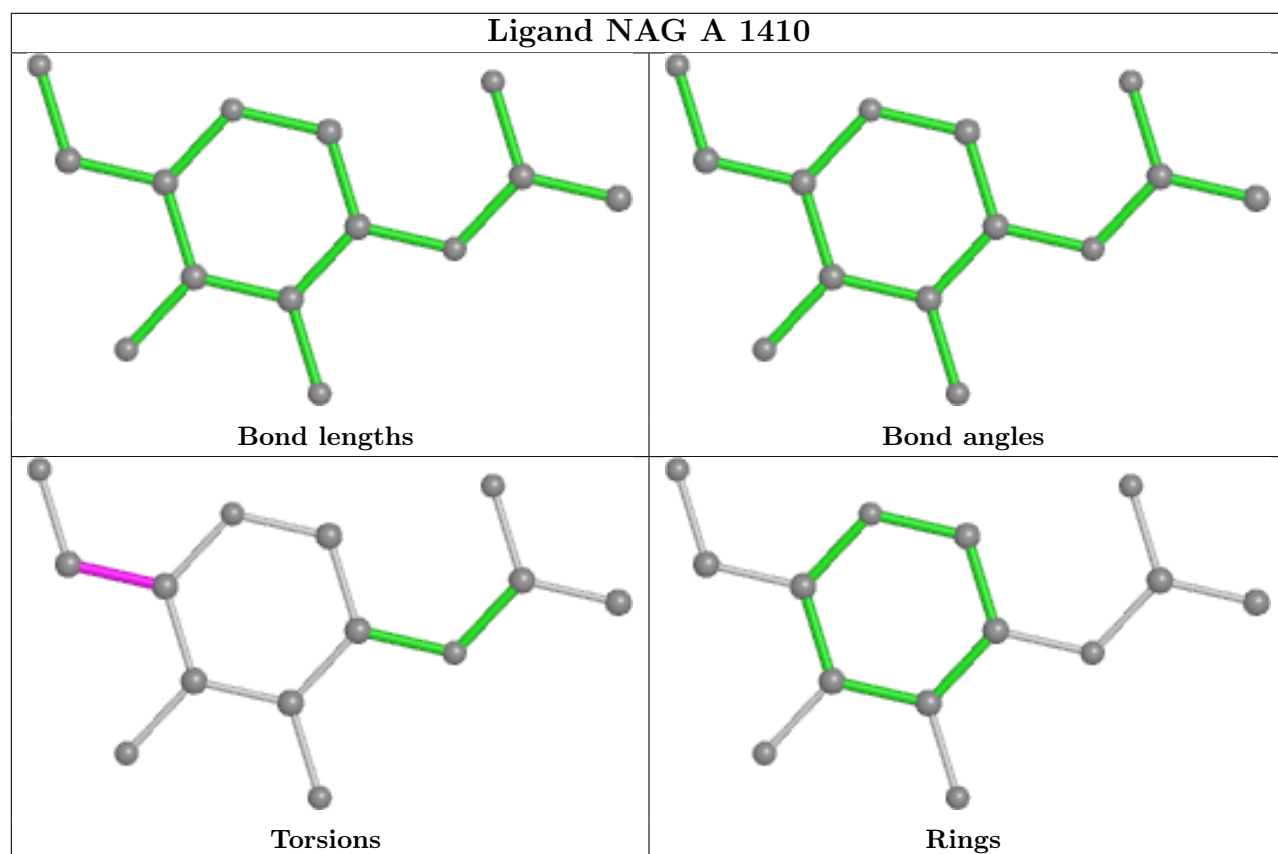
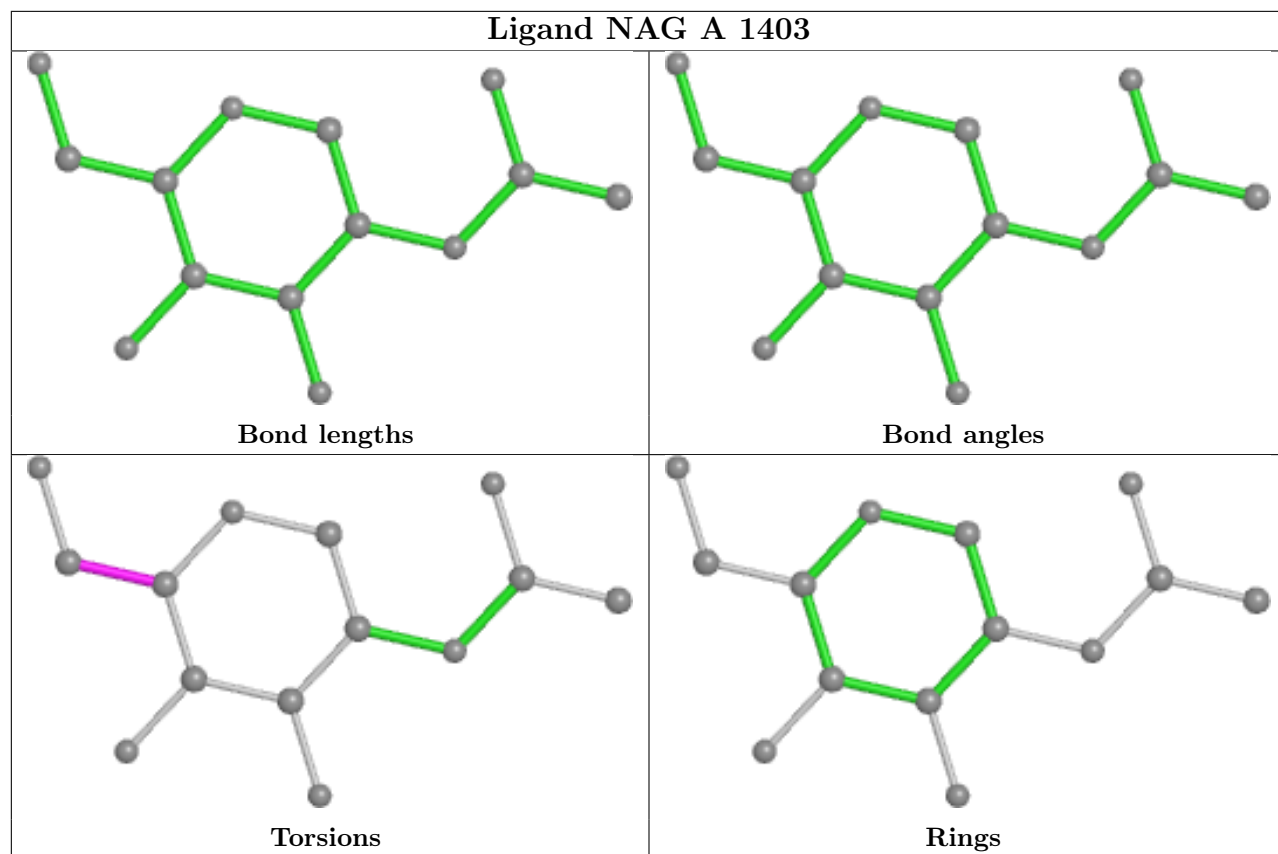
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

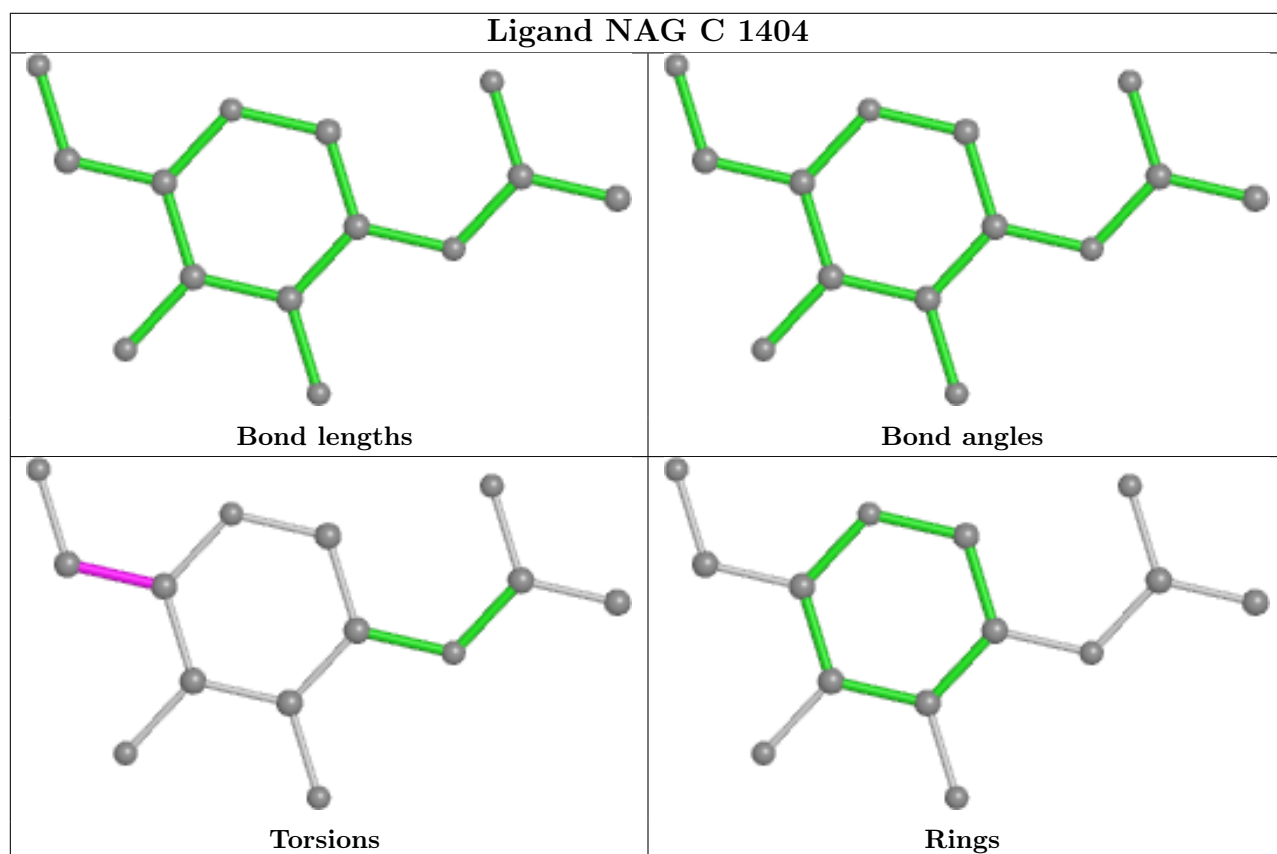
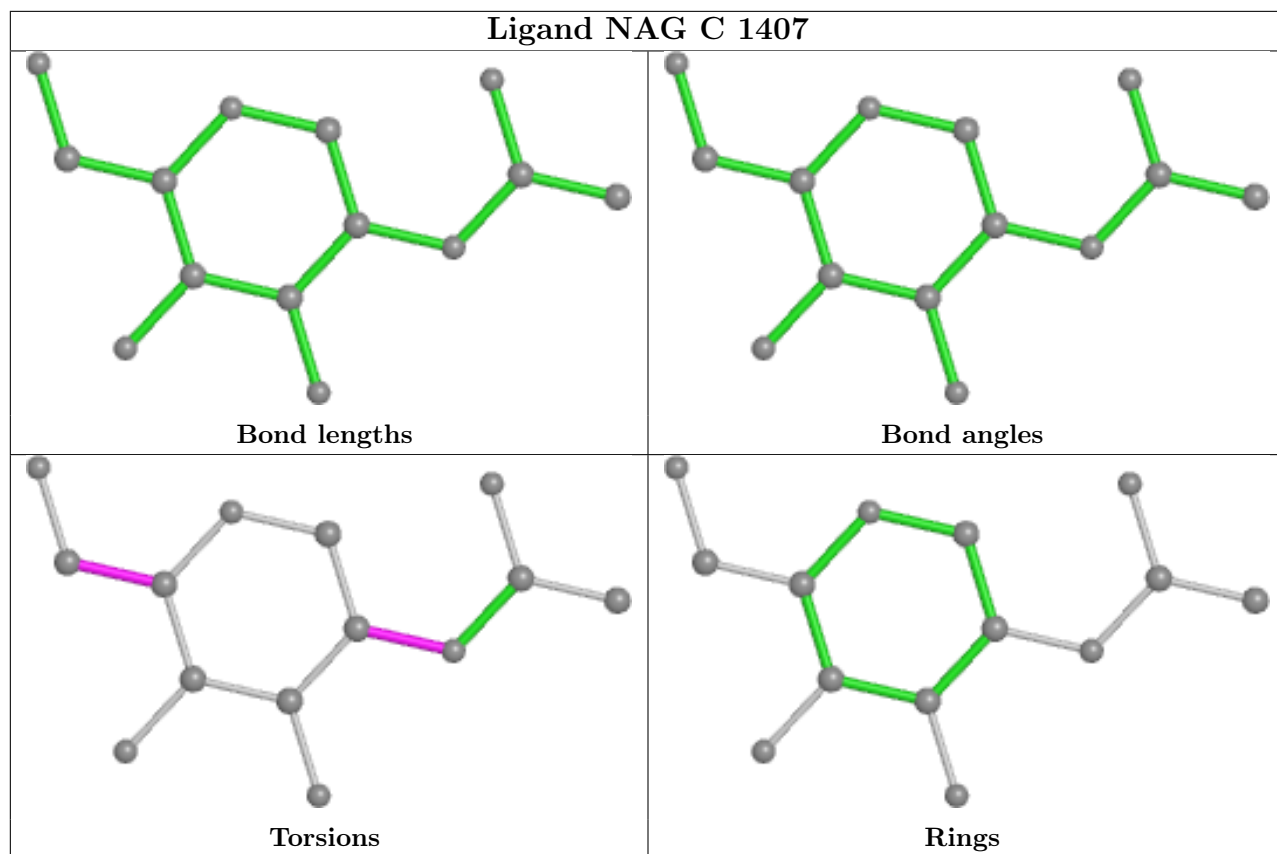


