



Full wwPDB EM Validation Report ⓘ

Jul 4, 2023 – 02:22 PM JST

PDB ID : 8GTO
EMDB ID : EMD-34259
Title : cryo-EM structure of Omicron BA.5 S protein in complex with XGv282
Authors : Xia, X.Y.; Zhang, Y.Y.; Chi, X.M.; Huang, B.D.; Wu, L.S.; Zhou, Q.
Deposited on : 2022-09-08
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev50
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) : 2.34

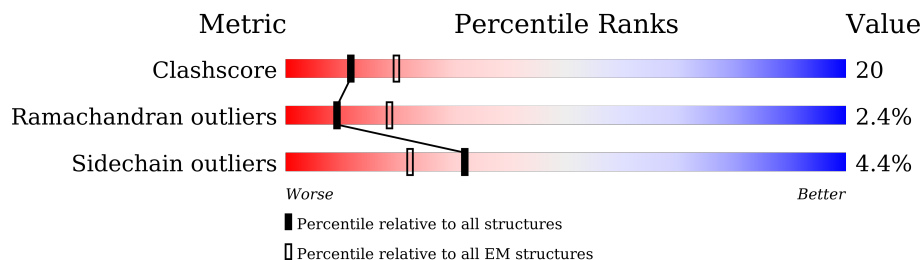
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	1271	
1	B	1271	
1	C	1271	
2	H	117	
2	I	117	
2	J	117	
3	L	111	
3	M	111	

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Mol	Chain	Length	Quality of chain
3	N	111	<p>85% 77% 22%</p>
4	D	2	<p>50% 100%</p>
4	E	2	<p>50% 50% 50%</p>
4	F	2	<p>50% 50%</p>
4	G	2	<p>50% 50%</p>
4	K	2	<p>100%</p>
4	O	2	<p>100%</p>
4	P	2	<p>50% 50%</p>
4	Q	2	<p>50% 50% 50%</p>
4	R	2	<p>50% 50%</p>
4	S	2	<p>50% 50%</p>
4	T	2	<p>100%</p>
4	U	2	<p>100%</p>
4	V	2	<p>50% 50% 50%</p>
4	W	2	<p>50% 50% 50%</p>
4	X	2	<p>50% 50%</p>
4	Y	2	<p>50% 50%</p>
4	Z	2	<p>100%</p>
4	a	2	<p>100%</p>

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30234 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	1025	8043	5154	1338	1514	37	0	0
1	B	1025	8043	5154	1338	1514	37	0	0
1	C	1025	8043	5154	1338	1514	37	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
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B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2

- Molecule 2 is a protein called heavy chain of XGv282.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			910	576	153	177	4		
2	I	117	Total	C	N	O	S	0	0
			910	576	153	177	4		
2	J	117	Total	C	N	O	S	0	0
			910	576	153	177	4		

- Molecule 3 is a protein called light chain of XGv282.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			803	495	139	167	2		
3	M	111	Total	C	N	O	S	0	0
			803	495	139	167	2		
3	N	111	Total	C	N	O	S	0	0
			803	495	139	167	2		

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



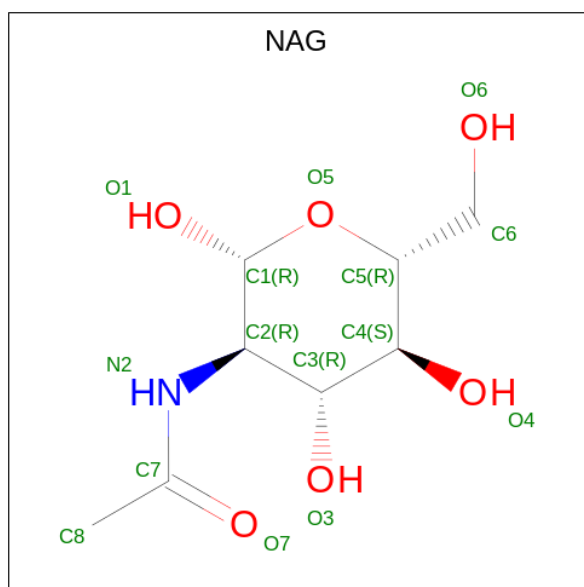
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	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	R	2	Total 28	C 16	N 2	O 10	0	0
4	S	2	Total 28	C 16	N 2	O 10	0	0
4	T	2	Total 28	C 16	N 2	O 10	0	0
4	U	2	Total 28	C 16	N 2	O 10	0	0
4	V	2	Total 28	C 16	N 2	O 10	0	0
4	W	2	Total 28	C 16	N 2	O 10	0	0
4	X	2	Total 28	C 16	N 2	O 10	0	0
4	Y	2	Total 28	C 16	N 2	O 10	0	0
4	Z	2	Total 28	C 16	N 2	O 10	0	0
4	a	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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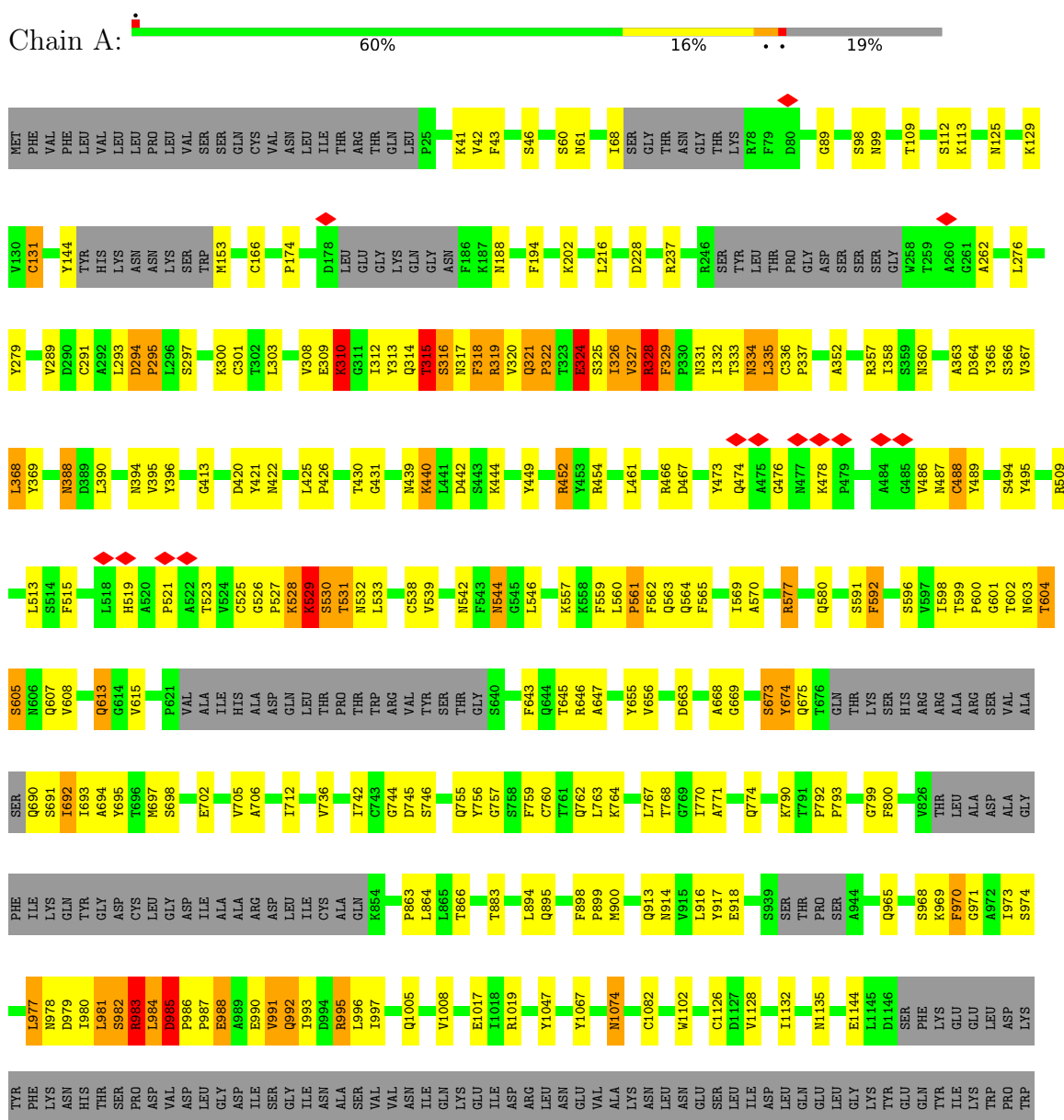
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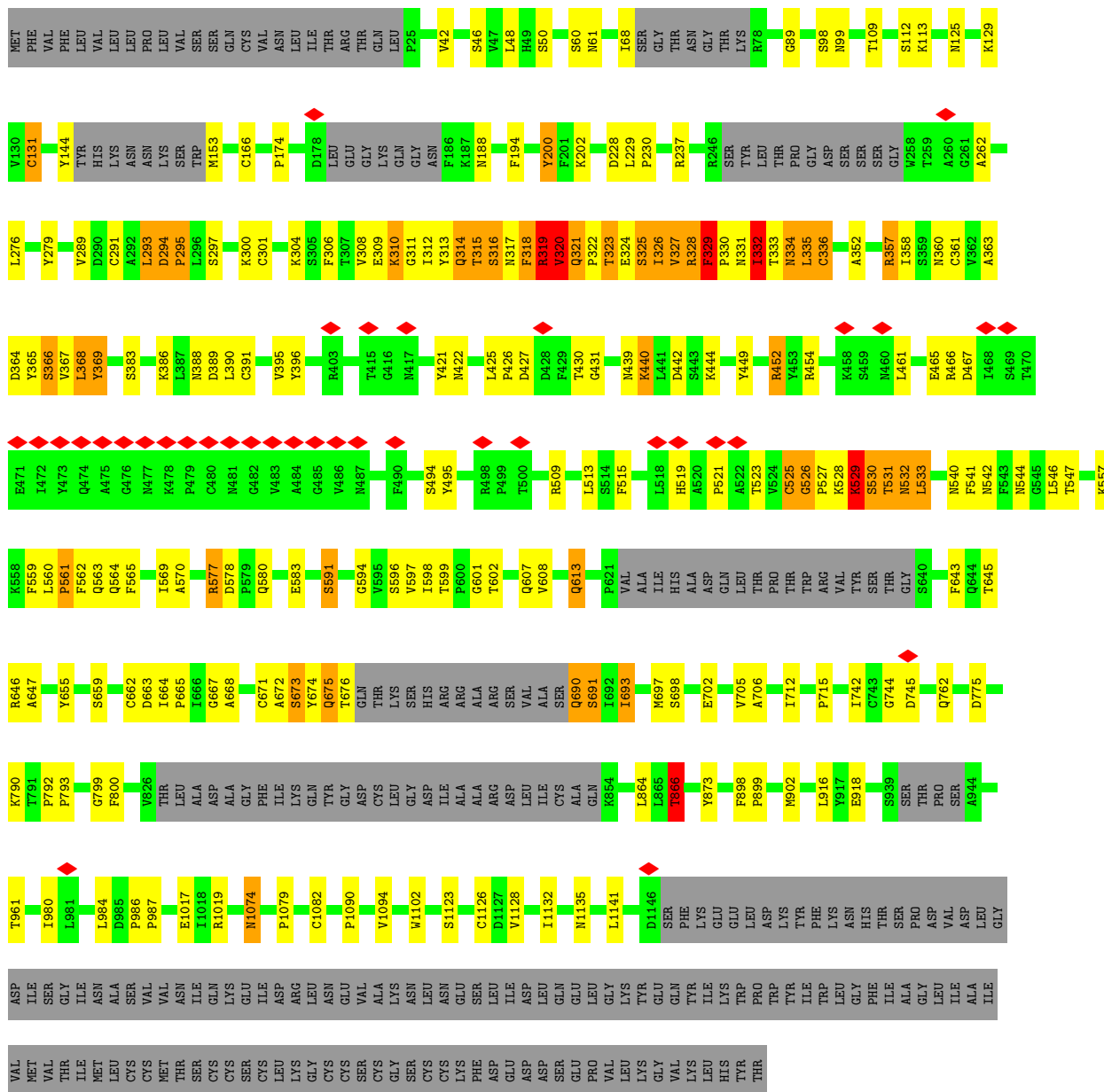
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1	5	0
5	C	1	Total 14	8	1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

3 Residue-property plots [i](#)

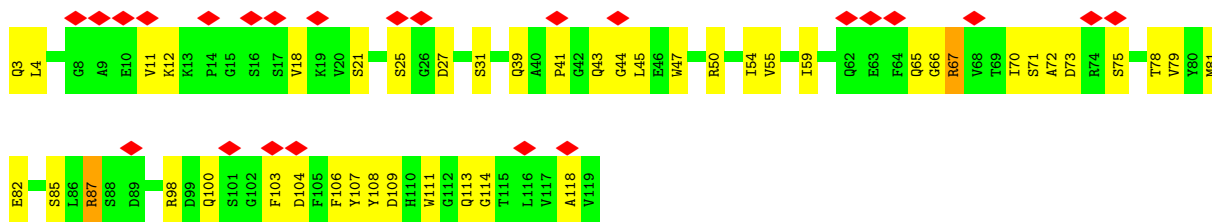
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein



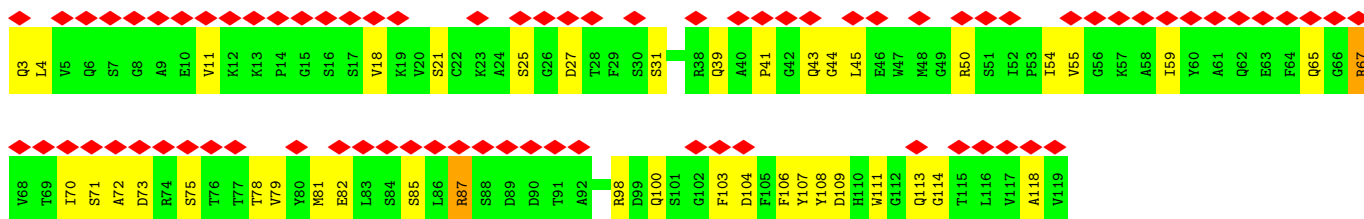


• Molecule 2: heavy chain of XGv282

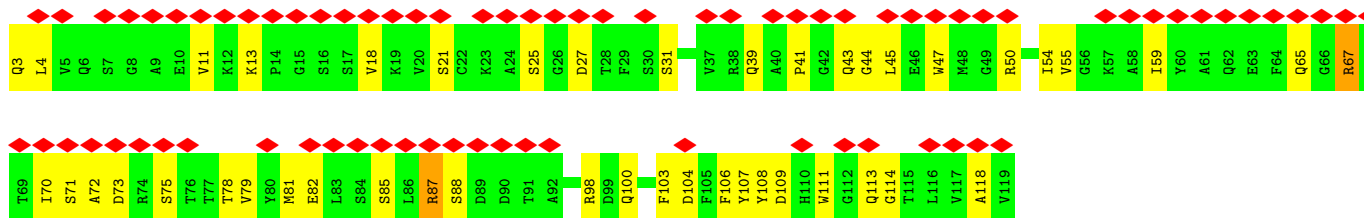


• Molecule 2: heavy chain of XGv282

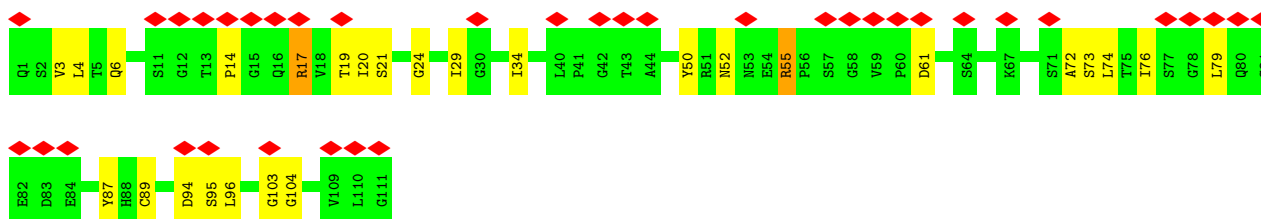
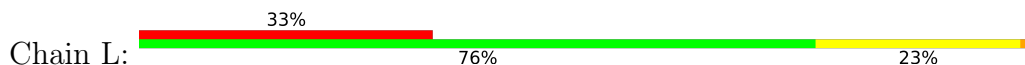




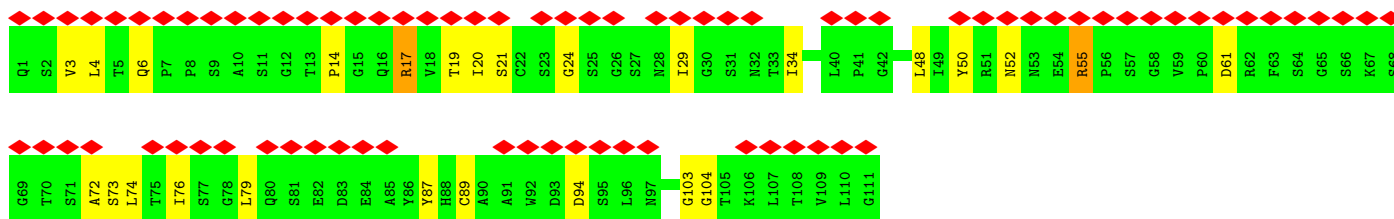
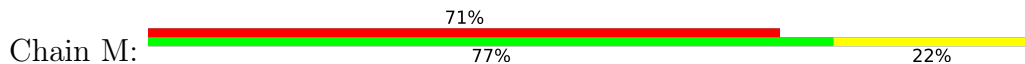
• Molecule 2: heavy chain of XGv282



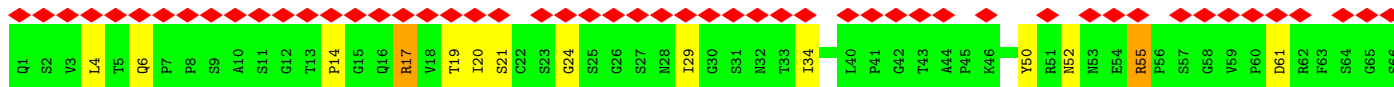
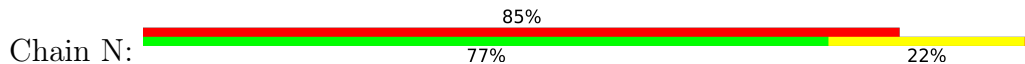
• Molecule 3: light chain of XGv282

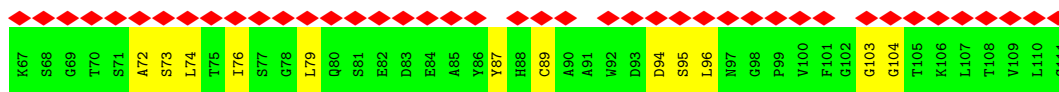


• Molecule 3: light chain of XGv282



• Molecule 3: light chain of XGv282





- 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



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



MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

- 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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	350760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.532	Depositor
Minimum map value	-2.719	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	344.64, 344.64, 344.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	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	0.54	0/8235	0.59	0/11204
1	B	0.54	0/8235	0.59	0/11204
1	C	0.55	0/8235	0.60	0/11204
2	H	0.39	0/932	0.59	0/1262
2	I	0.39	0/932	0.59	0/1262
2	J	0.39	0/932	0.59	0/1262
3	L	0.36	0/821	0.57	0/1120
3	M	0.36	0/821	0.57	0/1120
3	N	0.36	0/821	0.57	0/1120
All	All	0.52	0/29964	0.59	0/40758

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	8043	0	7848	421	0
1	B	8043	0	7847	394	0
1	C	8043	0	7849	372	0
2	H	910	0	866	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	910	0	866	29	0
2	J	910	0	866	33	0
3	L	803	0	765	16	0
3	M	803	0	765	17	0
3	N	803	0	765	15	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	K	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	3	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
5	A	154	0	142	8	0
5	B	154	0	142	7	0
5	C	154	0	142	6	0
All	All	30234	0	29313	1174	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 20.

All (1174) 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)
5:C:1410:NAG:O4	5:C:1411:NAG:C1	1.63	1.45
5:B:1410:NAG:O4	5:B:1411:NAG:C1	1.63	1.44
5:A:1410:NAG:O4	5:A:1411:NAG:C1	1.63	1.43
1:A:322:PRO:HB3	1:A:538:CYS:SG	1.63	1.39
1:A:486:VAL:HB	1:B:373:PRO:CB	1.60	1.30
1:A:605:SER:CB	1:A:674:TYR:HE2	1.46	1.27
1:A:486:VAL:CG2	1:B:373:PRO:HA	1.67	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.24	1.20
1:B:986:PRO:HB2	1:B:987:PRO:CD	1.71	1.20
1:C:675:GLN:HB2	1:C:693:ILE:CD1	1.72	1.20
1:B:308:VAL:O	1:B:601:GLY:HA2	1.38	1.19
1:C:328:ARG:NH2	1:C:531:THR:HB	1.55	1.19
1:B:315:THR:CG2	1:B:597:VAL:HG23	1.74	1.17
1:A:294:ASP:HB2	1:A:295:PRO:CD	1.75	1.17
1:B:294:ASP:HB2	1:B:295:PRO:HD2	1.25	1.17
1:C:294:ASP:HB2	1:C:295:PRO:HD2	1.21	1.16
1:B:315:THR:HG21	1:B:597:VAL:CG2	1.77	1.14
1:C:357:ARG:HG3	1:C:396:TYR:HE1	1.12	1.14
1:A:486:VAL:HG23	1:B:373:PRO:HA	1.16	1.13
1:B:326:ILE:HD11	1:B:533:LEU:HD12	1.15	1.13
1:C:530:SER:O	1:C:531:THR:CG2	1.96	1.13
1:A:41:LYS:HB2	1:C:519:HIS:NE2	1.63	1.13
1:B:332:ILE:CG1	1:B:362:VAL:HG11	1.78	1.13
1:A:329:PHE:HE2	1:A:528:LYS:CB	1.59	1.11
1:B:315:THR:HG21	1:B:597:VAL:HG23	1.27	1.11
1:C:675:GLN:HB2	1:C:693:ILE:HD11	1.22	1.11
1:A:295:PRO:HG2	1:A:608:VAL:HG21	1.33	1.10
1:A:313:TYR:O	1:A:596:SER:HB2	1.49	1.10
1:C:328:ARG:HH22	1:C:531:THR:CB	1.66	1.09
1:C:332:ILE:HG23	1:C:333:THR:H	1.15	1.08
1:A:486:VAL:CB	1:B:373:PRO:HB3	1.83	1.08
1:A:605:SER:CB	1:A:674:TYR:CE2	2.36	1.08
1:C:332:ILE:O	1:C:333:THR:HG22	1.54	1.07
1:B:675:GLN:O	1:B:690:GLN:HB2	1.53	1.07
1:A:294:ASP:HB2	1:A:295:PRO:HD2	1.08	1.07
1:A:866:THR:HG21	1:C:646:ARG:NH2	1.68	1.07
1:B:364:ASP:HA	1:B:527:PRO:HD3	1.30	1.07
1:A:309:GLU:N	1:A:309:GLU:OE1	1.87	1.07
1:A:605:SER:HB2	1:A:674:TYR:HE2	1.17	1.06
1:B:332:ILE:HD13	1:B:333:THR:N	1.70	1.06
1:B:294:ASP:HB2	1:B:295:PRO:CD	1.87	1.05
1:A:746:SER:OG	1:A:981:LEU:HD13	1.57	1.05
1:B:521:PRO:HB2	1:C:200:TYR:CE2	1.91	1.05
1:C:530:SER:O	1:C:531:THR:HG22	1.54	1.04
1:A:329:PHE:CE2	1:A:528:LYS:HB3	1.90	1.04
1:A:986:PRO:HG2	1:A:987:PRO:HD3	1.38	1.03
1:B:986:PRO:CB	1:B:987:PRO:HD3	1.89	1.03
1:C:294:ASP:HB2	1:C:295:PRO:CD	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HH22	1:C:531:THR:HB	0.88	1.02
1:B:332:ILE:HG12	1:B:362:VAL:HG11	1.36	1.02
1:A:646:ARG:NH2	1:B:866:THR:HG21	1.74	1.02
1:C:317:ASN:OD1	1:C:318:PHE:N	1.93	1.02
1:C:333:THR:HG21	1:C:361:CYS:HA	1.37	1.02
1:C:357:ARG:HG3	1:C:396:TYR:CE1	1.96	1.01
1:B:1017:GLU:HG2	1:C:1019:ARG:HH22	1.25	1.01
5:C:1410:NAG:C4	5:C:1411:NAG:C1	2.38	1.01
5:A:1410:NAG:C4	5:A:1411:NAG:C1	2.38	1.01
1:B:522:ALA:HB3	1:C:230:PRO:HG3	1.40	1.01
5:B:1410:NAG:C4	5:B:1411:NAG:C1	2.38	1.00
1:A:562:PHE:HD2	1:B:41:LYS:HG2	1.24	1.00
1:A:440:LYS:HE2	2:H:104:ASP:OD1	1.61	1.00
1:B:505:HIS:HD2	2:H:65:GLN:O	1.42	1.00
1:A:1017:GLU:HG2	1:B:1019:ARG:NH2	1.77	1.00
1:B:440:LYS:HE2	2:I:104:ASP:OD1	1.61	1.00
1:A:977:LEU:O	1:A:981:LEU:HD23	1.63	0.99
1:C:440:LYS:HE2	2:J:104:ASP:OD1	1.61	0.99
1:A:562:PHE:CD2	1:B:41:LYS:HG2	1.97	0.99
1:A:329:PHE:HE2	1:A:528:LYS:CG	1.75	0.99
1:A:329:PHE:CD2	1:A:528:LYS:HB3	1.97	0.98
1:A:866:THR:CG2	1:C:646:ARG:NH2	2.27	0.97
1:A:866:THR:CG2	1:C:646:ARG:HH21	1.76	0.97
1:B:1017:GLU:HG2	1:C:1019:ARG:NH2	1.79	0.96
1:A:866:THR:HG22	1:C:646:ARG:HH21	1.31	0.96
1:A:308:VAL:HG12	1:A:313:TYR:CE2	2.01	0.96
1:A:1019:ARG:HH22	1:C:1017:GLU:HG2	1.31	0.96
1:A:977:LEU:C	1:A:981:LEU:HD23	1.87	0.95
1:A:1017:GLU:HG2	1:B:1019:ARG:HH22	1.31	0.95
1:A:413:GLY:HA3	1:C:987:PRO:HG2	1.49	0.94
1:B:326:ILE:CD1	1:B:533:LEU:HD12	1.96	0.94
1:C:335:LEU:O	1:C:336:CYS:SG	2.24	0.94
3:M:17:ARG:HA	3:M:76:ILE:O	1.67	0.94
1:A:329:PHE:CE2	1:A:528:LYS:HB2	2.00	0.94
1:C:312:ILE:HG12	1:C:598:ILE:HG12	1.49	0.94
1:B:743:CYS:O	1:B:977:LEU:HD23	1.67	0.94
1:A:478:LYS:HZ2	1:A:487:ASN:HD22	1.16	0.94
1:B:329:PHE:HD1	1:B:330:PRO:HD3	1.32	0.94
3:L:17:ARG:HA	3:L:76:ILE:O	1.67	0.93
1:B:440:LYS:HE3	1:B:440:LYS:HA	1.50	0.93
3:N:17:ARG:HA	3:N:76:ILE:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HE3	1:A:440:LYS:HA	1.50	0.93
1:B:328:ARG:HG2	1:B:578:ASP:OD1	1.69	0.93
1:B:364:ASP:CA	1:B:527:PRO:HD3	1.99	0.93
1:A:983:ARG:HG3	1:C:390:LEU:CD1	1.99	0.93
1:C:333:THR:CG2	1:C:361:CYS:HA	1.99	0.93
1:C:312:ILE:HG12	1:C:598:ILE:CG1	1.99	0.92
1:C:440:LYS:HE3	1:C:440:LYS:HA	1.50	0.92
1:A:1017:GLU:CG	1:B:1019:ARG:HH22	1.82	0.92
1:B:312:ILE:HG12	1:B:598:ILE:HG12	1.47	0.92
1:B:973:ILE:HG23	1:B:992:GLN:OE1	1.69	0.92
1:A:291:CYS:HG	1:A:301:CYS:HG	1.13	0.92
1:A:605:SER:HB2	1:A:674:TYR:CE2	2.01	0.92
1:A:983:ARG:HG3	1:C:390:LEU:HD11	1.49	0.92
1:B:314:GLN:HE22	1:B:594:GLY:HA3	1.31	0.92
1:A:646:ARG:HH21	1:B:866:THR:CG2	1.82	0.91
1:B:1017:GLU:CG	1:C:1019:ARG:HH22	1.83	0.91
1:B:335:LEU:HD11	1:B:364:ASP:CG	1.89	0.91
1:A:985:ASP:HB2	1:A:987:PRO:HD2	1.51	0.91
1:B:969:LYS:HB3	1:B:974:SER:O	1.71	0.91
1:C:314:GLN:HA	1:C:596:SER:HB3	1.49	0.91
1:C:314:GLN:HE22	1:C:594:GLY:HA3	1.32	0.91
1:B:671:CYS:HB2	1:B:695:TYR:CE2	2.06	0.90
1:C:675:GLN:CB	1:C:693:ILE:HD11	2.01	0.90
1:C:332:ILE:HD13	1:C:333:THR:N	1.87	0.90
1:B:328:ARG:HG2	1:B:328:ARG:HH21	1.37	0.90
1:A:319:ARG:NH1	1:A:321:GLN:CG	2.35	0.90
1:A:562:PHE:HD2	1:B:41:LYS:CG	1.85	0.90
1:C:333:THR:HG21	1:C:361:CYS:CA	2.02	0.90
1:C:109:THR:HA	1:C:237:ARG:HH21	1.37	0.90
1:A:529:LYS:HD2	1:A:529:LYS:N	1.85	0.90
1:C:332:ILE:HD13	1:C:333:THR:O	1.71	0.89
1:B:324:GLU:HG3	1:B:539:VAL:HG12	1.53	0.89
1:B:986:PRO:HB2	1:B:987:PRO:HD3	0.93	0.89
1:C:294:ASP:CB	1:C:295:PRO:HD2	2.02	0.89
1:A:486:VAL:HB	1:B:373:PRO:HB3	0.89	0.89
1:B:675:GLN:O	1:B:690:GLN:CB	2.21	0.89
1:B:364:ASP:HA	1:B:527:PRO:CD	2.02	0.88
1:B:671:CYS:HB2	1:B:695:TYR:HE2	1.37	0.88
1:A:109:THR:HA	1:A:237:ARG:HH21	1.37	0.88
1:C:530:SER:O	1:C:531:THR:HG23	1.73	0.88
1:B:363:ALA:O	1:B:526:GLY:HA2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH21	1:B:230:PRO:CB	1.85	0.88
1:B:325:SER:O	1:B:327:VAL:HG23	1.74	0.88
1:A:995:ARG:HG3	1:A:995:ARG:HH11	1.36	0.88
1:A:1019:ARG:NH2	1:C:1017:GLU:HG2	1.88	0.88
1:A:965:GLN:NE2	1:B:762:GLN:HE22	1.70	0.88
1:C:323:THR:HG22	1:C:324:GLU:CD	1.93	0.88
1:A:41:LYS:HB2	1:C:519:HIS:CE1	2.09	0.88
1:A:530:SER:O	1:A:531:THR:OG1	1.91	0.88
1:B:109:THR:HA	1:B:237:ARG:HH21	1.37	0.88
1:A:322:PRO:CB	1:A:538:CYS:SG	2.58	0.88
1:B:505:HIS:CD2	2:H:65:GLN:O	2.26	0.87
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.55	0.87
1:B:319:ARG:HG3	1:B:319:ARG:HH21	1.38	0.87
1:C:289:VAL:HG12	1:C:301:CYS:SG	2.15	0.86
1:B:522:ALA:HB2	1:C:200:TYR:OH	1.73	0.86
1:A:363:ALA:HB3	1:A:525:CYS:O	1.75	0.86
1:C:675:GLN:CB	1:C:693:ILE:CD1	2.52	0.85
1:B:985:ASP:HB3	1:B:986:PRO:HD2	1.57	0.85
1:B:663:ASP:OD2	1:B:673:SER:HB3	1.75	0.85
1:B:328:ARG:NH2	1:B:533:LEU:HB2	1.89	0.85
1:A:866:THR:HG21	1:C:646:ARG:HH22	1.37	0.85
1:A:486:VAL:HB	1:B:373:PRO:CA	2.05	0.85
1:B:335:LEU:HD21	1:B:364:ASP:OD2	1.75	0.85
1:A:519:HIS:CE1	1:B:41:LYS:O	2.29	0.84
1:B:521:PRO:CB	1:C:200:TYR:CE2	2.58	0.84
1:B:315:THR:HG23	1:B:597:VAL:HG23	1.57	0.84
1:C:675:GLN:HB2	1:C:693:ILE:CG1	2.06	0.84
1:B:528:LYS:HA	1:B:528:LYS:NZ	1.93	0.84
1:C:289:VAL:HG13	1:C:297:SER:HB3	1.58	0.83
1:C:440:LYS:HA	1:C:440:LYS:CE	2.08	0.83
1:B:328:ARG:HH22	1:B:533:LEU:HD22	1.43	0.83
1:A:319:ARG:HH11	1:A:321:GLN:CB	1.91	0.82
1:A:324:GLU:HB2	1:A:539:VAL:HG12	1.60	0.82
1:A:332:ILE:HD12	1:A:332:ILE:O	1.78	0.82
1:B:985:ASP:HB3	1:B:986:PRO:CD	2.08	0.82
1:A:1017:GLU:CD	1:B:1019:ARG:HH22	1.81	0.82
1:A:1019:ARG:HH22	1:C:1017:GLU:CG	1.91	0.82
1:C:326:ILE:HG21	1:C:533:LEU:HA	1.62	0.82
1:A:978:ASN:HA	1:A:981:LEU:CD2	2.08	0.82
1:C:530:SER:C	1:C:531:THR:HG23	2.00	0.82
1:A:440:LYS:HA	1:A:440:LYS:CE	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:O	1:B:362:VAL:HG12	1.80	0.82
1:C:533:LEU:HD13	1:C:533:LEU:O	1.80	0.82
1:C:326:ILE:HG22	1:C:532:ASN:O	1.80	0.82
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.10	0.82
1:C:329:PHE:CB	1:C:330:PRO:CD	2.57	0.82
2:I:3:GLN:HB3	2:I:25:SER:O	1.80	0.82
1:C:663:ASP:OD2	1:C:673:SER:HB3	1.80	0.82
1:A:663:ASP:OD2	1:A:673:SER:HB3	1.80	0.81
1:A:308:VAL:HG23	1:A:602:THR:OG1	1.79	0.81
2:H:3:GLN:HB3	2:H:25:SER:O	1.80	0.81
2:J:3:GLN:HB3	2:J:25:SER:O	1.80	0.81
1:A:986:PRO:CG	1:A:987:PRO:HD3	2.09	0.81
1:A:674:TYR:CE1	1:A:691:SER:O	2.34	0.81
1:B:294:ASP:CB	1:B:295:PRO:HD2	2.09	0.81
1:C:308:VAL:O	1:C:601:GLY:HA2	1.81	0.81
1:A:519:HIS:NE2	1:B:41:LYS:HB2	1.94	0.80
1:B:332:ILE:CD1	1:B:333:THR:N	2.44	0.80
1:B:440:LYS:HA	1:B:440:LYS:CE	2.08	0.80
1:C:308:VAL:CG1	1:C:313:TYR:CE2	2.63	0.80
1:A:486:VAL:CG2	1:B:373:PRO:CA	2.57	0.80
1:B:294:ASP:CB	1:B:295:PRO:CD	2.59	0.80
1:B:308:VAL:O	1:B:601:GLY:CA	2.24	0.80
1:B:965:GLN:NE2	1:C:762:GLN:HE22	1.79	0.80
1:C:308:VAL:HG11	1:C:599:THR:HG21	1.63	0.80
1:C:332:ILE:HG23	1:C:333:THR:N	1.94	0.80
1:A:603:ASN:O	1:A:604:THR:OG1	1.99	0.80
1:A:977:LEU:C	1:A:981:LEU:CD2	2.51	0.80
1:A:314:GLN:HA	1:A:596:SER:CB	2.13	0.79
1:A:319:ARG:NH1	1:A:321:GLN:HG3	1.96	0.79
1:A:329:PHE:HE2	1:A:528:LYS:CD	1.95	0.79
1:C:357:ARG:CG	1:C:396:TYR:HE1	1.92	0.79
1:C:527:PRO:O	1:C:529:LYS:HD2	1.82	0.79
1:C:365:TYR:HA	1:C:368:LEU:HD23	1.64	0.79
1:B:504:GLY:HA3	2:H:65:GLN:NE2	1.98	0.79
1:B:315:THR:HG21	1:B:597:VAL:HG21	1.65	0.79
1:A:390:LEU:HD21	1:B:983:ARG:HG2	1.65	0.78
1:A:319:ARG:NH1	1:A:321:GLN:CB	2.47	0.78
1:A:365:TYR:HA	1:A:368:LEU:HD23	1.65	0.78
1:A:977:LEU:HD23	1:A:981:LEU:HD22	1.66	0.78
1:C:314:GLN:HA	1:C:596:SER:CB	2.13	0.78
1:A:486:VAL:CB	1:B:373:PRO:HA	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ILE:CG1	1:C:598:ILE:HG12	2.12	0.78
1:B:528:LYS:HA	1:B:528:LYS:HZ3	1.46	0.78
1:C:332:ILE:O	1:C:333:THR:CG2	2.32	0.78
1:A:313:TYR:O	1:A:596:SER:CB	2.32	0.77
1:A:46:SER:HA	1:A:279:TYR:O	1.85	0.77
1:A:978:ASN:O	1:A:982:SER:HB3	1.82	0.77
1:A:605:SER:OG	1:A:674:TYR:CE2	2.36	0.77
1:C:315:THR:H	1:C:596:SER:HA	1.49	0.77
1:A:486:VAL:CB	1:B:373:PRO:CB	2.54	0.77
1:B:365:TYR:HA	1:B:368:LEU:HD23	1.64	0.77
1:B:521:PRO:HG2	1:C:200:TYR:CZ	2.19	0.77
1:A:478:LYS:HZ2	1:A:487:ASN:ND2	1.83	0.77
1:A:529:LYS:HD2	1:A:529:LYS:H	1.48	0.77
1:A:41:LYS:O	1:C:519:HIS:CE1	2.38	0.76
1:A:605:SER:OG	1:A:674:TYR:HE2	1.67	0.76
1:C:46:SER:HA	1:C:279:TYR:O	1.85	0.76
1:C:521:PRO:HB3	1:C:564:GLN:HG3	1.66	0.76
1:A:983:ARG:CG	1:C:390:LEU:HD11	2.15	0.76
1:A:478:LYS:NZ	1:A:487:ASN:ND2	2.34	0.76
1:B:365:TYR:HB3	1:B:368:LEU:HD21	1.68	0.76
1:B:388:ASN:OD1	1:B:526:GLY:HA3	1.85	0.76
1:B:326:ILE:HD11	1:B:533:LEU:CD1	2.08	0.76
1:A:413:GLY:HA3	1:C:987:PRO:CG	2.14	0.76
1:B:46:SER:HA	1:B:279:TYR:O	1.85	0.76
1:C:388:ASN:HD21	1:C:527:PRO:HD2	1.51	0.76
1:A:563:GLN:HG2	1:B:41:LYS:C	2.06	0.76
1:B:328:ARG:NH2	1:B:533:LEU:CB	2.49	0.76
1:C:365:TYR:HB3	1:C:368:LEU:HD21	1.68	0.76
1:A:308:VAL:CG1	1:A:313:TYR:CE2	2.69	0.75
1:B:979:ASP:O	1:B:983:ARG:HG3	1.85	0.75
1:A:357:ARG:NH2	1:B:230:PRO:CB	2.50	0.75
1:B:364:ASP:HB3	1:B:527:PRO:CG	2.16	0.75
1:A:308:VAL:O	1:A:601:GLY:HA2	1.86	0.75
1:B:328:ARG:HG2	1:B:328:ARG:NH2	2.00	0.74
1:C:308:VAL:CG1	1:C:599:THR:HG21	2.17	0.74
1:C:329:PHE:CG	1:C:330:PRO:CD	2.71	0.74
1:B:334:ASN:OD1	1:B:361:CYS:HB2	1.87	0.74
1:A:41:LYS:O	1:C:519:HIS:HE1	1.68	0.74
1:A:918:GLU:HG2	1:C:1128:VAL:CG2	2.18	0.74
1:B:315:THR:CG2	1:B:597:VAL:CG2	2.48	0.74
1:A:478:LYS:NZ	1:A:487:ASN:HD22	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:SER:OG	1:B:980:ILE:CD1	2.36	0.74
1:B:985:ASP:CB	1:B:986:PRO:CD	2.63	0.73
1:C:308:VAL:HG12	1:C:313:TYR:CE2	2.23	0.73
1:A:978:ASN:N	1:A:981:LEU:HD21	2.04	0.73
1:C:329:PHE:CG	1:C:330:PRO:HD3	2.23	0.73
1:B:743:CYS:O	1:B:977:LEU:CD2	2.36	0.73
1:C:334:ASN:O	1:C:335:LEU:HG	1.88	0.73
1:A:365:TYR:HB3	1:A:368:LEU:HD21	1.68	0.73
1:A:329:PHE:CE2	1:A:528:LYS:CD	2.71	0.73
1:A:965:GLN:HE21	1:B:762:GLN:HE22	1.35	0.73
1:B:329:PHE:CD1	1:B:330:PRO:HD3	2.20	0.73
1:A:314:GLN:HA	1:A:596:SER:HB3	1.70	0.73
1:A:691:SER:C	1:A:692:ILE:HG22	2.09	0.73
1:B:522:ALA:HB3	1:C:230:PRO:CG	2.17	0.73
1:B:530:SER:O	1:B:531:THR:HG23	1.89	0.73
1:B:605:SER:HB2	1:B:674:TYR:CE2	2.23	0.73
1:A:316:SER:OG	1:A:317:ASN:N	2.19	0.73
1:A:476:GLY:HA3	1:A:487:ASN:HB3	1.69	0.72
1:C:326:ILE:CD1	1:C:541:PHE:HA	2.19	0.72
1:C:530:SER:C	1:C:531:THR:CG2	2.53	0.72
1:A:289:VAL:HG13	1:A:297:SER:HB3	1.71	0.72
1:B:318:PHE:CE1	1:B:615:VAL:HG21	2.24	0.72
1:C:295:PRO:HG2	1:C:608:VAL:HG21	1.70	0.72
1:C:308:VAL:HG12	1:C:313:TYR:HE2	1.55	0.72
1:C:323:THR:CG2	1:C:324:GLU:CD	2.58	0.72
1:A:486:VAL:CB	1:B:373:PRO:CA	2.67	0.71
1:A:978:ASN:OD1	1:A:979:ASP:N	2.23	0.71
1:B:502:GLY:HA3	2:H:66:GLY:O	1.89	0.71
1:A:357:ARG:HH21	1:B:230:PRO:HB3	1.54	0.71
1:A:866:THR:CG2	1:C:668:ALA:O	2.37	0.71
1:C:319:ARG:O	1:C:319:ARG:HG3	1.91	0.71
3:L:87:TYR:O	3:L:104:GLY:HA2	1.90	0.71
5:C:1410:NAG:H4	5:C:1411:NAG:C1	2.21	0.71
1:C:332:ILE:CG2	1:C:333:THR:H	1.99	0.71
3:M:87:TYR:O	3:M:104:GLY:HA2	1.90	0.71
1:B:363:ALA:N	1:B:525:CYS:O	2.21	0.71
1:B:521:PRO:CG	1:C:200:TYR:CE2	2.73	0.71
1:A:422:ASN:HD21	1:A:454:ARG:H	1.37	0.71
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.21	0.71
1:A:294:ASP:CB	1:A:295:PRO:CD	2.56	0.71
1:A:985:ASP:OD2	1:A:985:ASP:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG13	1:B:362:VAL:HG11	1.70	0.70
1:B:1017:GLU:CD	1:C:1019:ARG:HH22	1.93	0.70
1:C:326:ILE:H	1:C:326:ILE:HD12	1.56	0.70
1:A:478:LYS:NZ	1:A:486:VAL:HG13	2.06	0.70
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.27	0.70
3:N:87:TYR:O	3:N:104:GLY:HA2	1.90	0.70
1:A:319:ARG:NH1	1:A:321:GLN:HB3	2.06	0.70
1:B:323:THR:C	1:B:324:GLU:HG2	2.11	0.70
5:B:1410:NAG:H4	5:B:1411:NAG:C1	2.21	0.70
1:A:746:SER:OG	1:A:981:LEU:CD1	2.39	0.70
1:B:582:LEU:CD1	4:P:1:NAG:H83	2.21	0.70
5:A:1410:NAG:H4	5:A:1411:NAG:C1	2.20	0.70
1:B:335:LEU:HD11	1:B:364:ASP:OD1	1.91	0.70
1:A:864:LEU:HD13	1:C:665:PRO:HB2	1.72	0.70
1:B:422:ASN:HD21	1:B:454:ARG:H	1.37	0.70
1:A:324:GLU:CB	1:A:539:VAL:HG12	2.20	0.70
1:B:319:ARG:HG3	1:B:319:ARG:NH2	2.00	0.69
1:C:422:ASN:HD21	1:C:454:ARG:H	1.37	0.69
1:A:295:PRO:HG2	1:A:608:VAL:CG2	2.16	0.69
1:C:314:GLN:NE2	1:C:594:GLY:HA3	2.05	0.69
1:B:604:THR:O	1:B:605:SER:HB2	1.91	0.69
1:B:671:CYS:O	1:B:694:ALA:HA	1.92	0.69
1:B:691:SER:OG	1:B:692:ILE:N	2.23	0.69
1:A:985:ASP:HB2	1:A:986:PRO:HD2	1.74	0.69
1:A:319:ARG:HH11	1:A:321:GLN:HB3	1.55	0.69
1:A:365:TYR:CA	1:A:368:LEU:HD23	2.23	0.69
1:A:978:ASN:HA	1:A:981:LEU:HD21	1.72	0.69
1:A:41:LYS:HG2	1:C:562:PHE:HD2	1.57	0.69
1:B:333:THR:OG1	1:B:334:ASN:N	2.19	0.69
1:B:365:TYR:CA	1:B:368:LEU:HD23	2.23	0.69
1:C:674:TYR:CE2	1:C:690:GLN:N	2.61	0.69
1:A:335:LEU:HD21	1:A:364:ASP:OD1	1.92	0.68
1:A:646:ARG:NH2	1:B:866:THR:CG2	2.43	0.68
1:B:332:ILE:HD13	1:B:333:THR:CA	2.23	0.68
1:C:674:TYR:CD2	1:C:690:GLN:N	2.61	0.68
1:A:984:LEU:HD12	1:A:988:GLU:HB3	1.76	0.68
1:B:335:LEU:CD2	1:B:364:ASP:OD2	2.40	0.68
1:C:328:ARG:NH2	1:C:328:ARG:HG2	2.08	0.68
1:A:521:PRO:HB3	1:A:564:GLN:HG3	1.75	0.68
1:C:313:TYR:O	1:C:315:THR:N	2.25	0.68
1:A:604:THR:O	1:A:605:SER:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:GLN:HA	1:A:992:GLN:NE2	2.06	0.68
1:B:560:LEU:O	1:B:562:PHE:N	2.27	0.68
1:C:332:ILE:CD1	1:C:333:THR:N	2.56	0.68
1:A:328:ARG:NH2	1:A:580:GLN:OE1	2.26	0.68
1:B:335:LEU:HD12	1:B:362:VAL:O	1.94	0.68
1:B:295:PRO:HG2	1:B:608:VAL:HG21	1.76	0.67
1:C:332:ILE:CD1	1:C:333:THR:O	2.41	0.67
1:C:365:TYR:CA	1:C:368:LEU:HD23	2.23	0.67
1:A:41:LYS:HG2	1:C:562:PHE:CD2	2.30	0.67
1:A:473:TYR:O	1:A:488:CYS:HA	1.95	0.67
1:A:560:LEU:O	1:A:562:PHE:N	2.27	0.67
1:B:364:ASP:HB3	1:B:527:PRO:HG2	1.76	0.67
1:C:315:THR:HG21	1:C:597:VAL:HG23	1.77	0.67
1:A:978:ASN:N	1:A:981:LEU:CD2	2.57	0.67
1:C:560:LEU:O	1:C:562:PHE:N	2.26	0.67
1:A:329:PHE:CE2	1:A:528:LYS:CG	2.67	0.67
1:A:995:ARG:HG3	1:A:995:ARG:NH1	2.04	0.67
1:A:530:SER:OG	1:A:531:THR:N	2.21	0.67
1:B:973:ILE:HD12	1:B:983:ARG:NH2	2.10	0.67
1:B:974:SER:OG	1:B:980:ILE:HD13	1.94	0.67
1:C:326:ILE:HD12	1:C:326:ILE:N	2.09	0.66
3:L:6:GLN:NE2	3:L:89:CYS:SG	2.69	0.66
3:N:6:GLN:NE2	3:N:89:CYS:SG	2.69	0.66
1:A:918:GLU:HG2	1:C:1128:VAL:HG23	1.77	0.66
1:B:672:ALA:HA	1:B:693:ILE:O	1.95	0.66
1:B:328:ARG:CG	1:B:578:ASP:OD1	2.44	0.66
1:C:300:LYS:CE	1:C:602:THR:HG21	2.25	0.66
1:C:365:TYR:CB	1:C:368:LEU:HD21	2.25	0.66
3:M:6:GLN:NE2	3:M:89:CYS:SG	2.69	0.66
1:B:314:GLN:HE22	1:B:594:GLY:CA	2.07	0.66
1:A:521:PRO:O	1:A:544:ASN:CG	2.34	0.66
1:C:289:VAL:CG1	1:C:301:CYS:SG	2.83	0.66
1:C:335:LEU:O	1:C:336:CYS:O	2.14	0.66
1:B:314:GLN:HA	1:B:596:SER:CB	2.26	0.66
1:B:365:TYR:CB	1:B:368:LEU:HD21	2.25	0.66
1:A:365:TYR:CB	1:A:368:LEU:HD21	2.25	0.66
1:A:563:GLN:HG2	1:B:42:VAL:N	2.11	0.66
1:A:646:ARG:HH21	1:B:866:THR:HG22	1.59	0.65
1:A:478:LYS:CE	1:A:486:VAL:HG13	2.26	0.65
1:A:986:PRO:CD	1:A:987:PRO:HD2	2.26	0.65
1:B:318:PHE:HE1	1:B:615:VAL:HG21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:103:PHE:HD1	2:I:104:ASP:OD1	1.80	0.65
1:A:978:ASN:ND2	1:C:547:THR:OG1	2.29	0.65
1:B:984:LEU:CD1	1:B:988:GLU:HG3	2.26	0.65
2:H:103:PHE:HD1	2:H:104:ASP:OD1	1.80	0.65
2:J:103:PHE:HD1	2:J:104:ASP:OD1	1.80	0.65
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.69	0.65
1:B:332:ILE:HD13	1:B:332:ILE:C	2.16	0.65
1:A:978:ASN:CA	1:A:981:LEU:CD2	2.75	0.65
1:B:976:VAL:O	1:B:978:ASN:N	2.30	0.65
1:C:864:LEU:O	1:C:864:LEU:HD12	1.97	0.65
1:A:691:SER:O	1:A:692:ILE:CB	2.45	0.64
1:B:582:LEU:HD11	4:P:1:NAG:C8	2.27	0.64
1:A:986:PRO:CD	1:A:987:PRO:CD	2.75	0.64
1:A:144:TYR:HB3	1:A:153:MET:HB3	1.79	0.64
1:C:332:ILE:HD13	1:C:332:ILE:C	2.16	0.64
1:C:144:TYR:HB3	1:C:153:MET:HB3	1.79	0.64
1:A:977:LEU:HD23	1:A:981:LEU:CD2	2.28	0.64
1:C:308:VAL:CG1	1:C:599:THR:CG2	2.76	0.64
1:A:489:TYR:OH	1:B:375:PHE:HA	1.98	0.64