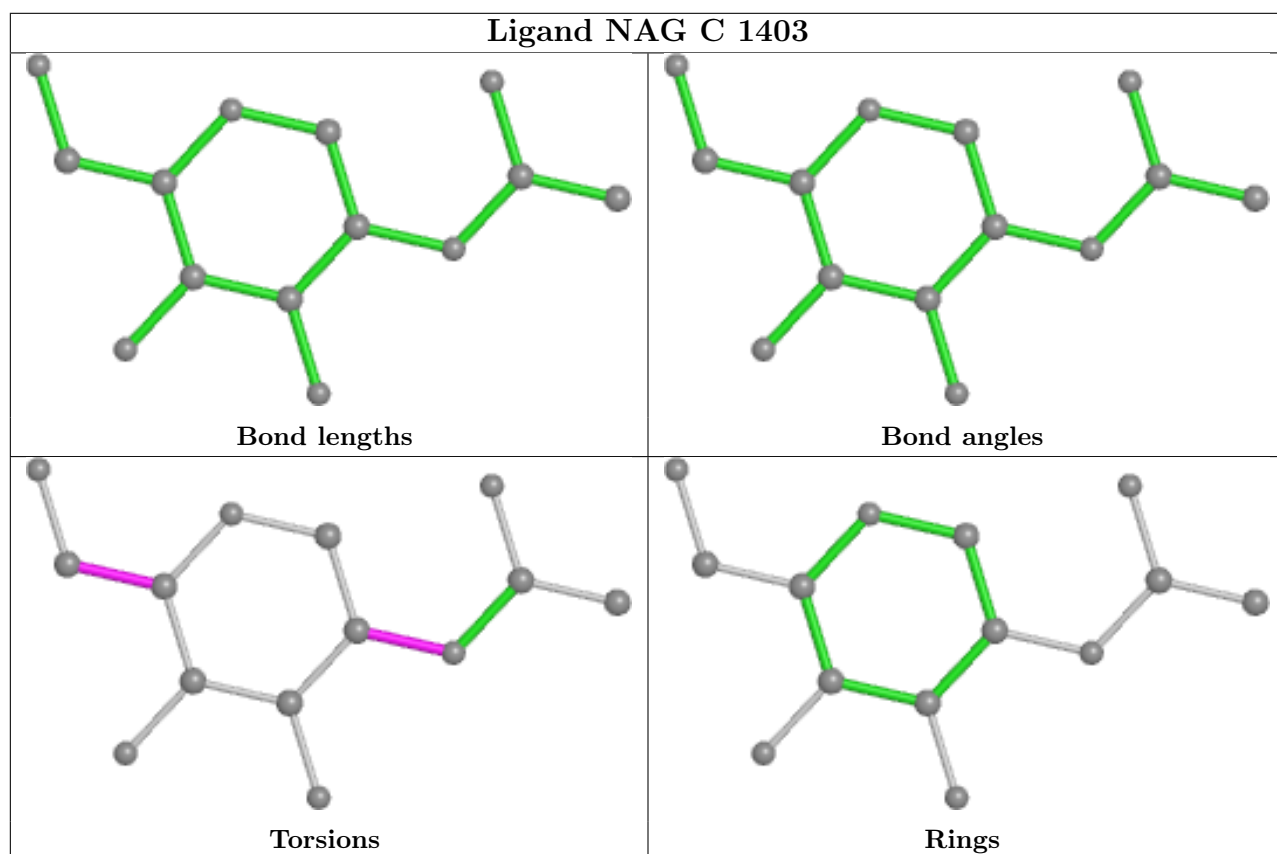
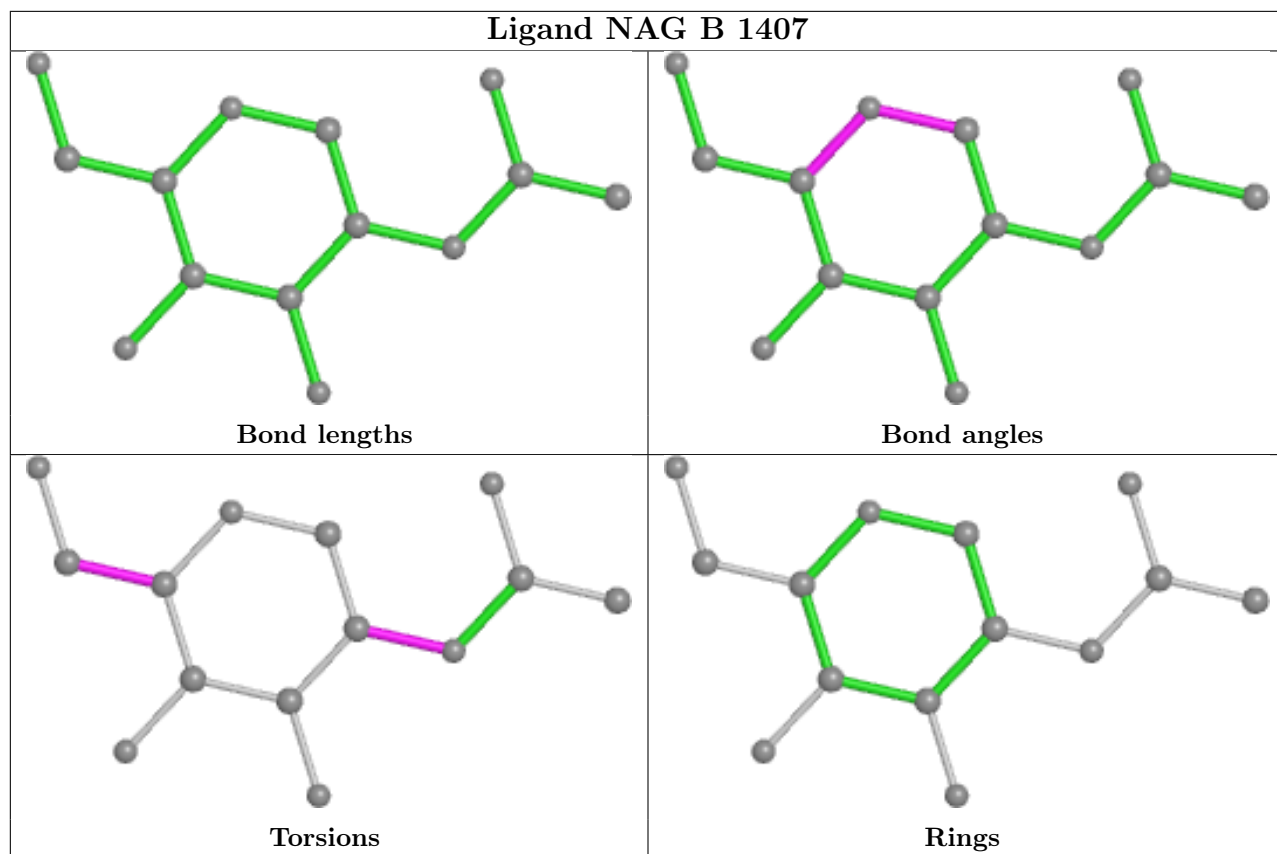


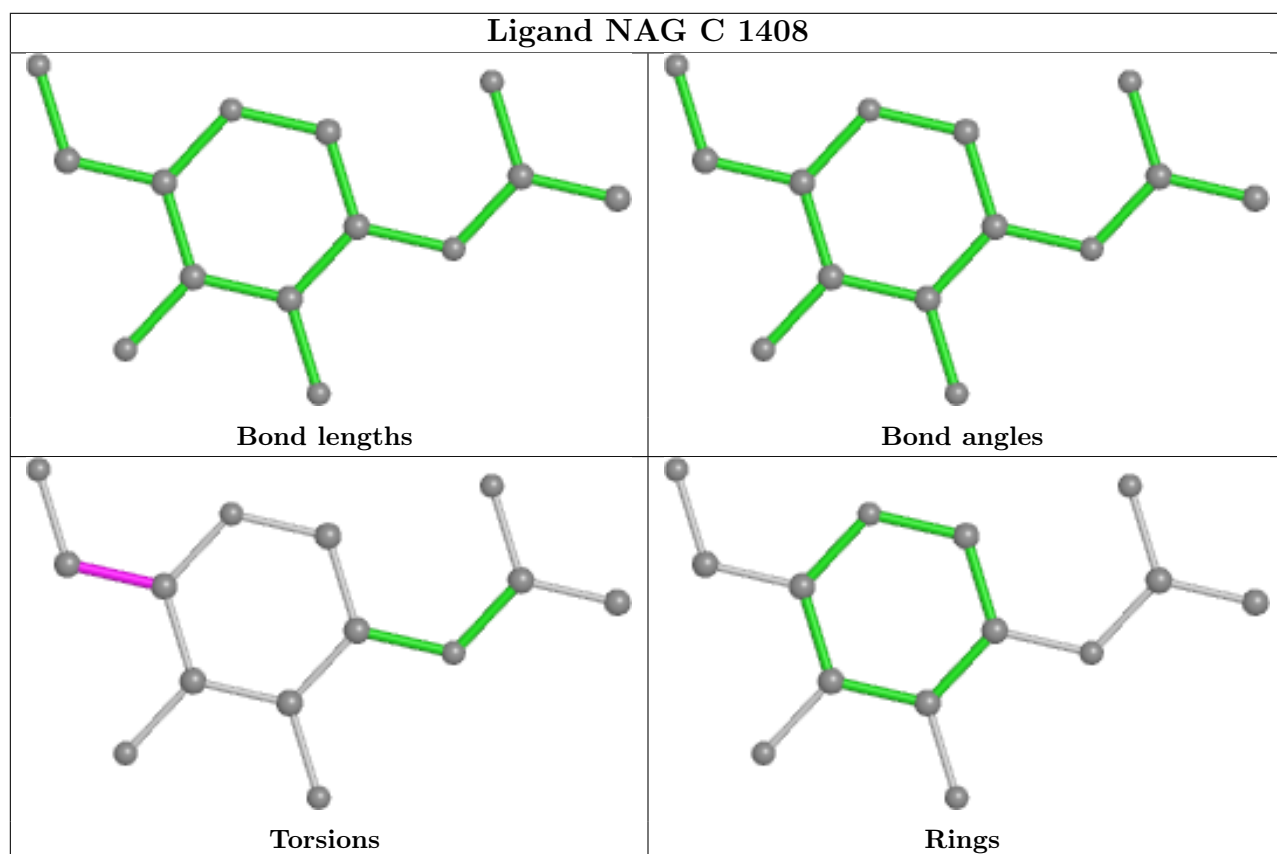
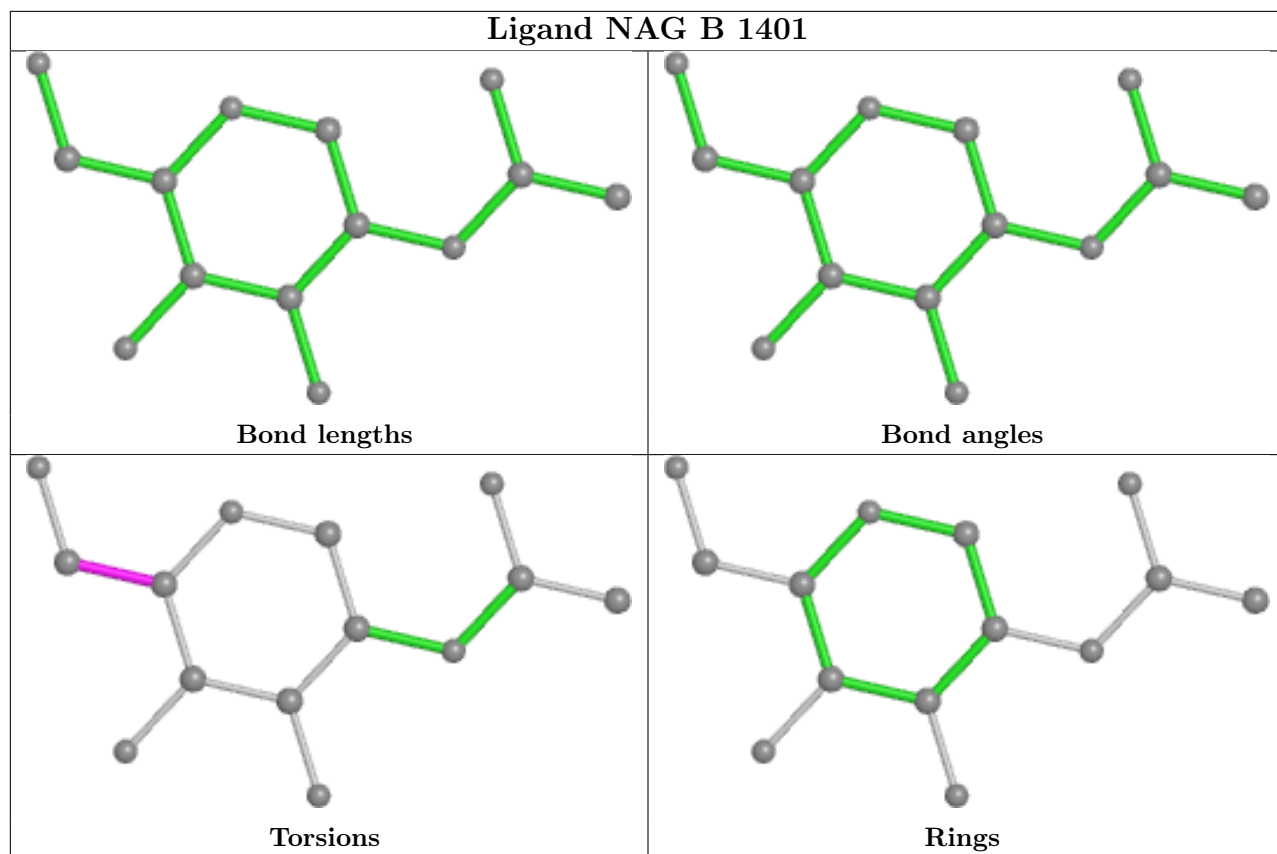


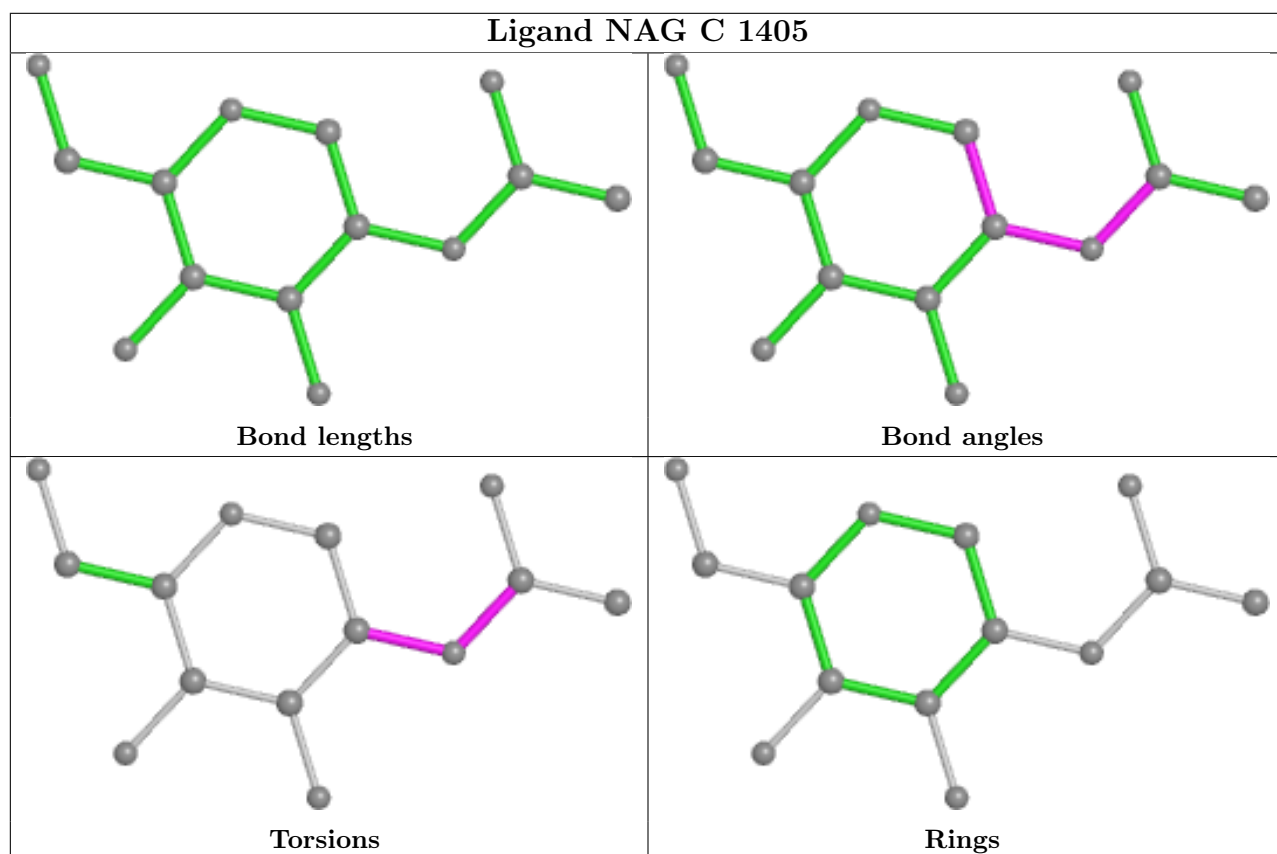
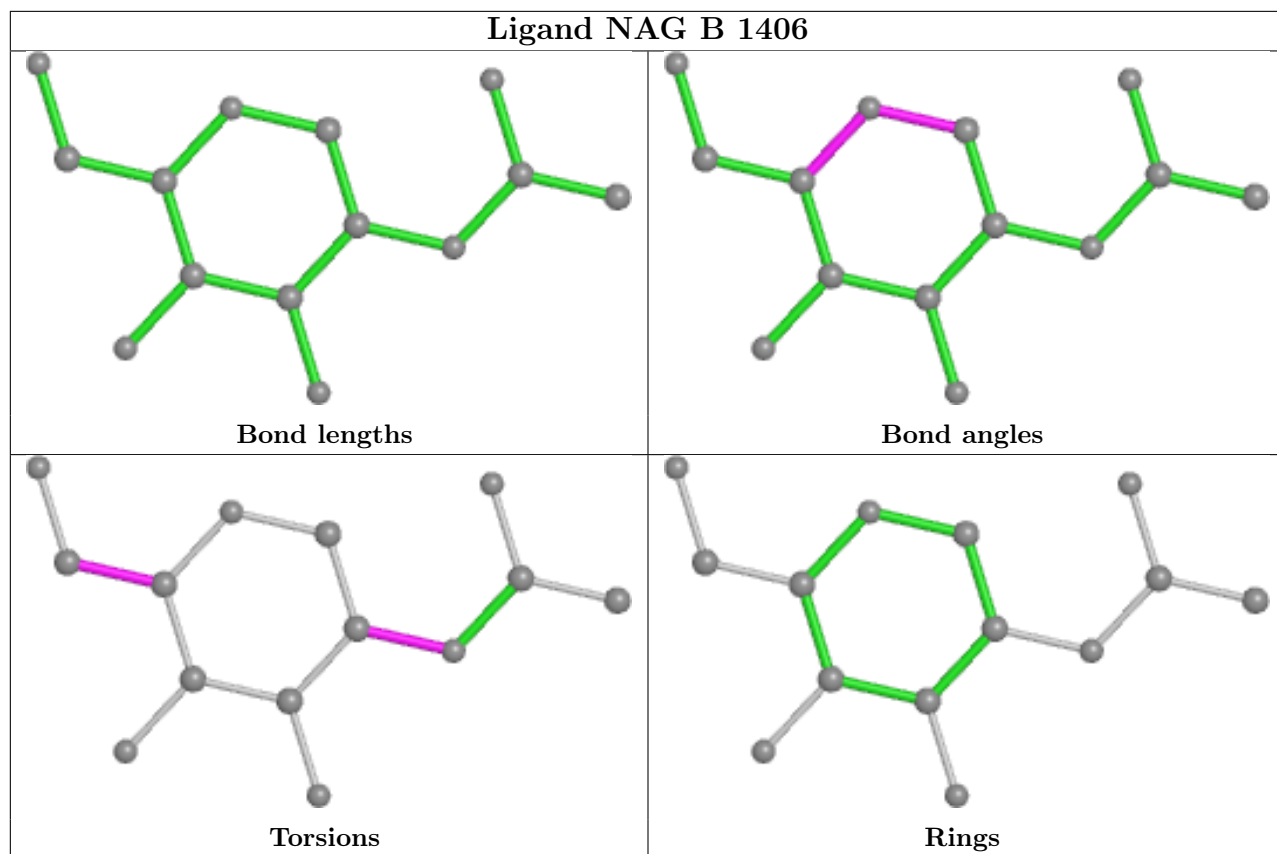