1:C:323:THR:CG2	1:C:324:GLU:OE2	2.46	0.64
1:C:367:VAL:O	1:C:368:LEU:HD23	1.99	0.64
1:B:144:TYR:HB3	1:B:153:MET:HB3	1.79	0.63
1:C:391:CYS:SG	1:C:525:CYS:HB3	2.38	0.63
1:C:675:GLN:HB2	1:C:693:ILE:HG12	1.78	0.63
1:B:314:GLN:HA	1:B:596:SER:HA	1.79	0.63
1:A:474:GLN:HG3	1:A:488:CYS:HB3	1.81	0.63
1:A:691:SER:O	1:A:692:ILE:HB	1.97	0.63
1:B:296:LEU:HD13	1:B:608:VAL:HG11	1.81	0.63
1:C:328:ARG:HG2	1:C:328:ARG:HH21	1.63	0.63
1:C:799:GLY:O	1:C:800:PHE:C	2.37	0.63
1:A:799:GLY:O	1:A:800:PHE:C	2.37	0.63
1:A:390:LEU:HD11	1:B:983:ARG:HB3	1.81	0.63
1:C:200:TYR:HD1	1:C:229:LEU:O	1.81	0.63
1:C:332:ILE:HD13	1:C:333:THR:C	2.19	0.63
1:A:977:LEU:CD2	1:A:981:LEU:HD22	2.28	0.63
1:A:978:ASN:CA	1:A:981:LEU:HD21	2.29	0.63
1:B:367:VAL:O	1:B:368:LEU:HD23	1.99	0.63
1:C:315:THR:HG21	1:C:597:VAL:CG2	2.29	0.63
1:C:391:CYS:SG	1:C:525:CYS:CB	2.87	0.63
1:A:318:PHE:HE1	1:A:615:VAL:HG21	1.63	0.62
1:A:332:ILE:HD12	1:A:332:ILE:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:O	1:A:368:LEU:HD23	1.99	0.62
1:B:799:GLY:O	1:B:800:PHE:C	2.37	0.62
1:A:329:PHE:HD2	1:A:528:LYS:HB3	1.62	0.62
1:B:986:PRO:CB	1:B:987:PRO:CD	2.55	0.62
1:C:529:LYS:O	1:C:529:LYS:HD3	1.99	0.62
1:B:695:TYR:HD2	1:B:695:TYR:O	1.83	0.62
1:A:312:ILE:HG23	1:A:312:ILE:O	2.00	0.62
1:A:1019:ARG:HH22	1:C:1017:GLU:CD	2.03	0.62
1:A:984:LEU:CD1	1:A:988:GLU:HB3	2.30	0.61
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.33	0.61
1:B:315:THR:H	1:B:596:SER:HA	1.63	0.61
1:A:318:PHE:CE1	1:A:615:VAL:HG21	2.35	0.61
1:A:527:PRO:O	1:A:529:LYS:NZ	2.33	0.61
1:B:326:ILE:HG23	1:B:326:ILE:O	2.00	0.61
1:A:978:ASN:HA	1:A:981:LEU:CG	2.31	0.61
1:A:329:PHE:CE2	1:A:528:LYS:HD3	2.35	0.61
1:A:368:LEU:HD12	1:A:368:LEU:O	2.01	0.61
1:A:519:HIS:CD2	1:B:41:LYS:HB2	2.35	0.61
1:B:335:LEU:CD1	1:B:364:ASP:CG	2.66	0.61
1:B:522:ALA:CB	1:C:230:PRO:HG3	2.22	0.61
1:C:318:PHE:O	1:C:319:ARG:HB3	1.99	0.61
1:A:295:PRO:CG	1:A:608:VAL:HG21	2.21	0.61
1:A:413:GLY:CA	1:C:987:PRO:HG2	2.29	0.61
1:A:692:ILE:HG23	1:A:692:ILE:O	2.00	0.61
1:A:986:PRO:N	1:A:987:PRO:CD	2.64	0.61
1:B:368:LEU:HD12	1:B:368:LEU:O	2.01	0.61
1:C:330:PRO:HG2	1:C:525:CYS:SG	2.41	0.61
1:C:368:LEU:HD12	1:C:368:LEU:O	2.01	0.61
1:A:986:PRO:N	1:A:987:PRO:HD2	2.15	0.60
1:B:974:SER:OG	1:B:980:ILE:HD11	2.00	0.60
1:A:357:ARG:NH2	1:B:230:PRO:CA	2.63	0.60
1:B:985:ASP:CB	1:B:986:PRO:HD2	2.27	0.60
1:B:327:VAL:HG12	1:B:327:VAL:O	2.01	0.60
1:B:675:GLN:OE1	1:B:675:GLN:HA	2.00	0.60
1:A:706:ALA:CB	5:A:1410:NAG:H5	2.32	0.60
1:A:978:ASN:HA	1:A:981:LEU:HG	1.82	0.60
1:A:598:ILE:HG22	1:A:598:ILE:O	2.01	0.60
1:B:668:ALA:H	1:C:864:LEU:HA	1.65	0.60
1:A:971:GLY:O	1:A:995:ARG:CD	2.50	0.60
1:B:325:SER:O	1:B:326:ILE:C	2.39	0.60
1:C:316:SER:OG	1:C:317:ASN:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:GLN:HA	1:C:321:GLN:OE1	2.01	0.60
1:A:918:GLU:HG2	1:C:1128:VAL:HG21	1.83	0.60
1:B:1128:VAL:CG2	1:C:918:GLU:HG2	2.32	0.60
1:C:706:ALA:CB	5:C:1410:NAG:H5	2.32	0.60
1:A:746:SER:HB3	1:A:977:LEU:CD2	2.32	0.59
1:B:335:LEU:CD1	1:B:364:ASP:OD1	2.49	0.59
1:B:977:LEU:CD2	1:B:1000:ARG:HH12	2.15	0.59
1:B:582:LEU:HD11	4:P:1:NAG:H83	1.82	0.59
1:C:328:ARG:HH21	1:C:328:ARG:CG	2.15	0.59
1:B:706:ALA:CB	5:B:1410:NAG:H5	2.32	0.59
1:A:973:ILE:HG23	1:A:992:GLN:OE1	2.03	0.59
1:A:983:ARG:HG3	1:C:390:LEU:CD2	2.33	0.59
1:A:790:LYS:CE	1:C:702:GLU:OE2	2.51	0.59
1:B:969:LYS:CE	1:B:974:SER:O	2.51	0.59
1:C:48:LEU:HD21	1:C:306:PHE:CE1	2.38	0.59
1:C:312:ILE:HG12	1:C:598:ILE:CD1	2.31	0.59
1:C:332:ILE:HD13	1:C:333:THR:CA	2.32	0.59
1:A:312:ILE:HG13	1:A:598:ILE:HG12	1.84	0.59
1:A:646:ARG:HH22	1:B:866:THR:HG21	1.66	0.59
1:A:41:LYS:HD2	1:C:519:HIS:CD2	2.38	0.58
1:A:669:GLY:N	1:B:864:LEU:O	2.36	0.58
1:C:328:ARG:HH22	1:C:531:THR:CG2	2.15	0.58
1:A:308:VAL:HG12	1:A:313:TYR:CZ	2.36	0.58
1:B:328:ARG:HH22	1:B:533:LEU:CD2	2.16	0.58
1:B:969:LYS:HE2	1:B:974:SER:O	2.02	0.58
1:B:521:PRO:HB2	1:C:200:TYR:HE2	1.59	0.58
1:B:521:PRO:HG2	1:C:200:TYR:CE1	2.38	0.58
1:A:289:VAL:HG12	1:A:301:CYS:SG	2.43	0.58
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.37	0.58
1:B:965:GLN:HE21	1:C:762:GLN:HE22	1.52	0.58
1:A:357:ARG:HH22	1:B:230:PRO:HA	1.68	0.58
1:A:592:PHE:CZ	1:B:740:MET:SD	2.97	0.58
1:C:676:THR:HA	1:C:690:GLN:CB	2.33	0.58
2:H:113:GLN:NE2	2:H:114:GLY:O	2.37	0.58
2:I:27:ASP:OD1	2:I:98:ARG:NH2	2.37	0.58
1:B:980:ILE:O	1:B:982:SER:N	2.36	0.58
2:J:27:ASP:OD1	2:J:98:ARG:NH2	2.37	0.58
1:B:431:GLY:HA3	1:B:513:LEU:O	2.04	0.57
1:A:521:PRO:O	1:A:544:ASN:OD1	2.23	0.57
1:A:988:GLU:O	1:A:991:VAL:HG23	2.03	0.57
1:B:322:PRO:HB2	1:B:540:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HB2	1:C:540:ASN:ND2	2.19	0.57
1:A:109:THR:HA	1:A:237:ARG:NH2	2.15	0.57
1:A:431:GLY:HA3	1:A:513:LEU:O	2.05	0.57
1:A:971:GLY:O	1:A:995:ARG:HD3	2.04	0.57
1:B:604:THR:O	1:B:604:THR:HG22	2.03	0.57
1:C:109:THR:HA	1:C:237:ARG:NH2	2.15	0.57
2:H:27:ASP:OD1	2:H:98:ARG:NH2	2.37	0.57
1:A:41:LYS:CG	1:C:562:PHE:HD2	2.17	0.57
1:C:431:GLY:HA3	1:C:513:LEU:O	2.04	0.57
1:B:332:ILE:CG1	1:B:333:THR:N	2.67	0.57
1:B:604:THR:HG22	1:B:674:TYR:CD2	2.40	0.57
1:A:986:PRO:HD2	1:A:987:PRO:HD2	1.85	0.57
2:I:113:GLN:NE2	2:I:114:GLY:O	2.37	0.57
1:A:331:ASN:O	1:A:332:ILE:HG23	2.05	0.57
1:C:291:CYS:SG	1:C:301:CYS:CB	2.92	0.57
1:C:357:ARG:CG	1:C:396:TYR:CE1	2.78	0.57
1:A:746:SER:CB	1:A:977:LEU:HD23	2.35	0.57
1:B:333:THR:O	1:B:335:LEU:N	2.37	0.57
1:C:294:ASP:CB	1:C:295:PRO:CD	2.55	0.57
1:C:329:PHE:CD1	1:C:330:PRO:HD3	2.40	0.57
1:B:984:LEU:HD12	1:B:988:GLU:HG3	1.87	0.56
1:C:388:ASN:ND2	1:C:527:PRO:HD2	2.17	0.56
1:C:388:ASN:OD1	1:C:526:GLY:HA3	2.05	0.56
3:L:34:ILE:H	3:L:52:ASN:HD21	1.54	0.56
3:N:34:ILE:H	3:N:52:ASN:HD21	1.53	0.56
1:A:985:ASP:CB	1:A:986:PRO:HD2	2.35	0.56
1:B:985:ASP:OD1	1:B:986:PRO:HD3	2.05	0.56
1:C:276:LEU:HD22	1:C:301:CYS:HA	1.87	0.56
1:C:326:ILE:CG2	1:C:533:LEU:HA	2.35	0.56
1:C:365:TYR:HA	1:C:368:LEU:CD2	2.34	0.56
2:J:113:GLN:NE2	2:J:114:GLY:O	2.37	0.56
1:A:763:LEU:HD23	1:A:1008:VAL:HG11	1.87	0.56
1:B:365:TYR:HA	1:B:368:LEU:CD2	2.34	0.56
1:C:309:GLU:HG2	1:C:313:TYR:OH	2.05	0.56
1:C:333:THR:CG2	1:C:361:CYS:CA	2.73	0.56
1:A:770:ILE:O	1:A:770:ILE:HG22	2.06	0.56
1:A:770:ILE:O	1:A:774:GLN:HG2	2.06	0.56
1:B:522:ALA:HB2	1:C:200:TYR:HH	1.70	0.56
1:C:308:VAL:HG11	1:C:599:THR:CG2	2.35	0.56
1:A:763:LEU:HD11	1:A:1005:GLN:HE21	1.69	0.56
1:C:323:THR:HG22	1:C:324:GLU:OE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:C	1:C:336:CYS:SG	2.83	0.56
1:A:531:THR:HG22	1:A:532:ASN:N	2.20	0.56
1:A:656:VAL:CG2	1:A:695:TYR:HB3	2.36	0.56
1:B:655:TYR:HA	1:B:694:ALA:O	2.05	0.56
3:L:55:ARG:NH2	3:L:61:ASP:OD1	2.39	0.56
3:M:55:ARG:NH2	3:M:61:ASP:OD1	2.39	0.56
1:A:866:THR:HG23	1:C:668:ALA:O	2.05	0.56
1:B:521:PRO:CG	1:C:200:TYR:CZ	2.89	0.56
1:A:602:THR:O	1:A:602:THR:HG22	2.05	0.55
1:C:308:VAL:O	1:C:601:GLY:CA	2.53	0.55
1:C:526:GLY:C	1:C:528:LYS:H	2.10	0.55
1:C:690:GLN:O	1:C:691:SER:HB2	2.06	0.55
1:B:315:THR:OG1	1:B:316:SER:N	2.38	0.55
1:A:365:TYR:HA	1:A:368:LEU:CD2	2.35	0.55
3:N:55:ARG:NH2	3:N:61:ASP:OD1	2.39	0.55
1:B:984:LEU:HD12	1:B:988:GLU:CG	2.36	0.55
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.42	0.55
1:B:109:THR:HA	1:B:237:ARG:NH2	2.15	0.55
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.88	0.55
1:C:314:GLN:O	1:C:314:GLN:HG3	2.05	0.55
1:C:315:THR:CG2	1:C:597:VAL:HG23	2.37	0.55
1:A:367:VAL:HG12	1:A:368:LEU:N	2.22	0.55
1:A:983:ARG:HG2	1:A:983:ARG:O	2.07	0.55
1:A:986:PRO:CG	1:A:987:PRO:CD	2.82	0.55
1:B:363:ALA:HB3	1:B:525:CYS:O	2.07	0.55
1:B:993:ILE:HG22	1:B:997:ILE:CD1	2.37	0.55
1:A:357:ARG:NH2	1:B:230:PRO:HA	2.22	0.55
1:A:308:VAL:HG12	1:A:313:TYR:HE2	1.66	0.54
1:B:335:LEU:HD13	1:B:362:VAL:HG13	1.87	0.54
1:B:646:ARG:HH21	1:C:866:THR:HG23	1.72	0.54
1:B:329:PHE:HD1	1:B:330:PRO:CD	2.13	0.54
3:M:24:GLY:H	3:M:29:ILE:HG21	1.72	0.54
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.41	0.54
3:M:34:ILE:H	3:M:52:ASN:HD21	1.53	0.54
1:B:314:GLN:HA	1:B:596:SER:CA	2.38	0.54
1:B:365:TYR:CB	1:B:368:LEU:CD2	2.85	0.54
1:B:690:GLN:O	1:B:690:GLN:HG3	2.07	0.54
1:C:521:PRO:HB3	1:C:564:GLN:CG	2.35	0.54
1:C:676:THR:HA	1:C:690:GLN:HB3	1.88	0.54
1:A:315:THR:OG1	1:A:316:SER:N	2.40	0.54
1:A:365:TYR:CB	1:A:368:LEU:CD2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:HA	1:B:602:THR:OG1	2.08	0.54
1:A:519:HIS:HE1	1:B:41:LYS:O	1.88	0.54
1:A:790:LYS:HE3	1:C:702:GLU:OE2	2.07	0.54
1:B:973:ILE:O	1:B:974:SER:HB3	2.06	0.54
1:C:365:TYR:CA	1:C:368:LEU:CD2	2.85	0.54
1:C:367:VAL:HG12	1:C:368:LEU:N	2.22	0.54
3:N:24:GLY:H	3:N:29:ILE:HG21	1.72	0.54
1:A:365:TYR:CA	1:A:368:LEU:CD2	2.85	0.54
1:A:656:VAL:HG22	1:A:694:ALA:O	2.08	0.54
1:B:365:TYR:CA	1:B:368:LEU:CD2	2.85	0.54
1:B:329:PHE:CD1	1:B:330:PRO:CD	2.90	0.54
1:B:367:VAL:HG12	1:B:368:LEU:N	2.22	0.54
1:C:365:TYR:CB	1:C:368:LEU:CD2	2.85	0.54
1:B:985:ASP:O	1:B:989:ALA:CB	2.56	0.54
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.72	0.53
1:B:984:LEU:HG	1:B:988:GLU:HG3	1.90	0.53
3:L:24:GLY:H	3:L:29:ILE:HG21	1.73	0.53
1:A:691:SER:O	1:A:692:ILE:HG22	2.06	0.53
1:C:200:TYR:CE1	1:C:230:PRO:CB	2.90	0.53
1:A:478:LYS:CE	1:A:486:VAL:CG1	2.87	0.53
1:B:504:GLY:O	2:H:65:GLN:HG2	2.08	0.53
1:C:319:ARG:O	1:C:320:VAL:O	2.27	0.53
1:C:646:ARG:NH2	1:C:668:ALA:O	2.42	0.53
1:B:296:LEU:HD13	1:B:608:VAL:CG1	2.38	0.53
1:B:440:LYS:HE3	1:B:440:LYS:CA	2.34	0.53
1:C:425:LEU:HD12	1:C:426:PRO:HD2	1.91	0.53
1:C:671:CYS:SG	1:C:697:MET:HB3	2.49	0.53
1:A:746:SER:CB	1:A:977:LEU:CD2	2.86	0.53
1:B:977:LEU:CD2	1:B:1000:ARG:NH1	2.71	0.53
3:L:14:PRO:HA	3:L:79:LEU:HD23	1.90	0.53
1:A:605:SER:HB3	1:A:674:TYR:CE2	2.41	0.53
1:B:364:ASP:OD1	1:B:364:ASP:N	2.42	0.53
1:B:528:LYS:HA	1:B:528:LYS:HZ2	1.74	0.53
3:N:14:PRO:HA	3:N:79:LEU:HD23	1.91	0.53
1:A:327:VAL:O	1:A:542:ASN:O	2.26	0.53
1:A:333:THR:OG1	1:A:334:ASN:N	2.41	0.53
1:C:331:ASN:O	1:C:332:ILE:HB	2.09	0.53
1:A:981:LEU:HG	1:A:981:LEU:O	2.10	0.52
1:A:332:ILE:HD13	1:A:333:THR:O	2.08	0.52
1:A:562:PHE:HB2	1:B:41:LYS:HD3	1.90	0.52
1:B:289:VAL:HG12	1:B:301:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:VAL:HG22	2:I:118:ALA:HB3	1.91	0.52
1:B:335:LEU:CG	1:B:364:ASP:OD2	2.58	0.52
1:C:521:PRO:O	1:C:544:ASN:ND2	2.42	0.52
1:C:530:SER:OG	1:C:531:THR:N	2.42	0.52
1:C:578:ASP:OD1	1:C:583:GLU:HG3	2.09	0.52
1:C:690:GLN:O	1:C:691:SER:CB	2.56	0.52
1:A:973:ILE:HD12	1:A:983:ARG:NH2	2.24	0.52
1:B:522:ALA:CB	1:C:200:TYR:OH	2.53	0.52
1:C:531:THR:OG1	1:C:532:ASN:N	2.42	0.52
1:A:319:ARG:HH11	1:A:321:GLN:CA	2.22	0.52
1:A:983:ARG:HG3	1:C:390:LEU:HD21	1.92	0.52
1:B:308:VAL:CG1	1:B:599:THR:HG21	2.39	0.52
2:J:11:VAL:HG22	2:J:118:ALA:HB3	1.91	0.52
1:A:1128:VAL:CG2	1:B:918:GLU:HG2	2.39	0.52
2:H:11:VAL:HG22	2:H:118:ALA:HB3	1.91	0.52
1:A:965:GLN:HE21	1:B:762:GLN:NE2	2.05	0.52
1:C:326:ILE:HD11	1:C:541:PHE:HA	1.89	0.52
1:A:478:LYS:HZ3	1:A:486:VAL:HG13	1.75	0.52
1:B:324:GLU:HG3	1:B:539:VAL:CG1	2.33	0.52
3:M:21:SER:HA	3:M:72:ALA:O	2.10	0.52
1:A:898:PHE:N	1:A:899:PRO:CD	2.73	0.52
1:A:973:ILE:CG1	1:A:974:SER:N	2.73	0.52
3:M:14:PRO:HA	3:M:79:LEU:HD23	1.91	0.52
1:C:200:TYR:CE1	1:C:230:PRO:CA	2.93	0.52
1:A:326:ILE:CG2	1:A:327:VAL:N	2.73	0.51
1:A:328:ARG:CZ	1:A:580:GLN:OE1	2.58	0.51
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.91	0.51
1:B:974:SER:HG	1:B:980:ILE:CD1	2.22	0.51
1:C:291:CYS:SG	1:C:301:CYS:HB3	2.50	0.51
2:J:3:GLN:NE2	2:J:4:LEU:O	2.43	0.51
1:B:898:PHE:N	1:B:899:PRO:CD	2.73	0.51
1:C:313:TYR:O	1:C:315:THR:HG23	2.10	0.51
1:C:898:PHE:N	1:C:899:PRO:CD	2.73	0.51
2:H:54:ILE:HG22	2:H:55:VAL:HG13	1.93	0.51
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.46	0.51
1:C:775:ASP:OD1	1:C:864:LEU:HB3	2.10	0.51
2:H:85:SER:O	2:H:87:ARG:NH1	2.44	0.51
2:I:54:ILE:HG22	2:I:55:VAL:HG13	1.93	0.51
1:A:746:SER:HB2	1:A:977:LEU:HD23	1.91	0.51
1:B:656:VAL:CG2	1:B:695:TYR:HB3	2.41	0.51
2:I:3:GLN:NE2	2:I:4:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.91	0.51
1:B:503:VAL:O	2:H:65:GLN:NE2	2.43	0.51
2:I:85:SER:O	2:I:87:ARG:NH1	2.44	0.51
2:J:21:SER:HA	2:J:79:VAL:O	2.11	0.51
2:J:85:SER:O	2:J:87:ARG:NH1	2.44	0.51
1:A:674:TYR:HE1	1:A:691:SER:O	1.88	0.51
1:B:332:ILE:CG1	1:B:362:VAL:CG1	2.70	0.51
3:L:21:SER:HA	3:L:72:ALA:O	2.10	0.51
1:A:41:LYS:C	1:C:563:GLN:HG2	2.32	0.51
1:B:421:TYR:HA	1:B:461:LEU:HB2	1.93	0.51
2:H:21:SER:HA	2:H:79:VAL:O	2.11	0.51
2:H:65:GLN:O	2:H:67:ARG:NH1	2.44	0.51
2:J:65:GLN:O	2:J:67:ARG:NH1	2.44	0.51
2:I:21:SER:HA	2:I:79:VAL:O	2.11	0.51
2:J:54:ILE:HG22	2:J:55:VAL:HG13	1.93	0.51
3:N:21:SER:HA	3:N:72:ALA:O	2.10	0.51
1:B:1128:VAL:HG21	1:C:918:GLU:HG2	1.93	0.51
1:C:528:LYS:O	1:C:528:LYS:HD3	2.11	0.51
1:C:675:GLN:CB	1:C:693:ILE:HG12	2.41	0.51
1:C:675:GLN:CG	1:C:693:ILE:HD11	2.40	0.51
1:C:421:TYR:HA	1:C:461:LEU:HB2	1.93	0.50
1:C:310:LYS:HA	1:C:599:THR:O	2.12	0.50
1:A:979:ASP:O	1:A:983:ARG:HB3	2.11	0.50
1:B:672:ALA:CB	1:B:693:ILE:O	2.59	0.50
1:B:1128:VAL:HG23	1:C:918:GLU:HG2	1.93	0.50
2:H:3:GLN:NE2	2:H:4:LEU:O	2.44	0.50
2:I:65:GLN:O	2:I:67:ARG:NH1	2.44	0.50
1:A:98:SER:OG	1:A:99:ASN:N	2.45	0.50
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.93	0.50
1:B:984:LEU:CD1	1:B:988:GLU:CG	2.89	0.50
1:B:521:PRO:HG3	1:C:200:TYR:CD2	2.47	0.50
1:A:388:ASN:HD22	1:A:388:ASN:H	1.59	0.50
1:B:293:LEU:O	1:B:294:ASP:HB3	2.12	0.50
1:B:332:ILE:HG12	1:B:333:THR:H	1.77	0.50
1:A:656:VAL:HG22	1:A:695:TYR:HB3	1.93	0.50
1:A:992:GLN:NE2	1:A:992:GLN:CA	2.72	0.50
1:B:112:SER:OG	1:B:113:LYS:N	2.45	0.50
1:B:318:PHE:C	1:B:319:ARG:HG2	2.32	0.50
1:B:365:TYR:CD2	1:B:368:LEU:HD21	2.47	0.50
1:C:312:ILE:HG12	1:C:598:ILE:HD11	1.92	0.50
1:C:329:PHE:HE2	1:C:528:LYS:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:72:ALA:HB2	2:I:79:VAL:HG13	1.94	0.50
1:A:365:TYR:CD2	1:A:368:LEU:HD21	2.47	0.50
1:B:98:SER:OG	1:B:99:ASN:N	2.45	0.50
1:C:320:VAL:CG2	1:C:321:GLN:N	2.75	0.50
2:J:44:GLY:HA3	3:N:103:GLY:HA2	1.94	0.50
1:A:112:SER:OG	1:A:113:LYS:N	2.45	0.49
1:B:310:LYS:HA	1:B:599:THR:O	2.12	0.49
1:B:521:PRO:CG	1:C:200:TYR:CD2	2.94	0.49
1:C:48:LEU:HD21	1:C:306:PHE:CD1	2.47	0.49
1:C:364:ASP:OD1	1:C:364:ASP:N	2.42	0.49
1:A:364:ASP:OD1	1:A:364:ASP:N	2.42	0.49
1:A:527:PRO:HB2	1:A:529:LYS:NZ	2.27	0.49
1:A:985:ASP:HB2	1:A:986:PRO:CD	2.37	0.49
1:C:365:TYR:CD2	1:C:368:LEU:HD21	2.47	0.49
2:J:72:ALA:HB2	2:J:79:VAL:HG13	1.94	0.49
1:A:388:ASN:N	1:A:388:ASN:ND2	2.60	0.49
1:A:864:LEU:CD1	1:C:665:PRO:HB2	2.40	0.49
2:H:50:ARG:HB3	2:H:59:ILE:HG23	1.95	0.49
1:A:315:THR:H	1:A:596:SER:HA	1.76	0.49
1:A:993:ILE:O	1:A:997:ILE:HG13	2.11	0.49
1:C:308:VAL:HG12	1:C:599:THR:CG2	2.41	0.49
1:A:755:GLN:O	1:A:757:GLY:N	2.39	0.49
1:B:335:LEU:CD1	1:B:362:VAL:O	2.59	0.49
1:C:98:SER:OG	1:C:99:ASN:N	2.45	0.49
1:C:112:SER:OG	1:C:113:LYS:N	2.45	0.49
1:C:324:GLU:OE2	1:C:324:GLU:N	2.45	0.49
1:A:643:PHE:CE1	1:A:655:TYR:CD2	3.01	0.49
1:A:668:ALA:H	1:B:864:LEU:HA	1.77	0.49
1:B:744:GLY:O	1:B:745:ASP:HB2	2.13	0.49
1:C:643:PHE:CE1	1:C:655:TYR:CD2	3.01	0.49
2:H:44:GLY:HA3	3:L:103:GLY:HA2	1.94	0.49
1:A:746:SER:CB	1:A:981:LEU:HD13	2.42	0.49
1:A:983:ARG:HB2	1:C:390:LEU:HD21	1.94	0.49
1:B:695:TYR:C	1:B:695:TYR:CD2	2.85	0.49
1:A:883:THR:OG1	1:C:705:VAL:HG11	2.13	0.49
1:B:643:PHE:CE1	1:B:655:TYR:CD2	3.01	0.49
1:B:974:SER:O	1:B:975:SER:HB3	2.13	0.49
2:J:108:TYR:HD2	2:J:111:TRP:HE1	1.61	0.49
1:A:478:LYS:HE2	1:A:486:VAL:HG13	1.95	0.49
1:C:529:LYS:HD3	1:C:529:LYS:C	2.34	0.49
2:H:108:TYR:HD2	2:H:111:TRP:HE1	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH21	1:B:230:PRO:HB2	1.70	0.49
1:B:989:ALA:O	1:B:992:GLN:N	2.46	0.49
2:I:44:GLY:HA3	3:M:103:GLY:HA2	1.94	0.49
2:I:108:TYR:HD2	2:I:111:TRP:HE1	1.61	0.49
3:N:94:ASP:OD1	3:N:94:ASP:N	2.41	0.49
1:A:303:LEU:CD1	1:A:308:VAL:HG13	2.43	0.48
1:A:321:GLN:H	1:A:321:GLN:CD	2.16	0.48
1:A:530:SER:C	1:A:531:THR:HG1	2.00	0.48
1:B:980:ILE:C	1:B:982:SER:H	2.15	0.48
1:A:439:ASN:O	1:A:440:LYS:CB	2.61	0.48
1:A:744:GLY:O	1:A:745:ASP:HB2	2.13	0.48
1:B:974:SER:HG	1:B:980:ILE:HD11	1.77	0.48
1:C:439:ASN:O	1:C:440:LYS:HB2	2.13	0.48
1:A:421:TYR:HA	1:A:461:LEU:HB2	1.93	0.48
1:C:676:THR:HG22	1:C:690:GLN:HB2	1.94	0.48
1:A:691:SER:O	1:A:692:ILE:CG2	2.61	0.48
1:A:985:ASP:CB	1:A:986:PRO:CD	2.90	0.48
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.46	0.48
1:C:439:ASN:O	1:C:440:LYS:CB	2.61	0.48
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.46	0.48
2:J:50:ARG:HB3	2:J:59:ILE:HG23	1.95	0.48
1:A:440:LYS:HE3	1:A:440:LYS:CA	2.33	0.48
1:C:48:LEU:CD2	1:C:306:PHE:CE1	2.95	0.48
2:I:50:ARG:HB3	2:I:59:ILE:HG23	1.95	0.48
1:B:695:TYR:HD2	1:B:695:TYR:C	2.16	0.48
1:C:315:THR:OG1	1:C:316:SER:N	2.46	0.48
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.47	0.48
1:C:323:THR:HB	1:C:324:GLU:OE2	2.14	0.48
1:C:744:GLY:O	1:C:745:ASP:HB2	2.13	0.48
2:H:72:ALA:HB2	2:H:79:VAL:HG13	1.94	0.48
2:J:41:PRO:O	2:J:43:GLN:NE2	2.47	0.48
1:A:276:LEU:HD22	1:A:301:CYS:HA	1.96	0.48
1:A:294:ASP:OD1	1:A:294:ASP:N	2.44	0.48
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.46	0.48
1:A:562:PHE:CD2	1:B:41:LYS:CG	2.73	0.48
1:B:973:ILE:HD11	1:B:984:LEU:CD2	2.44	0.48
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.47	0.48
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.74	0.48
1:B:324:GLU:CG	1:B:539:VAL:HG12	2.34	0.48
1:B:332:ILE:CD1	1:B:362:VAL:HG11	2.39	0.48
1:B:505:HIS:CD2	2:H:65:GLN:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CD2	1:B:528:LYS:HB3	2.49	0.48
1:C:673:SER:O	1:C:693:ILE:HG13	2.14	0.48
1:A:308:VAL:CG1	1:A:599:THR:HG21	2.44	0.47
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.54	0.47
1:B:439:ASN:O	1:B:440:LYS:CB	2.61	0.47
1:B:521:PRO:HB2	1:C:200:TYR:CZ	2.45	0.47
2:H:41:PRO:O	2:H:43:GLN:NE2	2.47	0.47
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.47	0.47
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.45	0.47
1:B:989:ALA:O	1:B:990:GLU:C	2.50	0.47
1:C:311:GLY:HA2	1:C:664:ILE:HG23	1.96	0.47
1:C:326:ILE:HD12	1:C:540:ASN:O	2.14	0.47
1:A:969:LYS:O	1:A:971:GLY:N	2.47	0.47
1:B:439:ASN:O	1:B:440:LYS:HB2	2.13	0.47
1:C:388:ASN:HD21	1:C:527:PRO:CD	2.25	0.47
1:C:1082:CYS:SG	1:C:1132:ILE:HD13	2.54	0.47
1:A:894:LEU:CD1	1:C:715:PRO:HD3	2.45	0.47
1:A:971:GLY:O	1:A:995:ARG:NE	2.48	0.47
1:B:564:GLN:O	1:B:577:ARG:HB3	2.14	0.47
1:A:521:PRO:HB3	1:A:564:GLN:CG	2.44	0.47
1:B:975:SER:O	1:B:1000:ARG:NH2	2.47	0.47
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.54	0.47
1:C:308:VAL:HG13	1:C:313:TYR:CE2	2.47	0.47
1:C:440:LYS:HE3	1:C:440:LYS:CA	2.34	0.47
1:A:365:TYR:CD1	1:A:365:TYR:N	2.82	0.47
1:B:605:SER:HB2	1:B:674:TYR:CZ	2.49	0.47
1:C:202:LYS:NZ	1:C:228:ASP:OD2	2.47	0.47
1:C:365:TYR:CD1	1:C:365:TYR:N	2.82	0.47
1:C:365:TYR:CG	1:C:368:LEU:HD21	2.50	0.47
1:A:519:HIS:NE2	1:B:41:LYS:O	2.48	0.47
1:A:864:LEU:HA	1:C:667:GLY:HA2	1.97	0.47
1:B:365:TYR:CG	1:B:368:LEU:HD21	2.50	0.47
1:B:452:ARG:NE	2:I:54:ILE:CG2	2.78	0.47
1:B:672:ALA:CA	1:B:693:ILE:O	2.60	0.47
2:I:41:PRO:O	2:I:43:GLN:NE2	2.47	0.47
1:A:439:ASN:O	1:A:440:LYS:HB2	2.13	0.47
1:B:969:LYS:HE3	1:B:974:SER:O	2.15	0.47
3:M:4:LEU:HD22	3:M:29:ILE:HD12	1.97	0.47
1:C:706:ALA:HB1	5:C:1410:NAG:H5	1.97	0.47
1:A:564:GLN:O	1:A:577:ARG:HB3	2.14	0.46
1:A:691:SER:C	1:A:692:ILE:CG2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:HA	1:B:596:SER:HB3	1.97	0.46
1:C:200:TYR:HE1	1:C:230:PRO:CB	2.28	0.46
1:C:659:SER:CB	1:C:698:SER:HB3	2.45	0.46
1:A:363:ALA:O	1:A:526:GLY:HA2	2.16	0.46
1:A:706:ALA:HB1	5:A:1410:NAG:H5	1.97	0.46
1:B:293:LEU:O	1:B:293:LEU:HD12	2.15	0.46
1:C:452:ARG:NE	2:J:54:ILE:CG2	2.78	0.46
1:C:564:GLN:O	1:C:577:ARG:HB3	2.14	0.46
1:A:557:LYS:HD3	1:B:43:PHE:CE2	2.50	0.46
1:A:607:GLN:HE21	1:A:607:GLN:HB3	1.60	0.46
1:B:329:PHE:CB	1:B:330:PRO:CD	2.94	0.46
1:B:977:LEU:HD21	1:B:1000:ARG:NH1	2.30	0.46
1:C:312:ILE:HG23	1:C:596:SER:OG	2.15	0.46
1:A:452:ARG:NE	2:H:54:ILE:CG2	2.78	0.46
1:B:528:LYS:C	1:B:529:LYS:HD2	2.36	0.46
2:I:73:ASP:OD2	2:I:75:SER:OG	2.34	0.46
1:C:300:LYS:NZ	1:C:602:THR:HG21	2.30	0.46
1:C:326:ILE:HD11	1:C:541:PHE:CB	2.46	0.46
1:C:330:PRO:CG	1:C:525:CYS:SG	3.03	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.49	0.46
1:A:592:PHE:CE2	1:B:740:MET:SD	3.09	0.46
1:B:328:ARG:HA	1:B:530:SER:HB2	1.96	0.46
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.45	0.46
1:B:607:GLN:O	1:B:608:VAL:HG13	2.15	0.46
1:C:607:GLN:O	1:C:608:VAL:HG13	2.15	0.46
1:C:326:ILE:HD11	1:C:541:PHE:CA	2.46	0.46
1:A:365:TYR:CG	1:A:368:LEU:HD21	2.50	0.46
1:A:995:ARG:NH1	1:A:995:ARG:CG	2.73	0.46
1:C:389:ASP:OD1	1:C:528:LYS:CE	2.64	0.46
3:N:4:LEU:HD22	3:N:29:ILE:HD12	1.97	0.46
1:A:489:TYR:OH	1:B:375:PHE:CA	2.64	0.46
1:B:467:ASP:OD1	1:B:467:ASP:N	2.49	0.46
1:C:533:LEU:H	1:C:533:LEU:HD12	1.81	0.46
1:C:676:THR:HA	1:C:690:GLN:HB2	1.97	0.46
1:B:973:ILE:O	1:B:974:SER:CB	2.63	0.45
1:B:980:ILE:H	1:B:980:ILE:HG12	1.57	0.45
1:C:334:ASN:HB3	1:C:335:LEU:H	1.54	0.45
1:C:613:GLN:H	1:C:613:GLN:HG2	1.48	0.45
2:H:73:ASP:OD2	2:H:75:SER:OG	2.34	0.45
3:L:4:LEU:HD22	3:L:29:ILE:HD12	1.97	0.45
1:A:569:ILE:O	1:A:570:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:VAL:HG23	1:B:918:GLU:HG2	1.99	0.45
1:B:365:TYR:N	1:B:365:TYR:CD1	2.82	0.45
1:C:467:ASP:N	1:C:467:ASP:OD1	2.49	0.45
1:A:746:SER:CB	1:A:981:LEU:CD1	2.93	0.45
1:C:89:GLY:HA2	1:C:194:PHE:O	2.17	0.45
1:C:333:THR:OG1	1:C:334:ASN:N	2.50	0.45
1:C:542:ASN:HA	1:C:546:LEU:O	2.17	0.45
1:A:531:THR:CG2	1:A:532:ASN:N	2.80	0.45
1:B:569:ILE:O	1:B:570:ALA:HB3	2.16	0.45
1:C:326:ILE:CD1	1:C:326:ILE:C	2.85	0.45
1:A:693:ILE:H	1:A:693:ILE:HG13	1.59	0.45
1:B:308:VAL:HG11	1:B:599:THR:HG21	1.99	0.45
1:C:494:SER:OG	1:C:495:TYR:N	2.50	0.45
2:J:73:ASP:OD2	2:J:75:SER:OG	2.34	0.45
1:B:60:SER:OG	1:B:61:ASN:N	2.50	0.45
1:B:542:ASN:HA	1:B:546:LEU:O	2.17	0.45
1:B:706:ALA:HB1	5:B:1410:NAG:H5	1.97	0.45
1:B:983:ARG:HE	1:B:983:ARG:HB2	1.56	0.45
1:A:318:PHE:O	1:A:318:PHE:CG	2.69	0.45
1:A:968:SER:HB2	1:A:970:PHE:CE2	2.52	0.45
1:C:295:PRO:CG	1:C:608:VAL:HG21	2.42	0.45
1:A:89:GLY:HA2	1:A:194:PHE:O	2.16	0.45
1:A:332:ILE:C	1:A:332:ILE:CD1	2.85	0.45
1:C:60:SER:OG	1:C:61:ASN:N	2.50	0.45
1:A:562:PHE:HD2	1:B:41:LYS:CB	2.30	0.45
1:B:559:PHE:HE2	1:B:565:PHE:HA	1.82	0.45
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.99	0.45
1:A:883:THR:CB	1:C:705:VAL:HG11	2.47	0.44
1:B:360:ASN:HD22	1:B:523:THR:HA	1.83	0.44
1:B:565:PHE:O	1:C:42:VAL:HA	2.17	0.44
1:B:984:LEU:CG	1:B:988:GLU:HG3	2.47	0.44
1:C:365:TYR:N	1:C:365:TYR:HD1	2.15	0.44
1:A:559:PHE:HE2	1:A:565:PHE:HA	1.82	0.44
1:A:763:LEU:HD11	1:A:1005:GLN:NE2	2.32	0.44
1:B:365:TYR:N	1:B:365:TYR:HD1	2.15	0.44
1:B:746:SER:OG	1:B:981:LEU:CD1	2.65	0.44
1:C:293:LEU:HD12	1:C:293:LEU:HA	1.77	0.44
1:C:526:GLY:O	1:C:528:LYS:N	2.51	0.44
2:I:18:VAL:O	2:I:82:GLU:HA	2.18	0.44
1:A:388:ASN:H	1:A:388:ASN:ND2	2.16	0.44
1:C:672:ALA:HA	1:C:693:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:VAL:O	2:H:82:GLU:HA	2.18	0.44
1:A:358:ILE:HB	1:A:395:VAL:HB	2.00	0.44
1:A:969:LYS:C	1:A:971:GLY:N	2.71	0.44
1:A:365:TYR:CG	1:A:368:LEU:CD2	3.01	0.44
1:A:965:GLN:NE2	1:B:762:GLN:NE2	2.53	0.44
1:B:712:ILE:O	1:B:1074:ASN:HA	2.18	0.44
1:A:542:ASN:HA	1:A:546:LEU:O	2.17	0.44
1:A:1126:CYS:SG	1:A:1132:ILE:HD13	2.58	0.44
1:B:89:GLY:HA2	1:B:194:PHE:O	2.17	0.44
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.85	0.44
1:B:528:LYS:NZ	1:B:528:LYS:CA	2.73	0.44
1:C:300:LYS:HE2	1:C:602:THR:HG21	1.98	0.44
1:C:569:ILE:O	1:C:570:ALA:HB3	2.16	0.44
2:J:50:ARG:HB3	2:J:59:ILE:CG2	2.48	0.44
1:A:60:SER:OG	1:A:61:ASN:N	2.50	0.44
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.44
1:B:494:SER:OG	1:B:495:TYR:N	2.50	0.44
1:B:646:ARG:NH2	1:B:668:ALA:O	2.51	0.44
1:C:109:THR:CA	1:C:237:ARG:HH21	2.21	0.44
1:C:333:THR:CG2	1:C:361:CYS:C	2.86	0.44
1:C:358:ILE:HB	1:C:395:VAL:HB	2.00	0.44
1:C:360:ASN:HD22	1:C:523:THR:HA	1.83	0.44
1:C:559:PHE:HE2	1:C:565:PHE:HA	1.82	0.44
3:L:19:THR:HA	3:L:74:LEU:O	2.18	0.44
1:A:303:LEU:HD11	1:A:308:VAL:HG13	2.00	0.44
1:A:763:LEU:HG	1:A:1005:GLN:NE2	2.33	0.44
1:A:980:ILE:O	1:A:982:SER:N	2.45	0.44
1:B:365:TYR:CG	1:B:368:LEU:CD2	3.01	0.44
1:B:669:GLY:O	1:B:697:MET:HG2	2.18	0.44
1:A:41:LYS:HB2	1:C:519:HIS:CD2	2.46	0.43
1:A:41:LYS:CB	1:C:519:HIS:NE2	2.57	0.43
1:A:982:SER:O	1:A:982:SER:OG	2.30	0.43
1:B:332:ILE:CG1	1:B:333:THR:H	2.30	0.43
1:A:866:THR:HG23	1:C:668:ALA:C	2.38	0.43
1:B:702:GLU:OE2	1:C:790:LYS:CE	2.66	0.43
2:I:71:SER:OG	2:I:72:ALA:N	2.51	0.43
1:A:319:ARG:HH11	1:A:321:GLN:HA	1.83	0.43
1:A:430:THR:OG1	1:A:515:PHE:O	2.37	0.43
1:A:916:LEU:C	1:A:916:LEU:HD23	2.39	0.43
5:A:1404:NAG:O3	1:C:465:GLU:OE2	2.23	0.43
1:B:109:THR:CA	1:B:237:ARG:HH21	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:HD22	1:C:873:TYR:OH	2.17	0.43
1:A:352:ALA:HB1	1:A:466:ARG:HH21	1.83	0.43
1:B:315:THR:N	1:B:595:VAL:O	2.51	0.43
1:B:352:ALA:HB1	1:B:466:ARG:HH21	1.83	0.43
1:B:607:GLN:HE21	1:B:607:GLN:HB3	1.68	0.43
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.58	0.43
1:C:333:THR:HG21	1:C:361:CYS:C	2.37	0.43
1:C:352:ALA:HB1	1:C:466:ARG:HH21	1.83	0.43
1:C:712:ILE:O	1:C:1074:ASN:HA	2.18	0.43
1:C:1126:CYS:SG	1:C:1132:ILE:HD13	2.58	0.43
2:H:71:SER:OG	2:H:72:ALA:N	2.51	0.43
2:J:18:VAL:O	2:J:82:GLU:HA	2.18	0.43
1:A:712:ILE:O	1:A:1074:ASN:HA	2.18	0.43
1:A:736:VAL:HG12	1:A:767:LEU:HD12	2.01	0.43
1:B:613:GLN:H	1:B:613:GLN:HG2	1.48	0.43
1:B:990:GLU:OE2	1:B:990:GLU:HA	2.19	0.43
1:C:430:THR:OG1	1:C:515:PHE:O	2.37	0.43
2:I:100:GLN:HG2	2:I:107:TYR:HD2	1.83	0.43
2:I:103:PHE:O	2:I:104:ASP:HB2	2.18	0.43
1:A:360:ASN:HD22	1:A:523:THR:HA	1.82	0.43
1:A:969:LYS:C	1:A:971:GLY:H	2.22	0.43
1:B:276:LEU:HD22	1:B:301:CYS:HA	2.01	0.43
1:B:328:ARG:NH2	1:B:533:LEU:HD13	2.34	0.43
1:B:335:LEU:HD11	1:B:364:ASP:CB	2.49	0.43
1:B:430:THR:OG1	1:B:515:PHE:O	2.37	0.43
2:H:50:ARG:HB3	2:H:59:ILE:CG2	2.48	0.43
2:J:71:SER:OG	2:J:72:ALA:N	2.51	0.43
1:B:323:THR:O	1:B:324:GLU:HG2	2.18	0.43
1:C:326:ILE:HD11	1:C:541:PHE:HB3	2.01	0.43
1:C:365:TYR:CG	1:C:368:LEU:CD2	3.01	0.43
2:H:103:PHE:O	2:H:104:ASP:HB2	2.18	0.43
2:J:100:GLN:HG2	2:J:107:TYR:HD2	1.83	0.43
3:N:19:THR:HA	3:N:74:LEU:O	2.18	0.43
1:A:365:TYR:N	1:A:365:TYR:HD1	2.15	0.43
1:A:863:PRO:O	1:C:668:ALA:N	2.44	0.43
1:B:335:LEU:HG	1:B:364:ASP:OD2	2.18	0.43
1:B:358:ILE:HB	1:B:395:VAL:HB	2.00	0.43
5:B:1410:NAG:O4	5:B:1411:NAG:O5	2.28	0.43
2:H:100:GLN:HG2	2:H:107:TYR:HD2	1.83	0.43
1:A:494:SER:OG	1:A:495:TYR:N	2.50	0.43
1:A:1128:VAL:HG21	1:B:918:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:C	1:B:324:GLU:CG	2.86	0.43
2:H:73:ASP:OD1	2:H:78:THR:OG1	2.35	0.43
3:M:19:THR:HA	3:M:74:LEU:O	2.18	0.43
1:B:916:LEU:C	1:B:916:LEU:HD23	2.39	0.43
1:B:969:LYS:O	1:B:971:GLY:N	2.52	0.43
1:C:50:SER:CB	1:C:304:LYS:HE3	2.49	0.43
1:C:328:ARG:HH21	1:C:328:ARG:HA	1.84	0.43
1:C:389:ASP:OD1	1:C:528:LYS:HE2	2.19	0.43
1:A:129:LYS:HG2	1:A:131:CYS:SG	2.59	0.42
1:A:985:ASP:OD2	1:C:383:SER:OG	2.36	0.42
1:B:976:VAL:C	1:B:978:ASN:N	2.72	0.42
1:C:519:HIS:CD2	1:C:519:HIS:O	2.72	0.42
1:C:916:LEU:C	1:C:916:LEU:HD23	2.39	0.42
2:J:85:SER:O	2:J:85:SER:OG	2.34	0.42
4:T:1:NAG:H4	4:T:2:NAG:C7	2.49	0.42
4:Z:1:NAG:H4	4:Z:2:NAG:C7	2.49	0.42
1:B:592:PHE:CD1	1:B:592:PHE:C	2.92	0.42
1:B:674:TYR:HD1	1:B:674:TYR:HA	1.70	0.42
1:C:315:THR:HG23	1:C:597:VAL:H	1.84	0.42
1:C:672:ALA:HB1	1:C:693:ILE:O	2.19	0.42
2:J:73:ASP:OD1	2:J:78:THR:OG1	2.35	0.42
1:A:289:VAL:CG1	1:A:301:CYS:SG	3.07	0.42
1:A:613:GLN:H	1:A:613:GLN:HG2	1.48	0.42
1:A:792:PRO:HA	1:A:793:PRO:HD3	1.91	0.42
3:L:94:ASP:OD1	3:L:94:ASP:N	2.41	0.42
2:I:73:ASP:OD1	2:I:78:THR:OG1	2.35	0.42
4:K:1:NAG:H4	4:K:2:NAG:C7	2.49	0.42
1:A:327:VAL:HG21	1:A:528:LYS:HE2	2.02	0.42
1:A:983:ARG:CG	1:C:390:LEU:HD21	2.49	0.42
1:C:129:LYS:HG2	1:C:131:CYS:SG	2.60	0.42
1:C:560:LEU:HB2	1:C:563:GLN:OE1	2.20	0.42
1:C:980:ILE:O	1:C:984:LEU:HB3	2.19	0.42
1:A:763:LEU:HG	1:A:1005:GLN:HE22	1.84	0.42
1:C:662:CYS:HG	1:C:671:CYS:HG	1.67	0.42
2:I:108:TYR:HB3	2:I:111:TRP:CD1	2.54	0.42
1:A:327:VAL:CG2	1:A:528:LYS:HE2	2.49	0.42
1:B:328:ARG:HH21	1:B:328:ARG:CG	2.15	0.42
1:B:328:ARG:HH22	1:B:533:LEU:CB	2.30	0.42
1:B:337:PRO:C	1:B:339:ASP:N	2.73	0.42
1:B:522:ALA:HB3	1:C:230:PRO:CB	2.48	0.42
1:C:326:ILE:CD1	1:C:326:ILE:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:TYR:HB3	2:H:111:TRP:CD1	2.54	0.42
2:J:103:PHE:O	2:J:104:ASP:HB2	2.18	0.42
1:A:43:PHE:CE2	1:C:557:LYS:HD3	2.55	0.42
1:A:363:ALA:HB1	1:A:365:TYR:HE1	1.85	0.42
1:B:332:ILE:HG13	1:B:362:VAL:CG1	2.44	0.42
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.01	0.42
2:H:47:TRP:HZ2	2:H:50:ARG:HB2	1.85	0.42
3:M:94:ASP:OD1	3:M:94:ASP:N	2.41	0.42
2:J:108:TYR:HB3	2:J:111:TRP:CD1	2.54	0.42
1:B:129:LYS:HG2	1:B:131:CYS:SG	2.60	0.42
1:B:993:ILE:HG22	1:B:997:ILE:HD12	2.02	0.42
1:C:320:VAL:HG22	1:C:321:GLN:N	2.34	0.42
1:C:324:GLU:O	1:C:325:SER:HB2	2.20	0.42
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.02	0.42
1:A:310:LYS:O	1:A:310:LYS:HG3	2.18	0.42
1:A:313:TYR:HE2	1:A:599:THR:CG2	2.32	0.42
5:A:1410:NAG:O4	5:A:1411:NAG:O5	2.28	0.42
1:C:326:ILE:O	1:C:327:VAL:HG23	2.20	0.42
1:C:327:VAL:HG12	1:C:327:VAL:O	2.19	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.92	0.42
1:A:394:ASN:OD1	1:A:394:ASN:N	2.52	0.42
1:A:898:PHE:HB3	1:A:899:PRO:HD3	2.01	0.42
1:B:335:LEU:CG	1:B:364:ASP:CG	2.87	0.42
1:B:339:ASP:O	1:B:343:ASN:N	2.49	0.42
1:B:363:ALA:HB1	1:B:365:TYR:HE1	1.85	0.42
1:C:332:ILE:C	1:C:333:THR:HG22	2.31	0.42
2:I:50:ARG:HB3	2:I:59:ILE:CG2	2.48	0.42
3:M:48:LEU:HD23	3:M:48:LEU:HA	1.91	0.42
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.83	0.41
1:A:560:LEU:HB2	1:A:563:GLN:OE1	2.20	0.41
1:A:668:ALA:N	1:B:863:PRO:O	2.52	0.41
1:C:449:TYR:HE2	2:J:50:ARG:HH12	1.67	0.41
2:I:70:ILE:HD13	2:I:81:MET:HB2	2.02	0.41
3:M:20:ILE:O	3:M:73:SER:HA	2.21	0.41
2:J:88:SER:O	2:J:88:SER:OG	2.34	0.41
1:A:762:GLN:NE2	1:C:961:THR:HG21	2.35	0.41
1:A:913:GLN:NE2	1:C:1090:PRO:O	2.54	0.41
1:A:973:ILE:HG12	1:A:974:SER:H	1.85	0.41
1:A:996:LEU:HA	1:A:996:LEU:HD23	1.86	0.41
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.36	0.41
1:B:329:PHE:C	1:B:579:PRO:HB2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:ASP:O	1:B:989:ALA:HB2	2.19	0.41
1:A:604:THR:O	1:A:604:THR:HG22	2.19	0.41
1:A:864:LEU:CD1	1:C:665:PRO:CB	2.98	0.41
1:B:325:SER:O	1:B:327:VAL:N	2.53	0.41
1:A:324:GLU:CB	1:A:539:VAL:CG1	2.97	0.41
1:A:478:LYS:NZ	1:A:486:VAL:CG1	2.80	0.41
1:A:968:SER:O	1:A:970:PHE:CD2	2.74	0.41
1:B:394:ASN:OD1	1:B:394:ASN:N	2.52	0.41
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.36	0.41
1:C:333:THR:HG23	1:C:361:CYS:HA	1.92	0.41
1:C:986:PRO:N	1:C:987:PRO:CD	2.83	0.41
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.36	0.41
2:I:39:GLN:HB2	2:I:45:LEU:HD23	2.02	0.41
3:N:20:ILE:O	3:N:73:SER:HA	2.20	0.41
1:A:42:VAL:N	1:C:563:GLN:HG2	2.35	0.41
1:A:367:VAL:O	1:A:368:LEU:CB	2.68	0.41
1:A:981:LEU:O	1:A:982:SER:CB	2.68	0.41
1:B:37:TYR:OH	1:B:54:LEU:O	2.31	0.41
1:B:367:VAL:O	1:B:368:LEU:CB	2.68	0.41
1:B:526:GLY:O	1:B:528:LYS:HE2	2.21	0.41
1:B:980:ILE:HG21	1:B:992:GLN:HB2	2.01	0.41
1:C:68:ILE:HG21	1:C:262:ALA:HA	2.03	0.41
1:C:188:ASN:OD1	1:C:188:ASN:N	2.52	0.41
2:I:107:TYR:CD1	3:M:50:TYR:HB3	2.56	0.41
2:J:47:TRP:HZ2	2:J:50:ARG:HB2	1.85	0.41
1:A:1144:GLU:OE1	1:C:1141:LEU:CD2	2.68	0.41
1:B:504:GLY:CA	2:H:65:GLN:NE2	2.76	0.41
1:C:898:PHE:HB3	1:C:899:PRO:HD3	2.01	0.41
3:L:20:ILE:O	3:L:73:SER:HA	2.21	0.41
1:A:333:THR:HG23	1:A:334:ASN:CG	2.41	0.41
1:A:449:TYR:HE2	2:H:50:ARG:HH12	1.67	0.41
1:A:900:MET:CE	1:C:1094:VAL:HG23	2.51	0.41
1:B:600:PRO:HG3	1:B:692:ILE:HD11	2.03	0.41
1:B:976:VAL:C	1:B:978:ASN:H	2.23	0.41
1:C:68:ILE:HD12	1:C:68:ILE:HA	1.92	0.41
1:C:659:SER:HB3	1:C:698:SER:HB3	2.03	0.41
1:C:792:PRO:HA	1:C:793:PRO:HD3	1.91	0.41
3:M:87:TYR:O	3:M:104:GLY:CA	2.67	0.41
2:J:70:ILE:HD13	2:J:81:MET:HB2	2.02	0.41
2:J:107:TYR:CD1	3:N:50:TYR:HB3	2.56	0.41
1:A:300:LYS:HE2	1:A:602:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TYR:OH	1:B:375:PHE:C	2.59	0.41
1:B:125:ASN:HD21	5:B:1402:NAG:H5	1.86	0.41
1:B:528:LYS:C	1:B:529:LYS:CD	2.88	0.41
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.20	0.41
1:B:986:PRO:C	1:B:988:GLU:H	2.24	0.41
1:A:125:ASN:HD21	5:A:1402:NAG:H5	1.86	0.41
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.86	0.41
1:A:645:THR:HG23	1:A:647:ALA:H	1.86	0.41
1:B:368:LEU:O	1:B:368:LEU:CG	2.69	0.41
1:B:420:ASP:OD1	1:B:420:ASP:N	2.54	0.41
1:B:444:LYS:HE3	1:B:444:LYS:HB2	1.85	0.41
1:B:504:GLY:O	2:H:65:GLN:CG	2.68	0.41
1:B:604:THR:HG22	1:B:674:TYR:HD2	1.85	0.41
1:B:645:THR:HG23	1:B:647:ALA:H	1.86	0.41
1:C:363:ALA:HB1	1:C:365:TYR:HE1	1.85	0.41
1:C:366:SER:O	1:C:369:TYR:HB2	2.21	0.41
2:J:39:GLN:HB2	2:J:45:LEU:HD23	2.02	0.41
1:A:188:ASN:OD1	1:A:188:ASN:N	2.52	0.41
1:A:420:ASP:N	1:A:420:ASP:OD1	2.54	0.41
1:A:489:TYR:OH	1:B:375:PHE:O	2.37	0.41
1:A:986:PRO:CD	1:A:987:PRO:HD3	2.45	0.41
1:B:449:TYR:HE2	2:I:50:ARG:HH12	1.67	0.41
1:C:125:ASN:HD21	5:C:1402:NAG:H5	1.86	0.41
1:C:326:ILE:CG2	1:C:532:ASN:O	2.61	0.41
2:H:12:LYS:HG2	2:H:18:VAL:HG22	2.03	0.41
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.53	0.40
1:A:974:SER:OG	1:A:980:ILE:HG13	2.20	0.40
1:A:982:SER:HA	1:C:386:LYS:NZ	2.37	0.40
1:A:992:GLN:CA	1:A:992:GLN:HE21	2.34	0.40
1:C:367:VAL:O	1:C:368:LEU:CB	2.68	0.40
3:L:3:VAL:HG23	3:L:4:LEU:HG	2.03	0.40
2:J:13:LYS:HD3	2:J:13:LYS:HA	1.99	0.40
1:A:68:ILE:HG21	1:A:262:ALA:HA	2.03	0.40
1:A:486:VAL:HG22	1:A:487:ASN:N	2.36	0.40
1:A:705:VAL:HG11	1:B:883:THR:CB	2.51	0.40
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	2.04	0.40
1:C:200:TYR:CD1	1:C:230:PRO:HA	2.56	0.40
1:C:367:VAL:CG1	1:C:368:LEU:N	2.85	0.40
3:M:3:VAL:HG23	3:M:4:LEU:HG	2.03	0.40
1:A:367:VAL:CG1	1:A:368:LEU:N	2.85	0.40
1:A:674:TYR:C	1:A:675:GLN:HG3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:TYR:CD1	1:A:691:SER:O	2.74	0.40
1:A:768:THR:O	1:A:771:ALA:HB3	2.20	0.40
1:A:895:GLN:O	1:C:712:ILE:HA	2.21	0.40
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.97	0.40
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.04	0.40
1:C:326:ILE:C	1:C:327:VAL:HG23	2.42	0.40
1:C:526:GLY:C	1:C:528:LYS:N	2.73	0.40
3:N:95:SER:OG	3:N:96:LEU:N	2.55	0.40
1:A:562:PHE:CE1	1:B:225:PRO:HD2	2.56	0.40
1:B:364:ASP:CA	1:B:527:PRO:CD	2.80	0.40
3:L:95:SER:OG	3:L:96:LEU:N	2.55	0.40
1:A:763:LEU:CD2	1:A:1008:VAL:HG11	2.50	0.40
1:B:233:ILE:HD13	1:B:233:ILE:HA	1.87	0.40
1:B:318:PHE:O	1:B:319:ARG:CB	2.70	0.40
1:B:328:ARG:HA	1:B:328:ARG:HD2	1.88	0.40
1:C:645:THR:HG23	1:C:647:ALA:H	1.86	0.40
1:C:902:MET:HB2	1:C:916:LEU:HD11	2.03	0.40
2:H:70:ILE:HD13	2:H:81:MET:HB2	2.02	0.40
2:H:107:TYR:CD1	3:L:50:TYR:HB3	2.56	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	1007/1271 (79%)	886 (88%)	89 (9%)	32 (3%)	4	26
1	B	1007/1271 (79%)	894 (89%)	85 (8%)	28 (3%)	5	29
1	C	1007/1271 (79%)	905 (90%)	76 (8%)	26 (3%)	5	31
2	H	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	17	56
2	I	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	17	56
3	L	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
3	M	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
3	N	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
All	All	3693/4497 (82%)	3282 (89%)	322 (9%)	89 (2%)	9	34