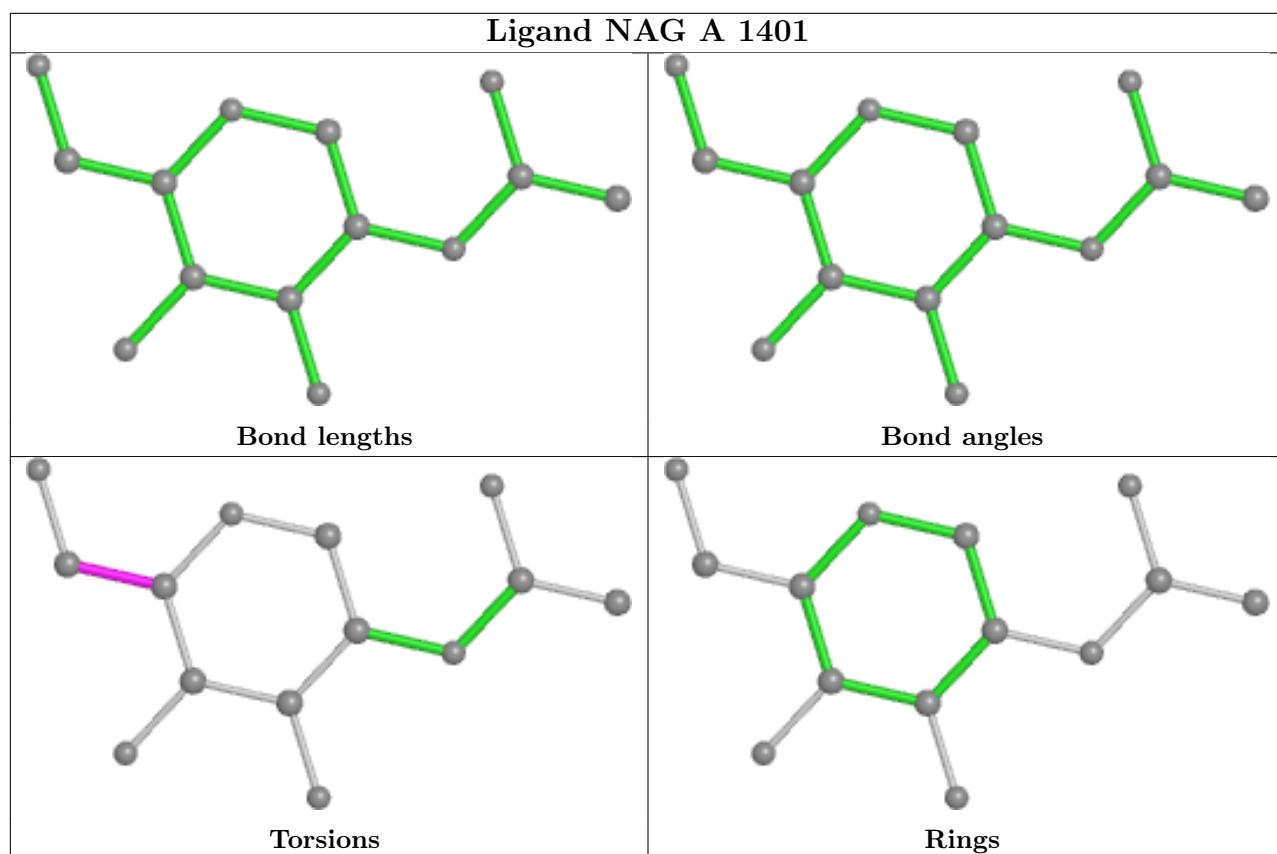
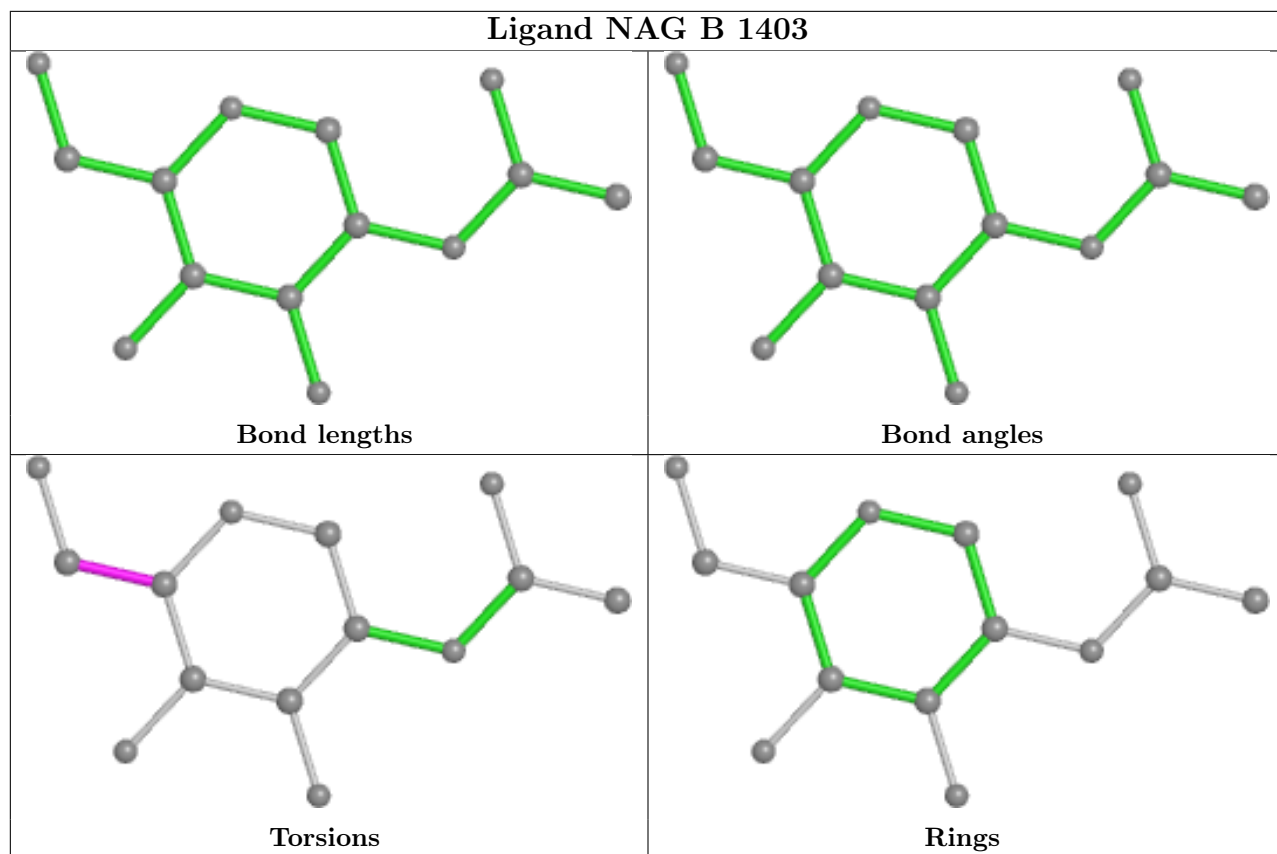


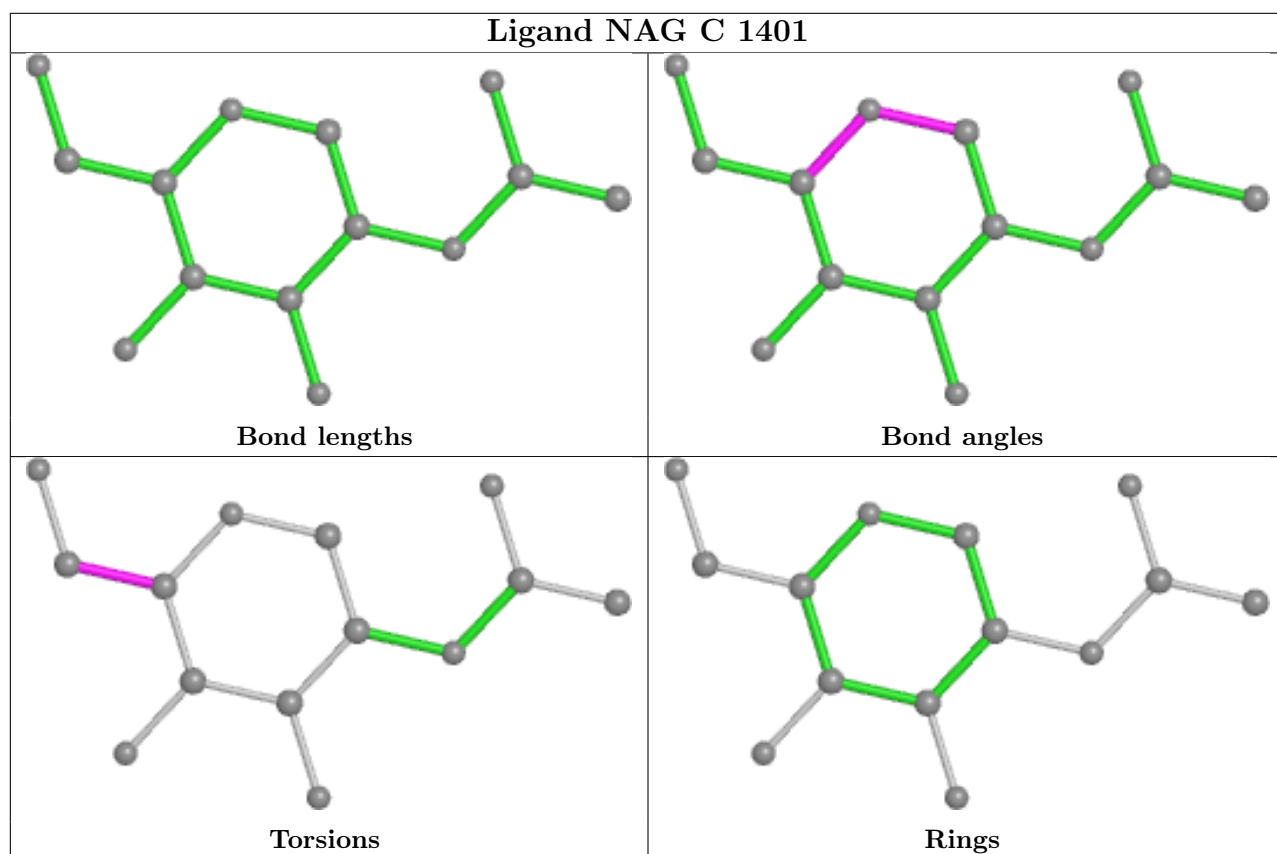
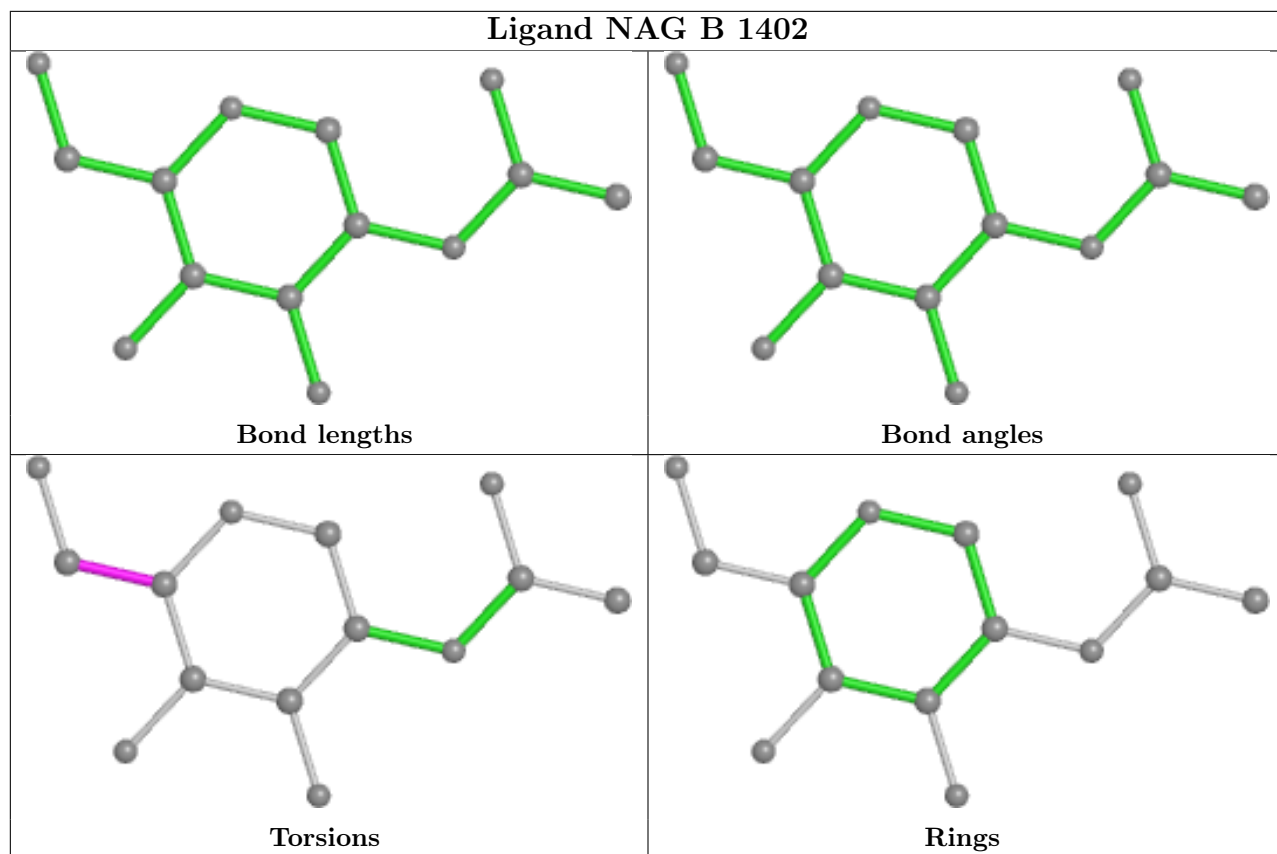


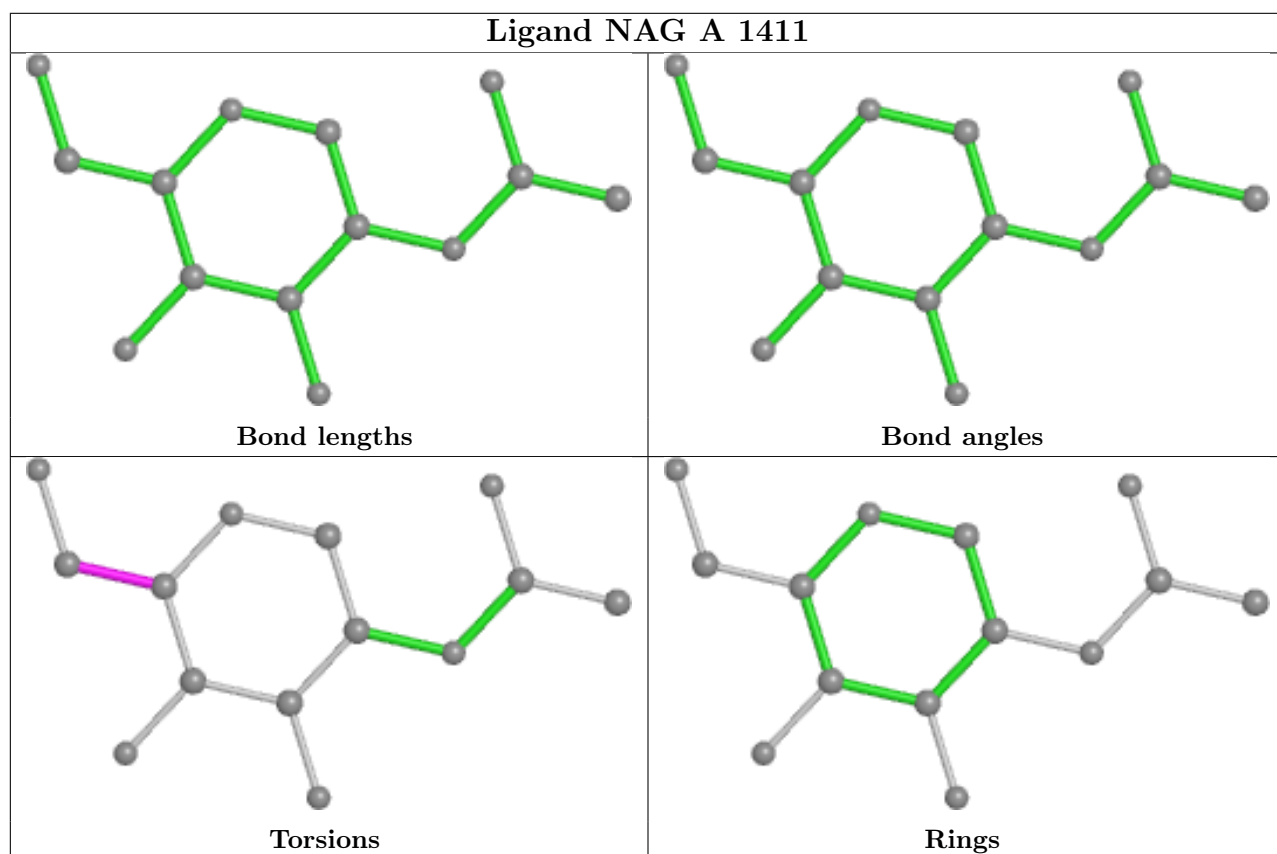
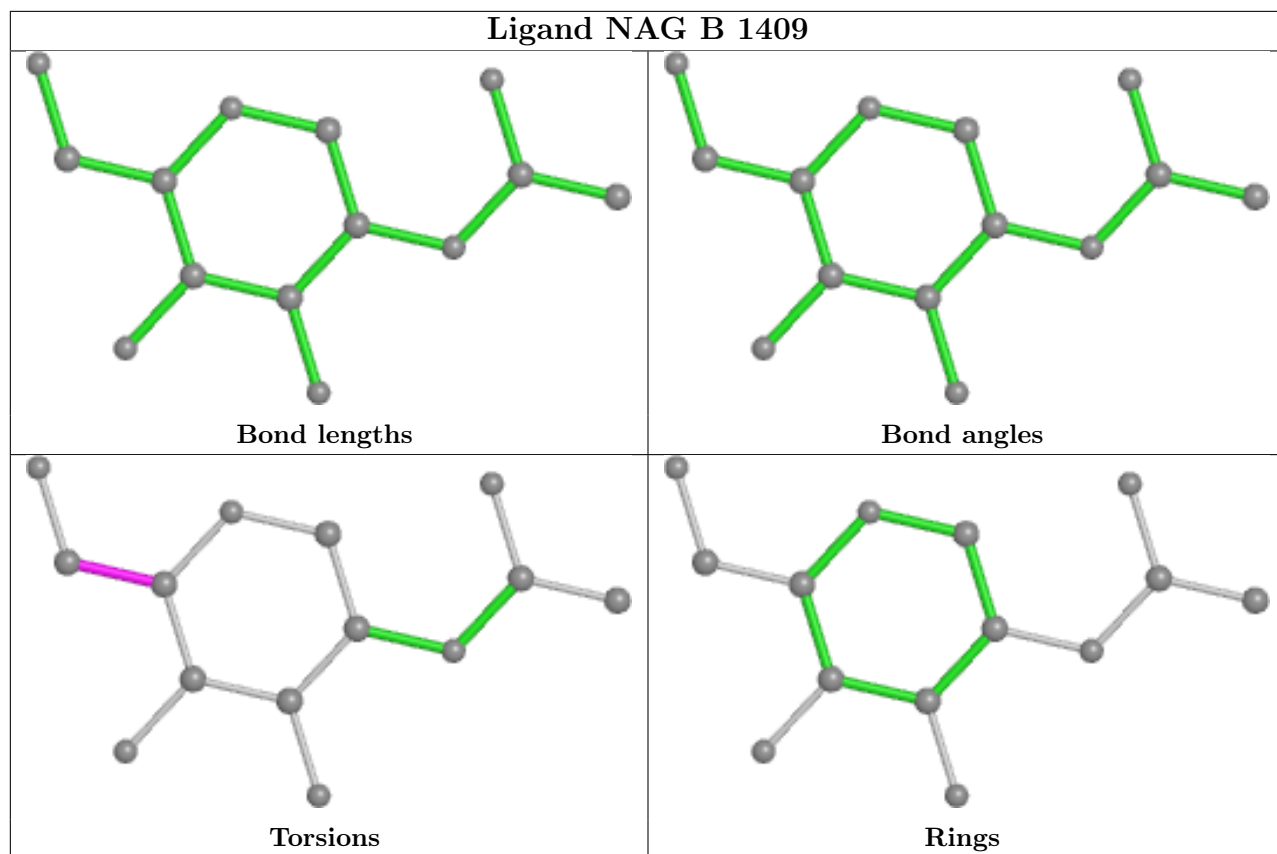