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	316	SER
1	A	325	SER
1	A	529	LYS
1	A	530	SER
1	A	561	PRO
1	A	591	SER
1	A	604	THR
1	A	692	ILE
1	A	756	TYR
1	A	982	SER
1	A	983	ARG
1	B	294	ASP
1	B	316	SER
1	B	326	ILE
1	B	332	ILE
1	B	334	ASN
1	B	336	CYS
1	B	561	PRO
1	B	591	SER
1	B	974	SER
1	B	975	SER
1	B	977	LEU
1	B	981	LEU
1	C	294	ASP
1	C	314	GLN
1	C	315	THR
1	C	316	SER
1	C	320	VAL
1	C	332	ILE
1	C	334	ASN
1	C	561	PRO

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Mol	Chain	Res	Type
1	C	691	SER
2	H	109	ASP
2	I	109	ASP
2	J	109	ASP
1	A	174	PRO
1	A	293	LEU
1	A	310	LYS
1	A	315	THR
1	A	324	GLU
1	A	334	ASN
1	B	174	PRO
1	B	315	THR
1	B	319	ARG
1	C	174	PRO
1	C	293	LEU
1	C	319	ARG
1	C	327	VAL
1	C	529	LYS
1	C	530	SER
1	C	531	THR
1	A	328	ARG
1	A	488	CYS
1	A	605	SER
1	A	970	PHE
1	B	295	PRO
1	B	331	ASN
1	B	691	SER
1	B	986	PRO
1	C	323	THR
1	C	325	SER
1	C	335	LEU
1	A	592	PHE
1	B	337	PRO
1	B	529	LYS
1	B	972	ALA
1	C	295	PRO
1	C	591	SER
1	C	866	THR
1	A	337	PRO
1	A	531	THR
1	A	985	ASP
1	B	970	PHE

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Mol	Chain	Res	Type
1	B	985	ASP
1	B	988	GLU
1	C	329	PHE
1	C	336	CYS
1	C	526	GLY
1	B	605	SER
1	A	326	ILE
1	A	600	PRO
1	A	327	VAL
1	B	973	ILE
1	A	322	PRO
1	A	742	ILE
1	B	742	ILE
1	C	742	ILE
1	A	295	PRO

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	896/1111 (81%)	850 (95%)	46 (5%)	24	60
1	B	896/1111 (81%)	850 (95%)	46 (5%)	24	60
1	C	896/1111 (81%)	862 (96%)	34 (4%)	33	67
2	H	97/97 (100%)	93 (96%)	4 (4%)	30	66
2	I	97/97 (100%)	93 (96%)	4 (4%)	30	66
2	J	97/97 (100%)	93 (96%)	4 (4%)	30	66
3	L	89/90 (99%)	87 (98%)	2 (2%)	52	79
3	M	89/90 (99%)	87 (98%)	2 (2%)	52	79
3	N	89/90 (99%)	87 (98%)	2 (2%)	52	79
All	All	3246/3894 (83%)	3102 (96%)	144 (4%)	32	64

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	CYS
1	A	166	CYS
1	A	310	LYS
1	A	315	THR
1	A	318	PHE
1	A	319	ARG
1	A	320	VAL
1	A	321	GLN
1	A	324	GLU
1	A	328	ARG
1	A	329	PHE
1	A	335	LEU
1	A	336	CYS
1	A	366	SER
1	A	368	LEU
1	A	369	TYR
1	A	388	ASN
1	A	440	LYS
1	A	444	LYS
1	A	452	ARG
1	A	528	LYS
1	A	529	LYS
1	A	533	LEU
1	A	544	ASN
1	A	561	PRO
1	A	577	ARG
1	A	613	GLN
1	A	673	SER
1	A	674	TYR
1	A	690	GLN
1	A	697	MET
1	A	698	SER
1	A	759	PHE
1	A	760	CYS
1	A	764	LYS
1	A	977	LEU
1	A	981	LEU
1	A	983	ARG
1	A	984	LEU
1	A	985	ASP
1	A	988	GLU
1	A	990	GLU
1	A	991	VAL

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Mol	Chain	Res	Type
1	A	992	GLN
1	A	995	ARG
1	A	1074	ASN
1	B	131	CYS
1	B	166	CYS
1	B	310	LYS
1	B	317	ASN
1	B	318	PHE
1	B	319	ARG
1	B	320	VAL
1	B	321	GLN
1	B	328	ARG
1	B	329	PHE
1	B	332	ILE
1	B	338	PHE
1	B	366	SER
1	B	368	LEU
1	B	369	TYR
1	B	440	LYS
1	B	444	LYS
1	B	452	ARG
1	B	505	HIS
1	B	528	LYS
1	B	529	LYS
1	B	531	THR
1	B	532	ASN
1	B	533	LEU
1	B	561	PRO
1	B	577	ARG
1	B	590	CYS
1	B	591	SER
1	B	602	THR
1	B	613	GLN
1	B	673	SER
1	B	674	TYR
1	B	675	GLN
1	B	692	ILE
1	B	695	TYR
1	B	697	MET
1	B	698	SER
1	B	969	LYS
1	B	977	LEU

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Mol	Chain	Res	Type
1	B	980	ILE
1	B	983	ARG
1	B	984	LEU
1	B	985	ASP
1	B	990	GLU
1	B	995	ARG
1	B	1074	ASN
1	C	131	CYS
1	C	166	CYS
1	C	200	TYR
1	C	310	LYS
1	C	318	PHE
1	C	319	ARG
1	C	320	VAL
1	C	321	GLN
1	C	326	ILE
1	C	328	ARG
1	C	329	PHE
1	C	332	ILE
1	C	357	ARG
1	C	366	SER
1	C	368	LEU
1	C	369	TYR
1	C	427	ASP
1	C	440	LYS
1	C	444	LYS
1	C	452	ARG
1	C	525	CYS
1	C	529	LYS
1	C	532	ASN
1	C	533	LEU
1	C	561	PRO
1	C	577	ARG
1	C	591	SER
1	C	613	GLN
1	C	673	SER
1	C	675	GLN
1	C	690	GLN
1	C	693	ILE
1	C	866	THR
1	C	1074	ASN
2	H	31	SER

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Mol	Chain	Res	Type
2	H	67	ARG
2	H	87	ARG
2	H	106	PHE
3	L	17	ARG
3	L	55	ARG
2	I	31	SER
2	I	67	ARG
2	I	87	ARG
2	I	106	PHE
3	M	17	ARG
3	M	55	ARG
2	J	31	SER
2	J	67	ARG
2	J	87	ARG
2	J	106	PHE
3	N	17	ARG
3	N	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	173	GLN
1	A	360	ASN
1	A	388	ASN
1	A	422	ASN
1	A	450	ASN
1	A	481	ASN
1	A	487	ASN
1	A	519	HIS
1	A	606	ASN
1	A	607	GLN
1	A	755	GLN
1	A	913	GLN
1	A	914	ASN
1	A	965	GLN
1	A	1005	GLN
1	B	164	ASN
1	B	173	GLN
1	B	314	GLN
1	B	321	GLN
1	B	360	ASN