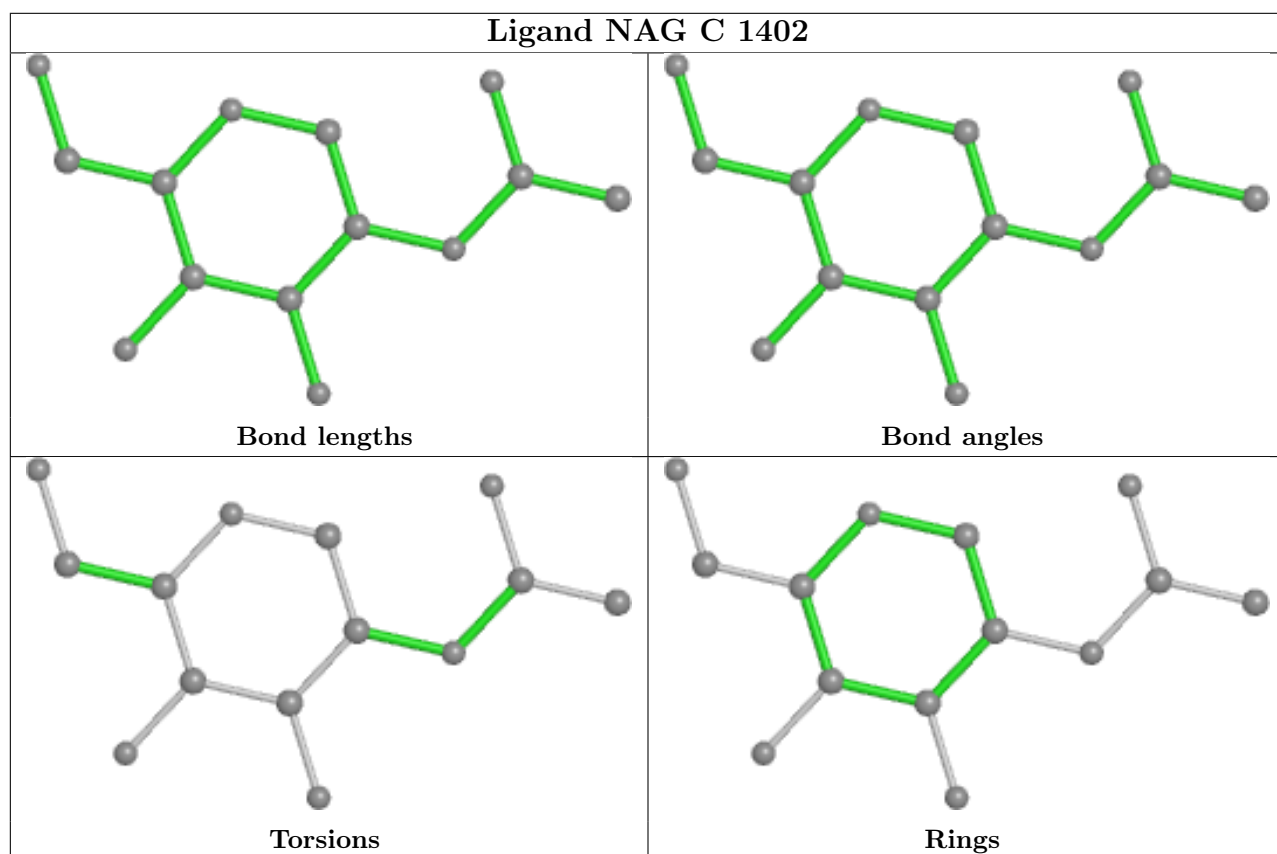
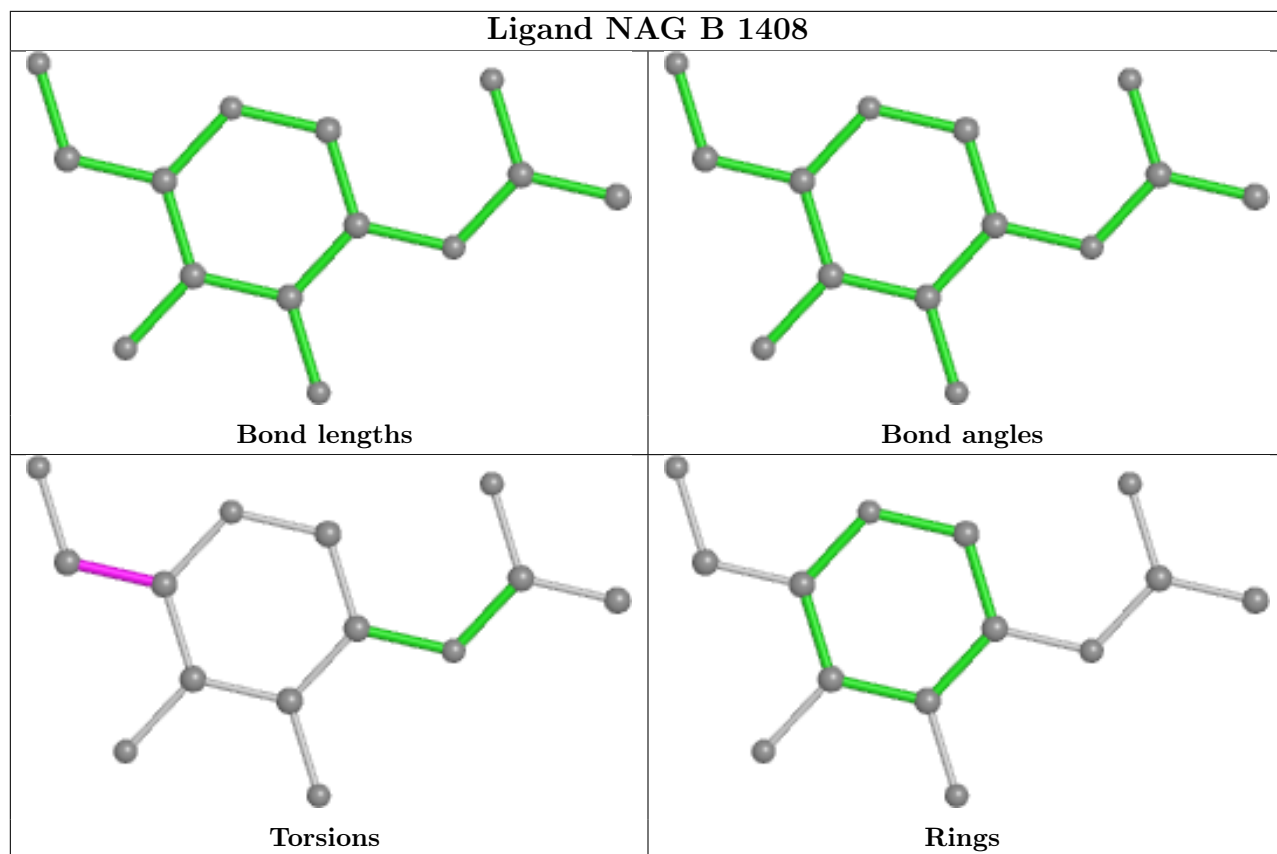












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

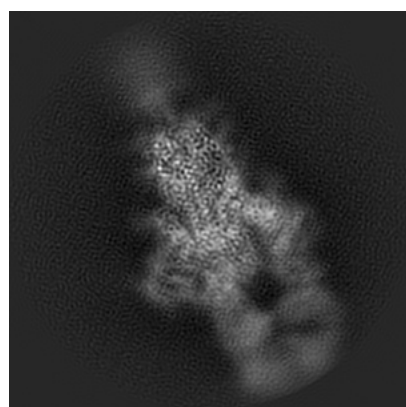
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30530. These allow visual inspection of the internal detail of the map and identification of artifacts.

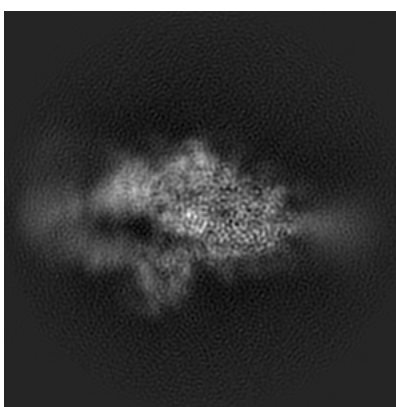
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

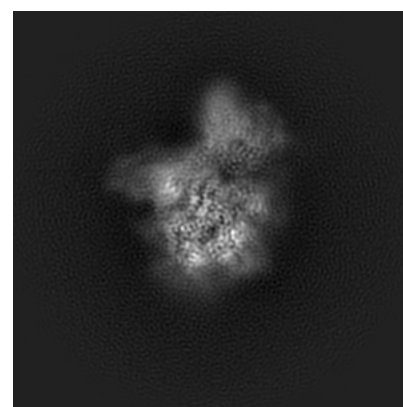
6.1.1 Primary map



X



Y

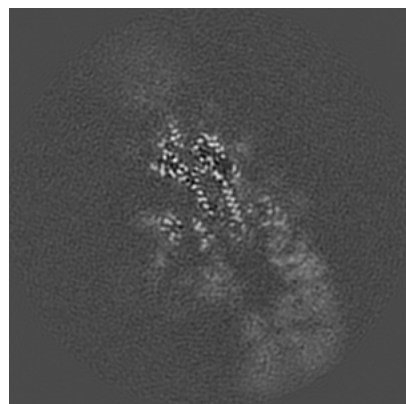


Z

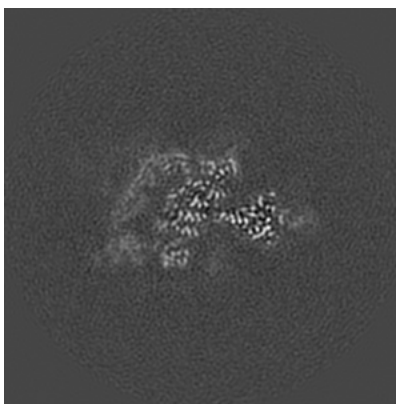
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

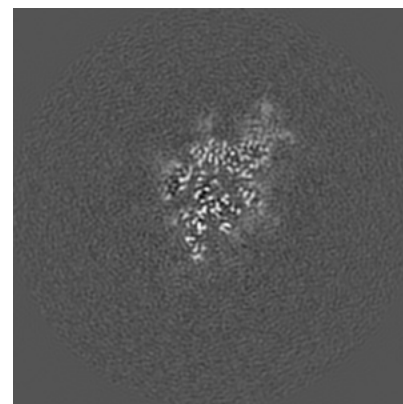
6.2.1 Primary map



X Index: 144



Y Index: 144

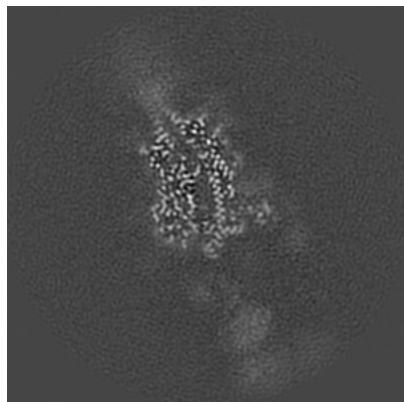


Z Index: 144

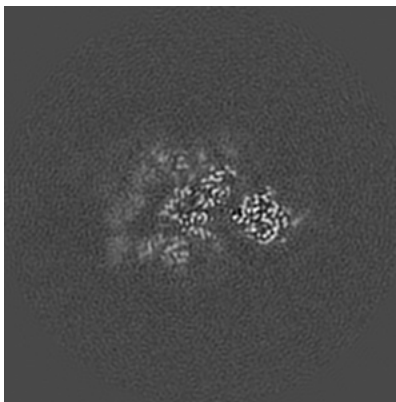
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