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Mol	Chain	Res	Type
1	B	422	ASN
1	B	450	ASN
1	B	481	ASN
1	B	505	HIS
1	B	607	GLN
1	B	965	GLN
1	C	164	ASN
1	C	173	GLN
1	C	314	GLN
1	C	360	ASN
1	C	422	ASN
1	C	450	ASN
1	C	519	HIS
1	C	532	ASN
1	C	913	GLN
2	H	65	GLN
3	L	52	ASN
3	L	88	HIS
3	M	52	ASN
3	M	88	HIS
3	N	52	ASN
3	N	88	HIS

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](#)

36 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	1,4	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	E	1	1,4	14,14,15	0.26	0	17,19,21	0.65	1 (5%)
4	NAG	E	2	4	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	F	1	1,4	14,14,15	0.34	0	17,19,21	1.14	1 (5%)
4	NAG	F	2	4	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	G	1	1,4	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	K	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	K	2	4	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
4	NAG	O	1	1,4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	O	2	4	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	P	1	1,4	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	P	2	4	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	Q	1	1,4	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
4	NAG	Q	2	4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	R	1	1,4	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	S	1	1,4	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
4	NAG	S	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	T	1	1,4	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	T	2	4	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
4	NAG	U	1	1,4	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	V	1	1,4	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	V	2	4	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	W	1	1,4	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
4	NAG	W	2	4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	X	1	1,4	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
4	NAG	X	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	Y	1	1,4	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
4	NAG	Y	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	Z	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	Z	2	4	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
4	NAG	a	1	1,4	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	a	2	4	14,14,15	0.28	0	17,19,21	0.38	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	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	O5-C1	-2.75	1.39	1.43
4	Z	1	NAG	O5-C1	-2.70	1.39	1.43
4	T	1	NAG	O5-C1	-2.67	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	1	NAG	C1-O5-C5	3.35	116.73	112.19
4	X	1	NAG	C1-O5-C5	3.35	116.73	112.19
4	F	1	NAG	C1-O5-C5	3.32	116.70	112.19
4	T	1	NAG	O4-C4-C3	-2.40	104.81	110.35
4	K	1	NAG	O4-C4-C3	-2.39	104.83	110.35
4	Z	1	NAG	O4-C4-C3	-2.36	104.89	110.35
4	V	1	NAG	C8-C7-N2	2.29	119.97	116.10
4	E	1	NAG	C1-O5-C5	2.26	115.26	112.19
4	Q	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	Y	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	W	1	NAG	C1-O5-C5	2.24	115.22	112.19
4	S	1	NAG	C1-O5-C5	2.23	115.21	112.19
4	G	1	NAG	C1-O5-C5	2.20	115.18	112.19
4	T	2	NAG	C1-O5-C5	2.13	115.08	112.19
4	Z	2	NAG	C1-O5-C5	2.10	115.04	112.19
4	K	2	NAG	C1-O5-C5	2.09	115.02	112.19
4	V	1	NAG	C2-N2-C7	-2.03	120.01	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6

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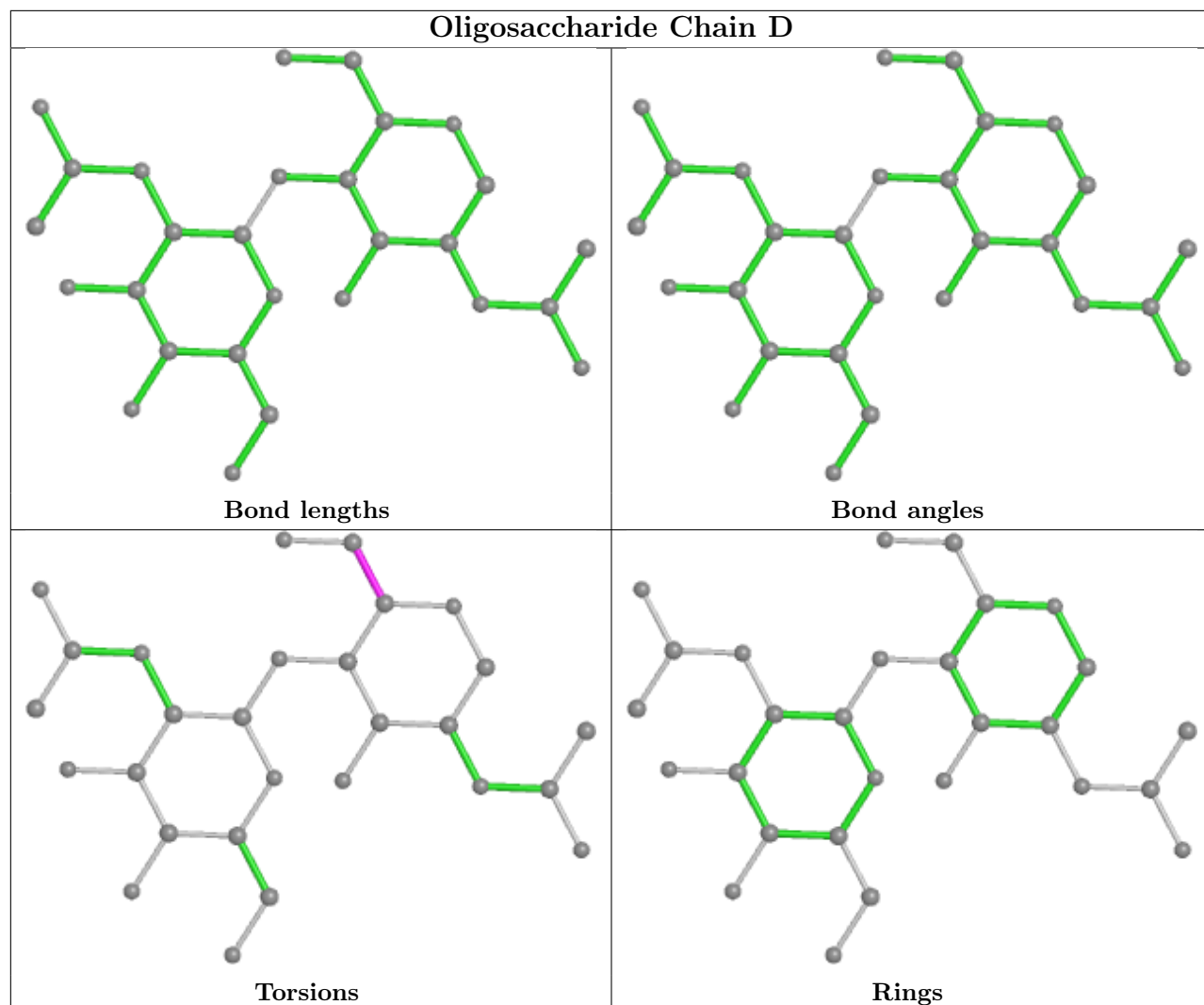
Mol	Chain	Res	Type	Atoms
4	W	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6

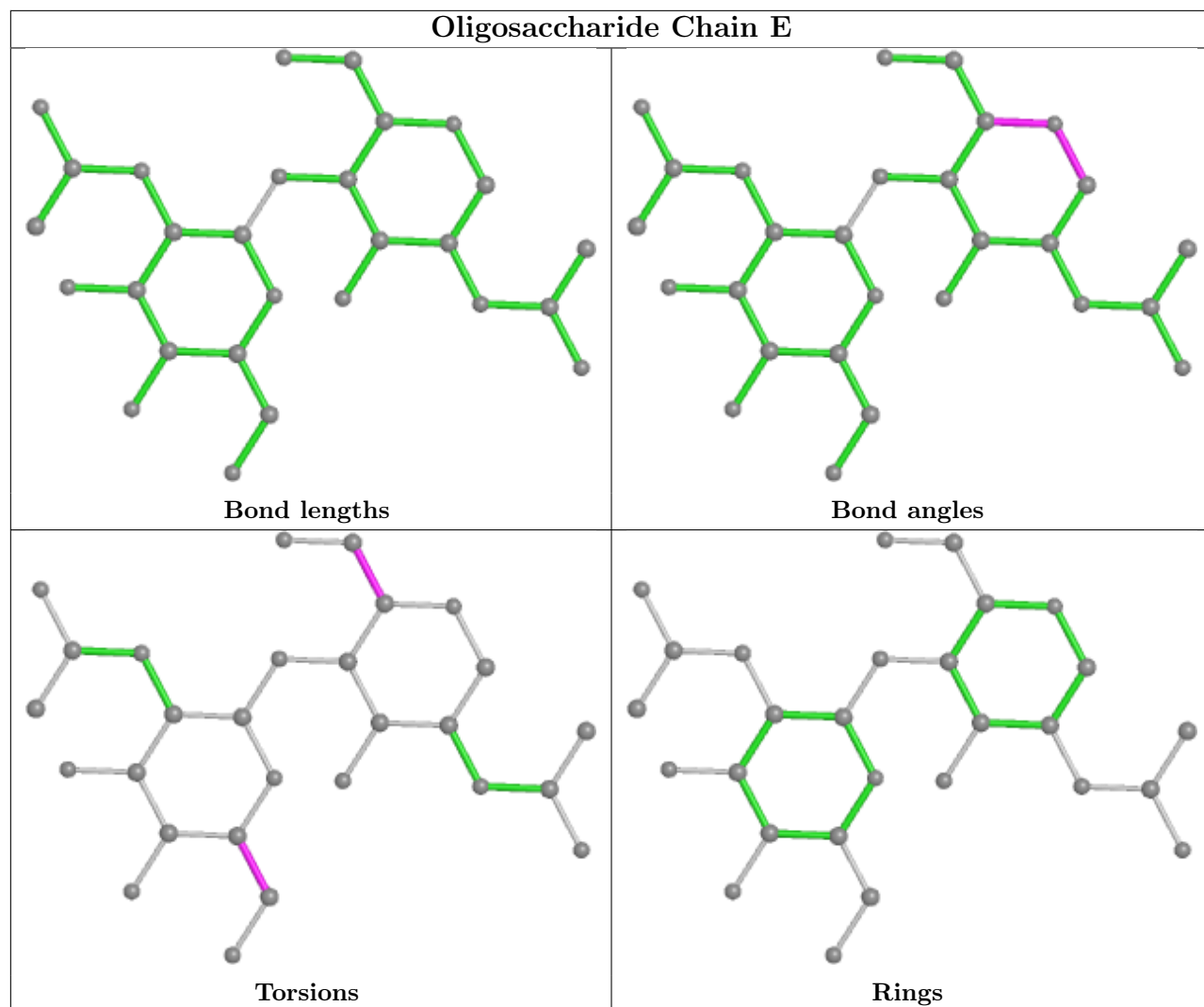
There are no ring outliers.

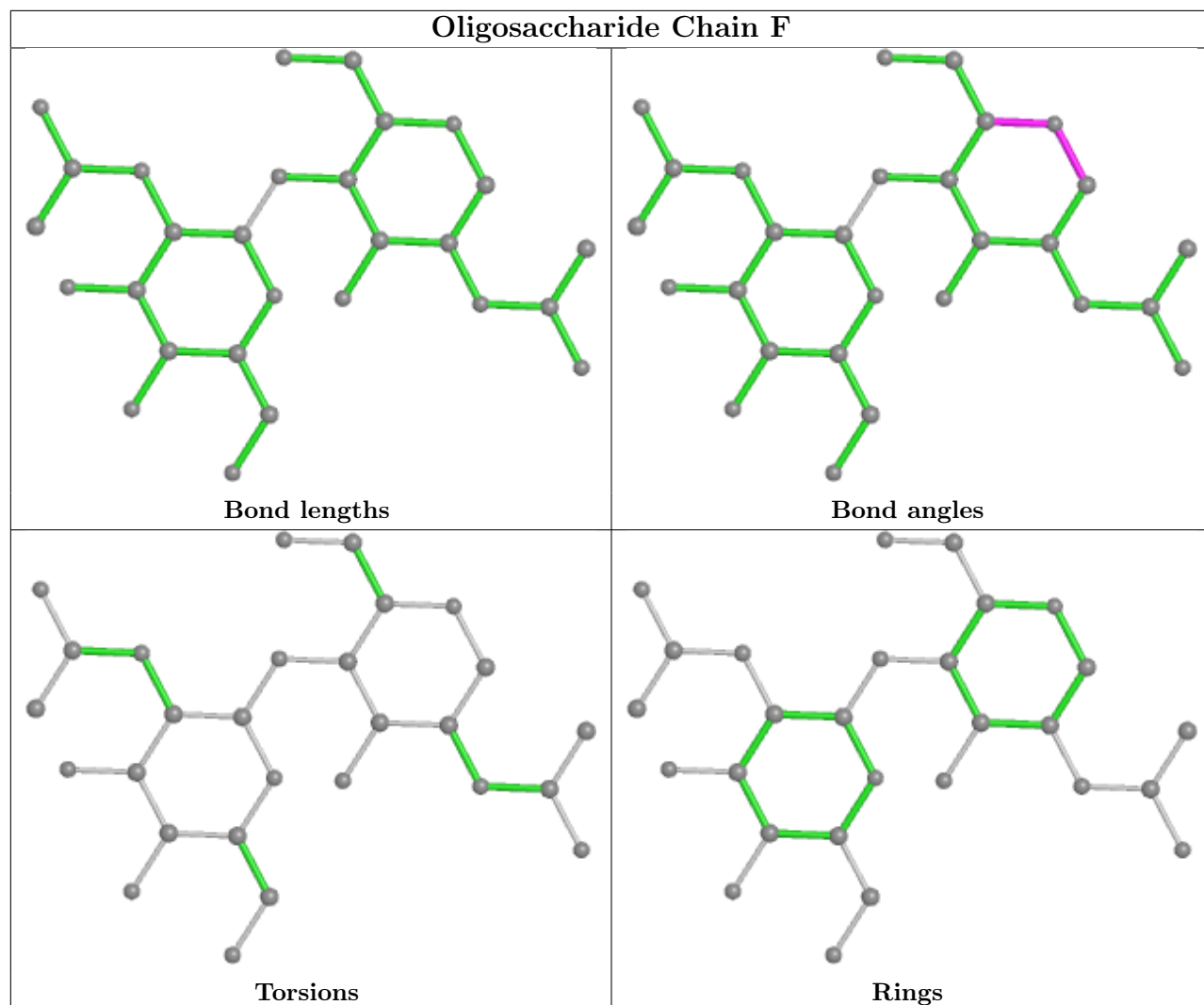
7 monomers are involved in 6 short contacts:

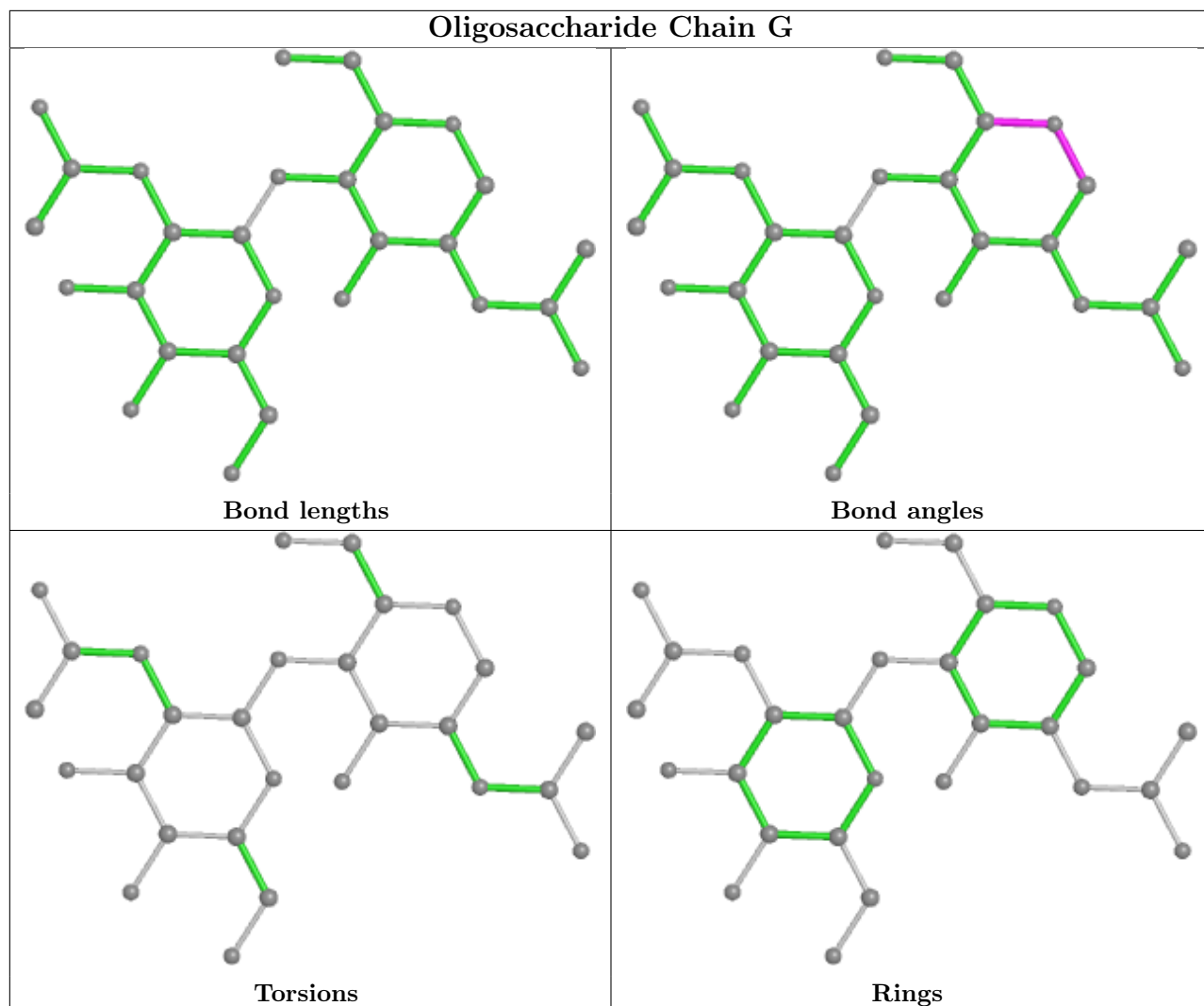
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2	NAG	1	0
4	P	1	NAG	3	0
4	T	2	NAG	1	0
4	Z	2	NAG	1	0
4	K	1	NAG	1	0
4	T	1	NAG	1	0
4	Z	1	NAG	1	0

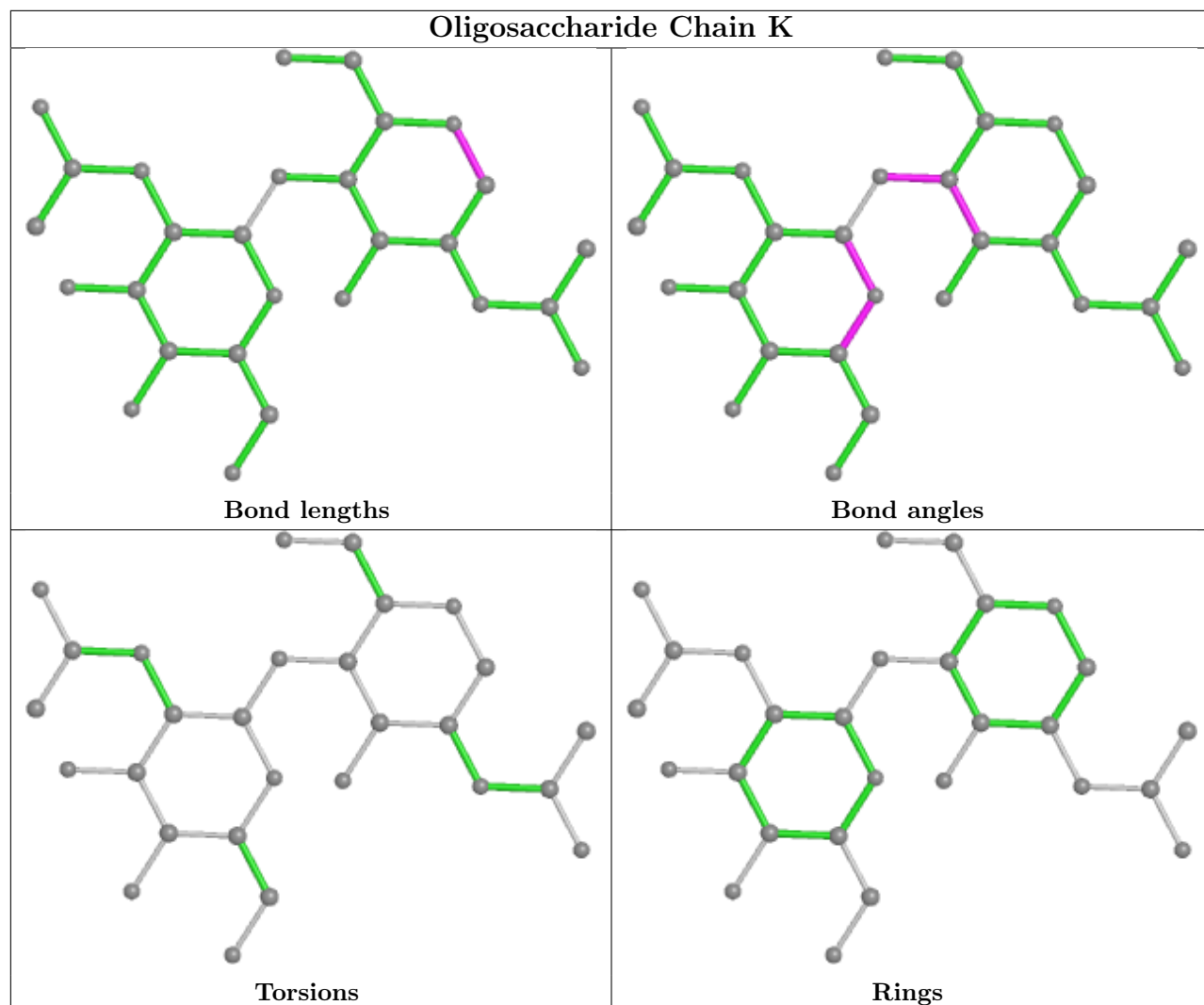
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