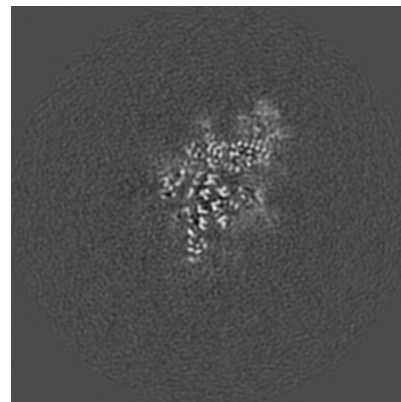
6.3.1 Primary map



X Index: 130



Y Index: 141

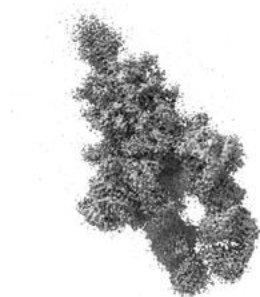


Z Index: 141

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

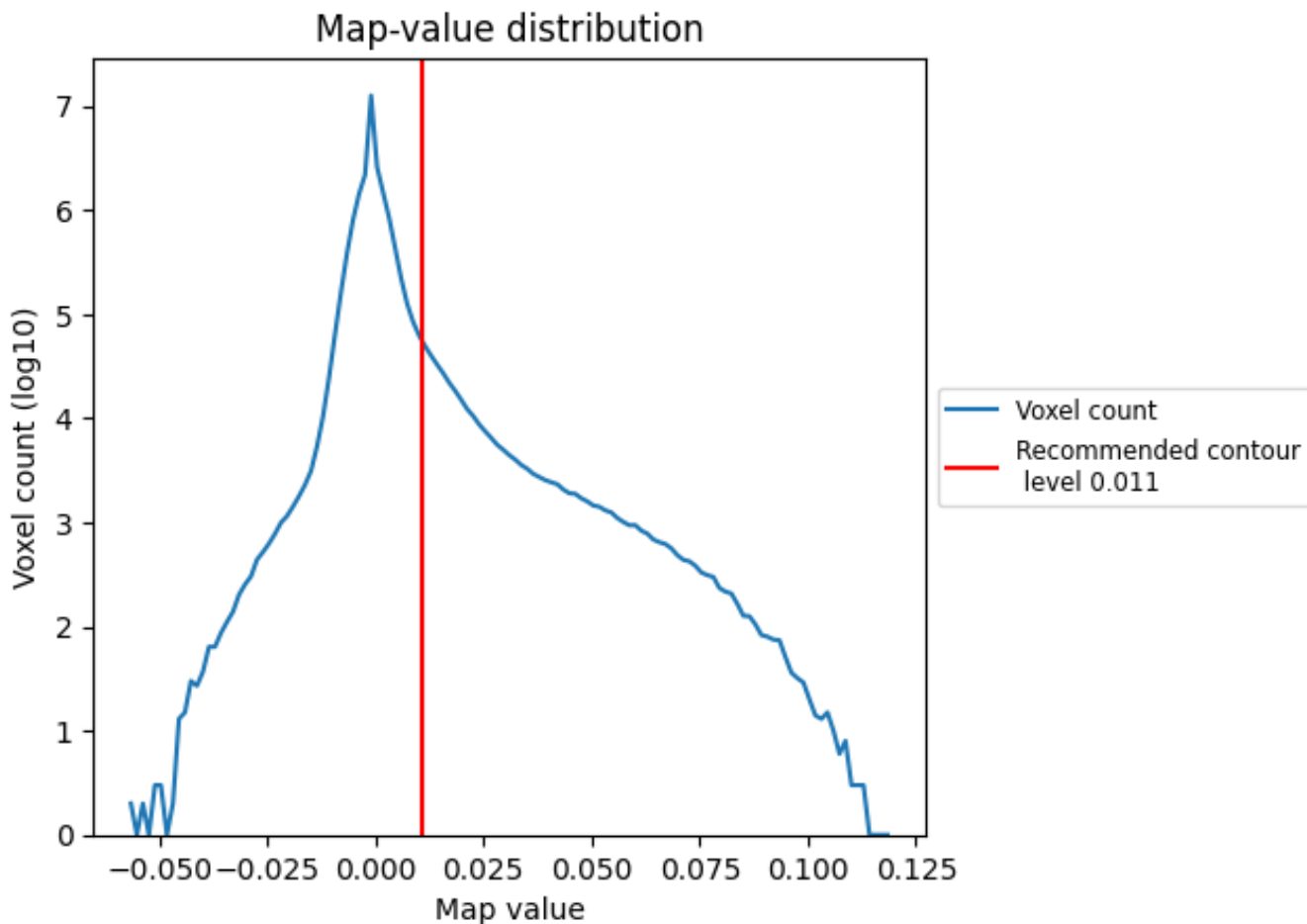
6.5 Mask visualisation

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

7 Map analysis [i](#)

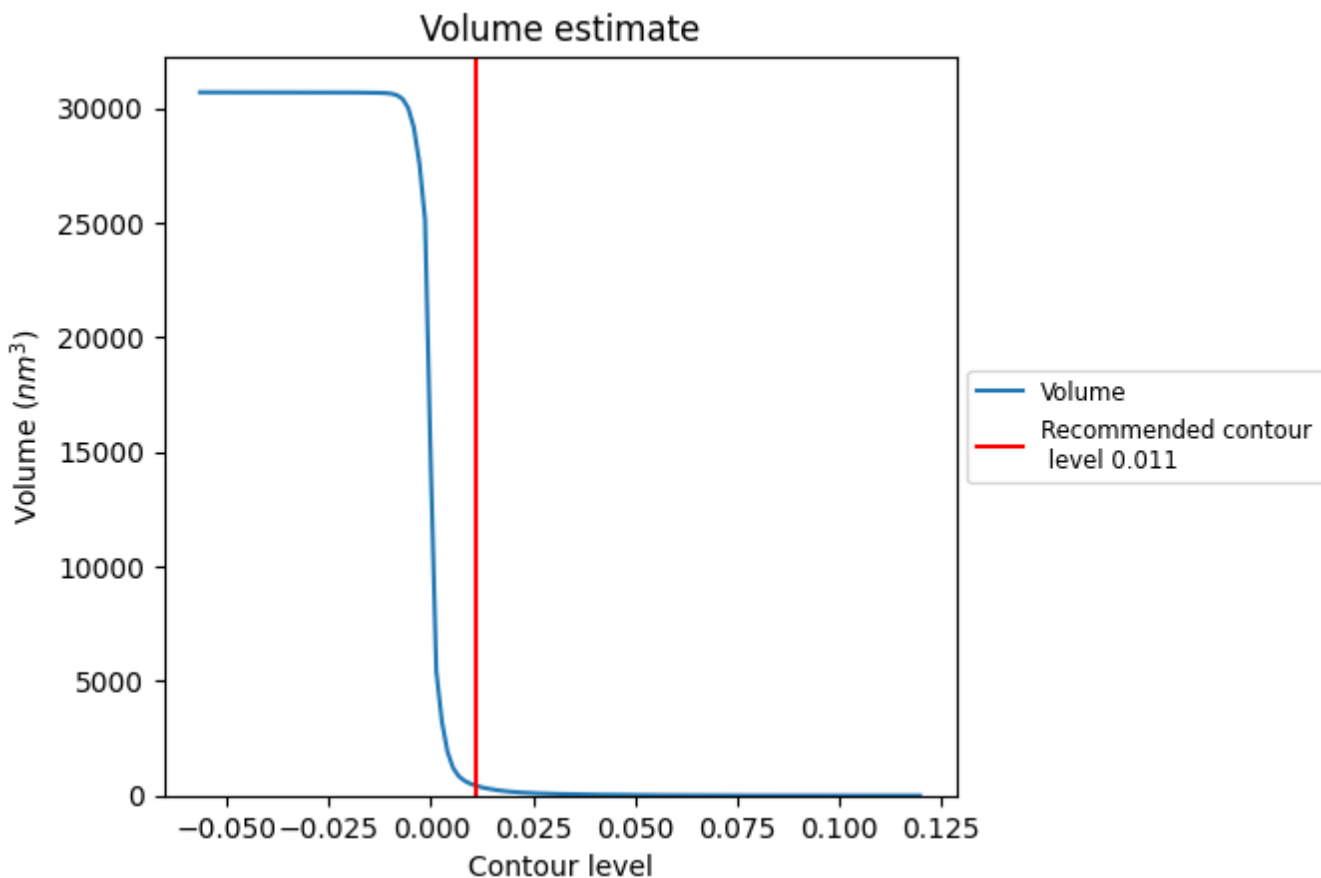
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

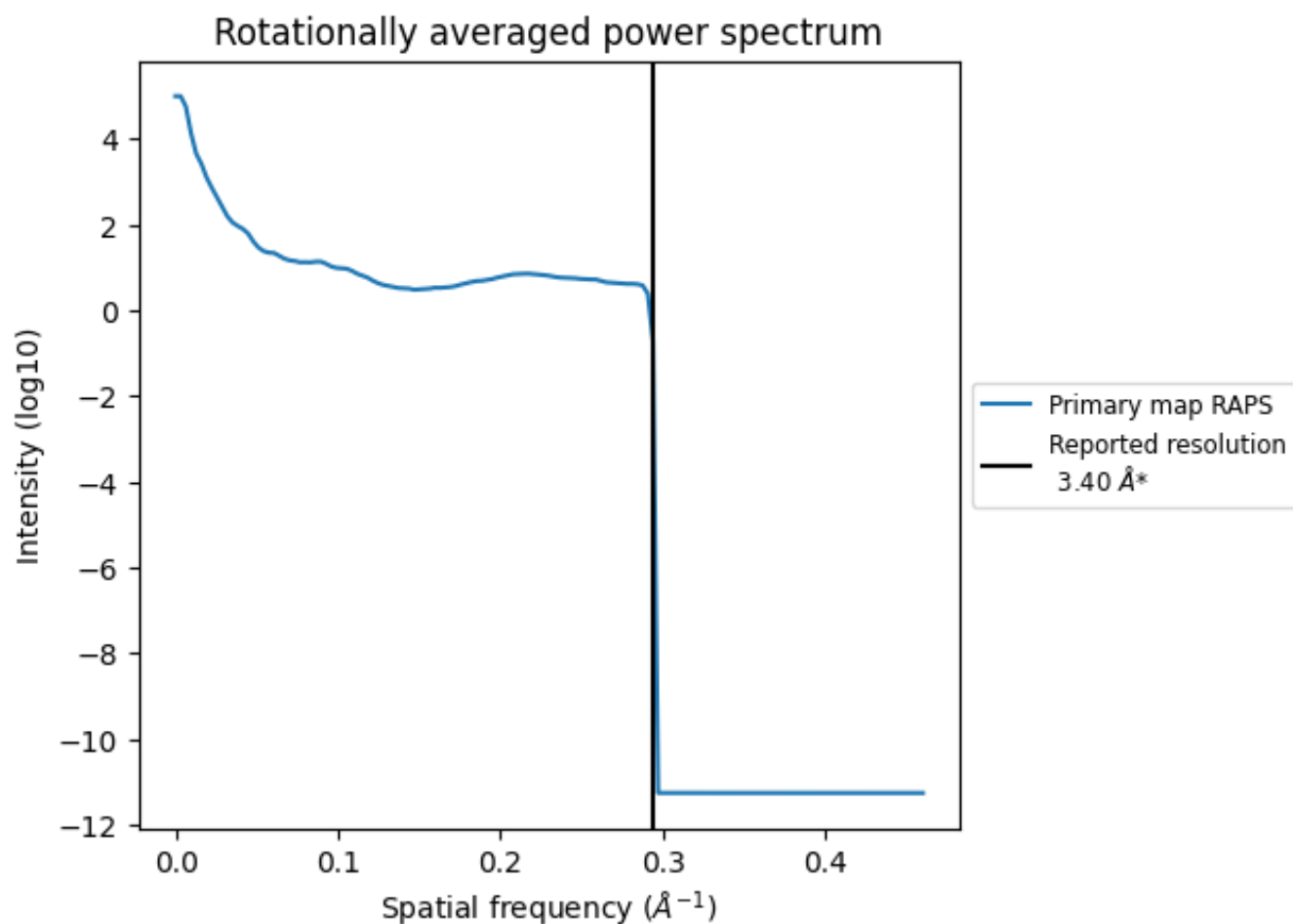
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 435 nm³; this corresponds to an approximate mass of 393 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

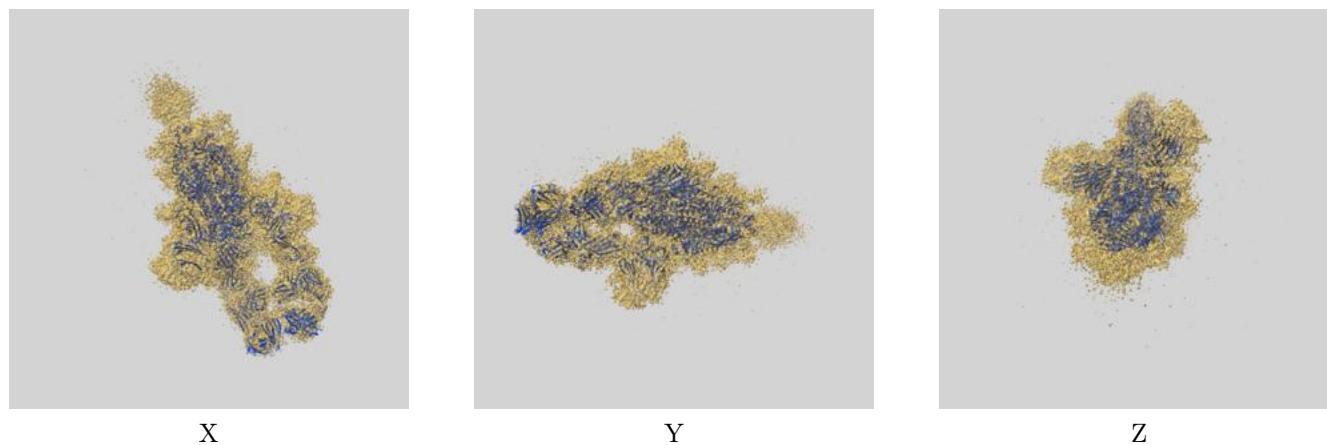
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

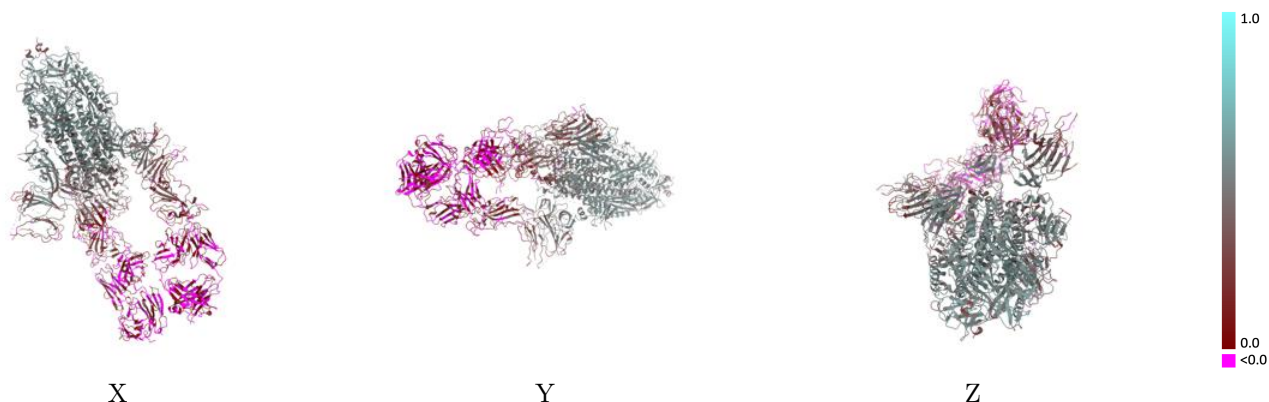
This section contains information regarding the fit between EMDB map EMD-30530 and PDB model 7D0C. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



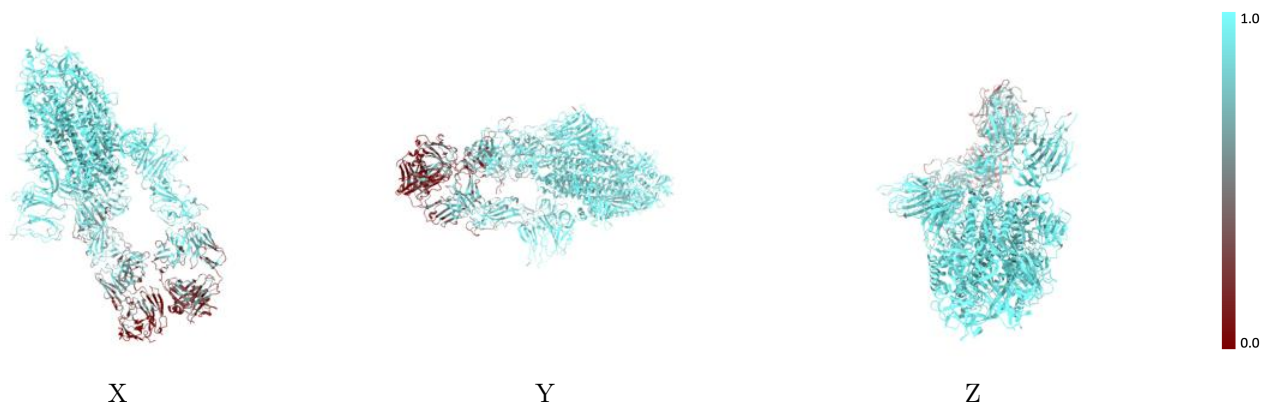
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



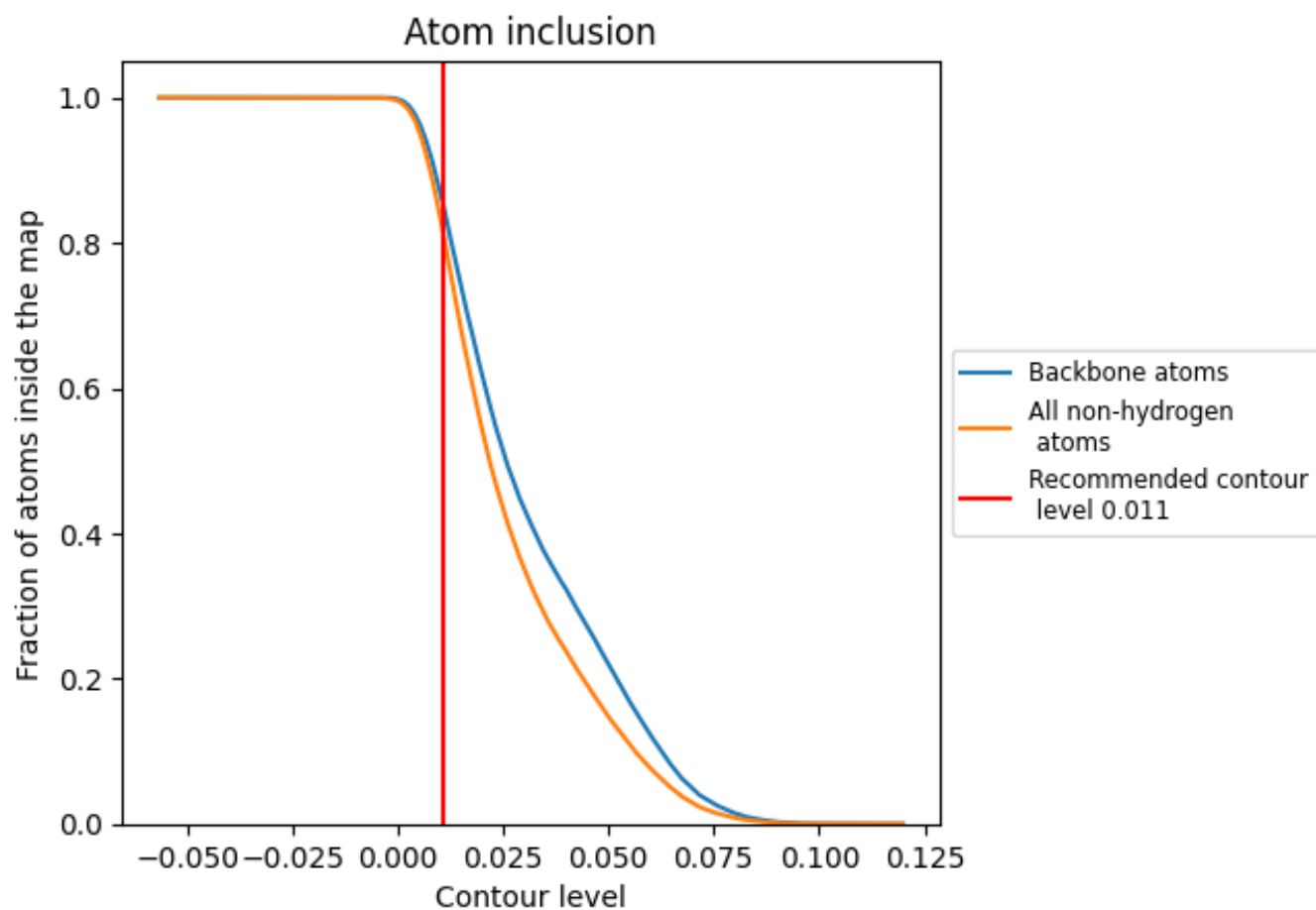
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8077	 0.3280
A	 0.9236	 0.4150
B	 0.8896	 0.4150
C	 0.9053	 0.4010
D	 0.5357	 0.0210
E	 0.9643	 0.4710
F	 0.3783	 0.0380
G	 0.4308	 0.0160
H	 0.5233	 0.0200
I	 0.8571	 0.3090
J	 0.8214	 0.3870
K	 0.9643	 0.3910
L	 0.4576	 0.0340
M	 0.9286	 0.3610
N	 0.6786	 0.2110
O	 0.8214	 0.3060
P	 0.9286	 0.4120
Q	 0.9643	 0.3920
R	 0.9286	 0.3750
S	 0.8929	 0.3860
T	 0.9643	 0.3470
U	 0.3571	 0.0710
V	 0.7857	 0.3410
W	 0.8929	 0.4430
X	 0.8571	 0.3590
Y	 0.6786	 0.2940
Z	 0.9286	 0.4200
a	 0.8571	 0.3770
b	 0.9286	 0.3580
c	 0.7857	 0.3810