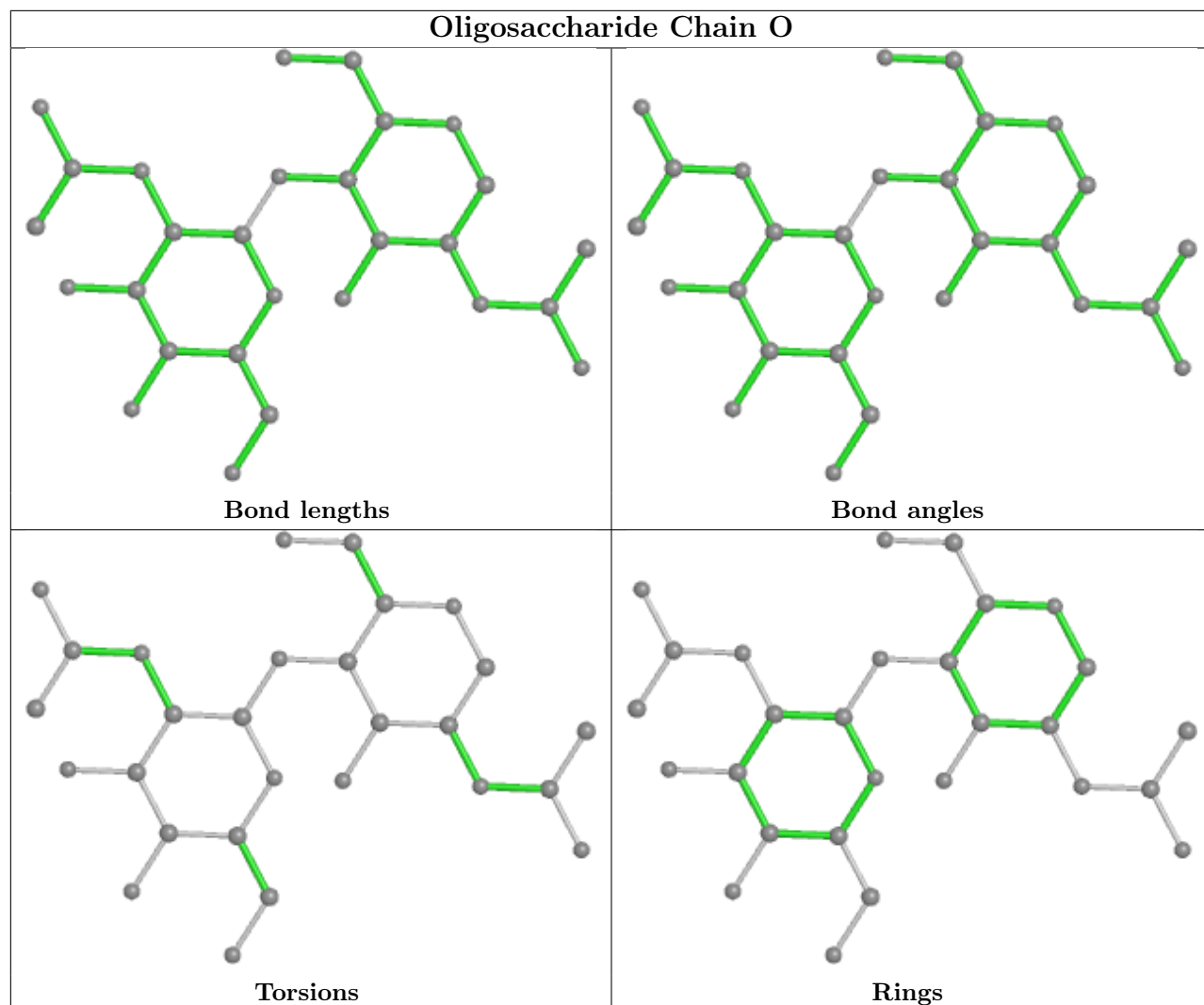


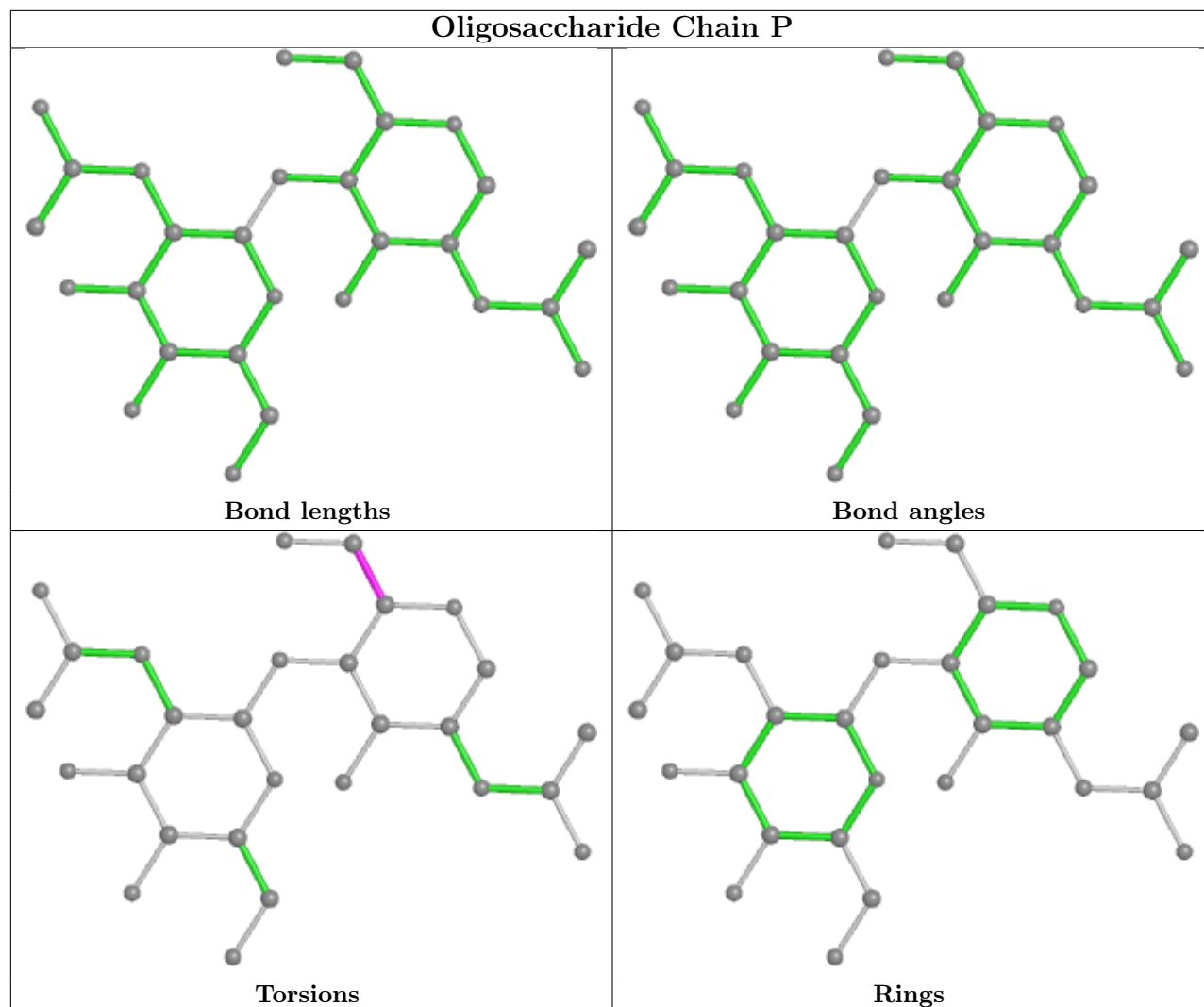


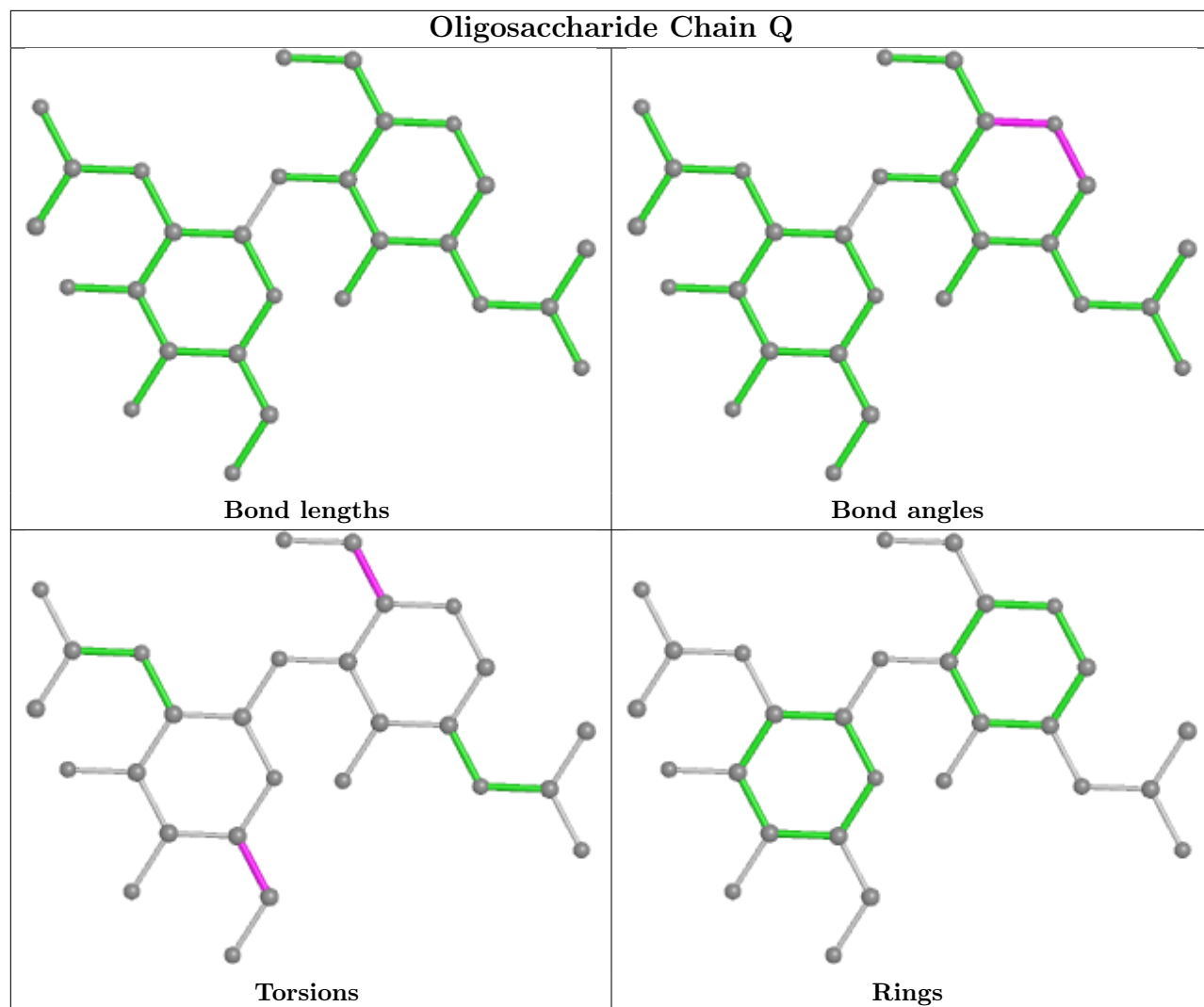


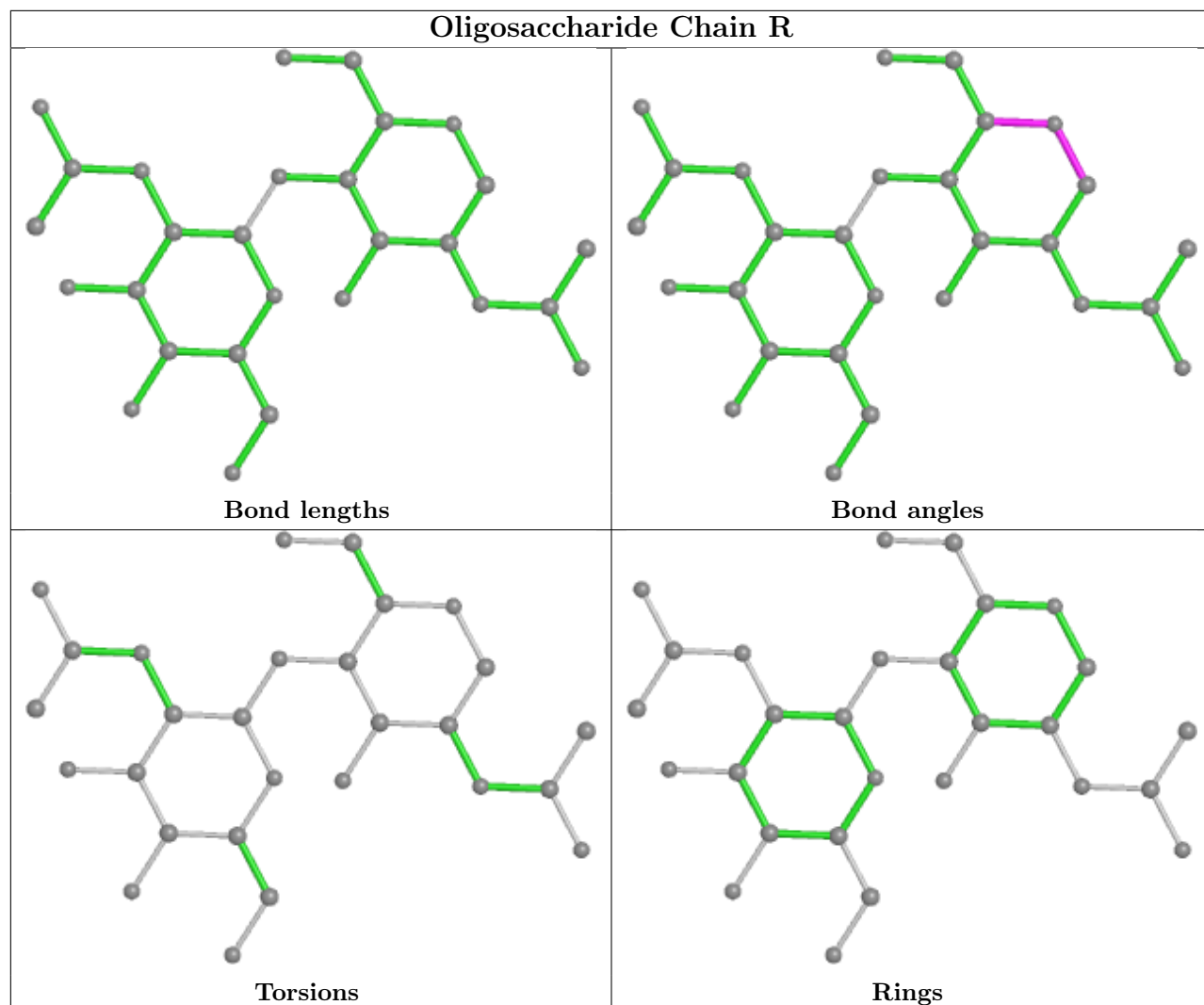


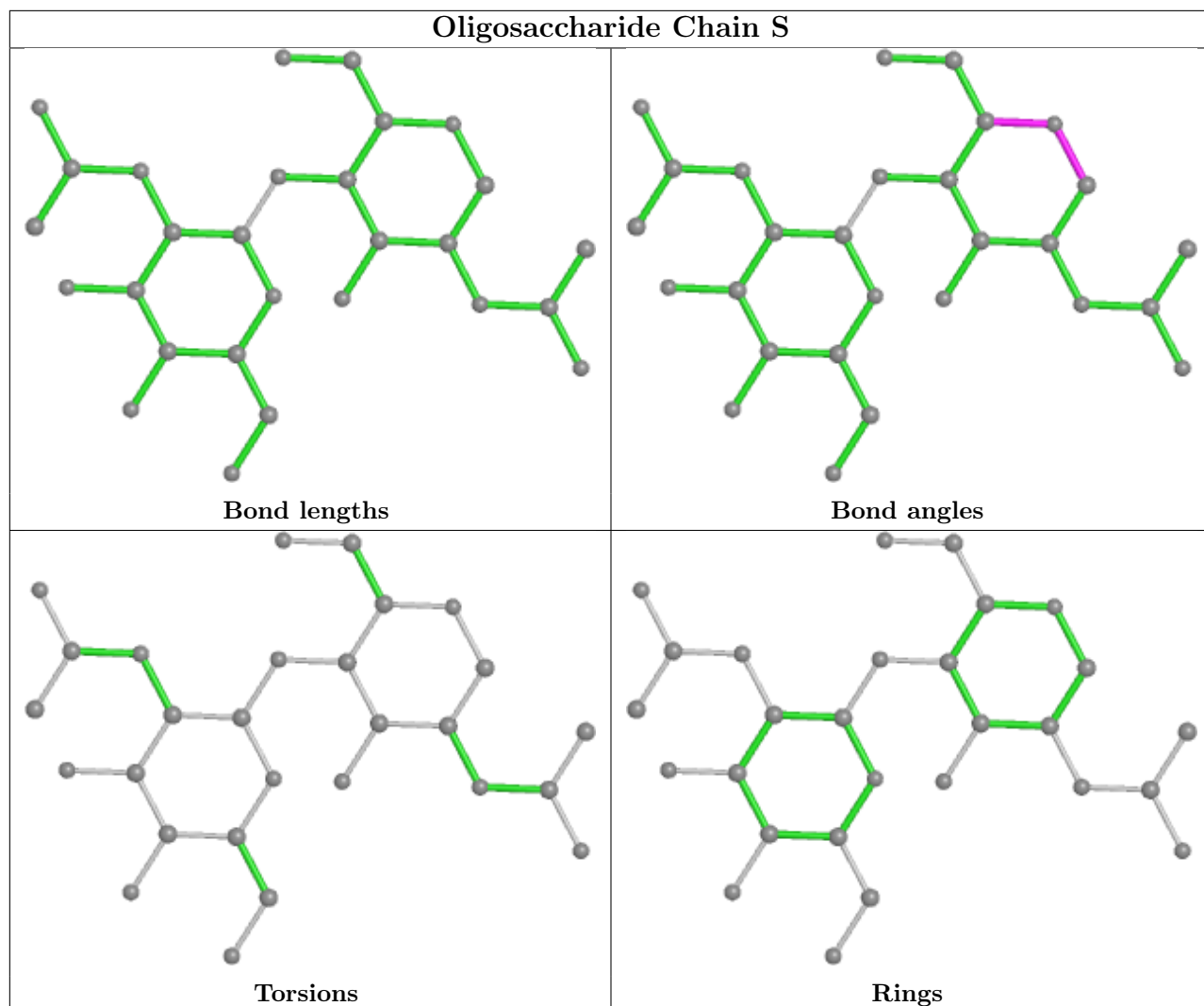


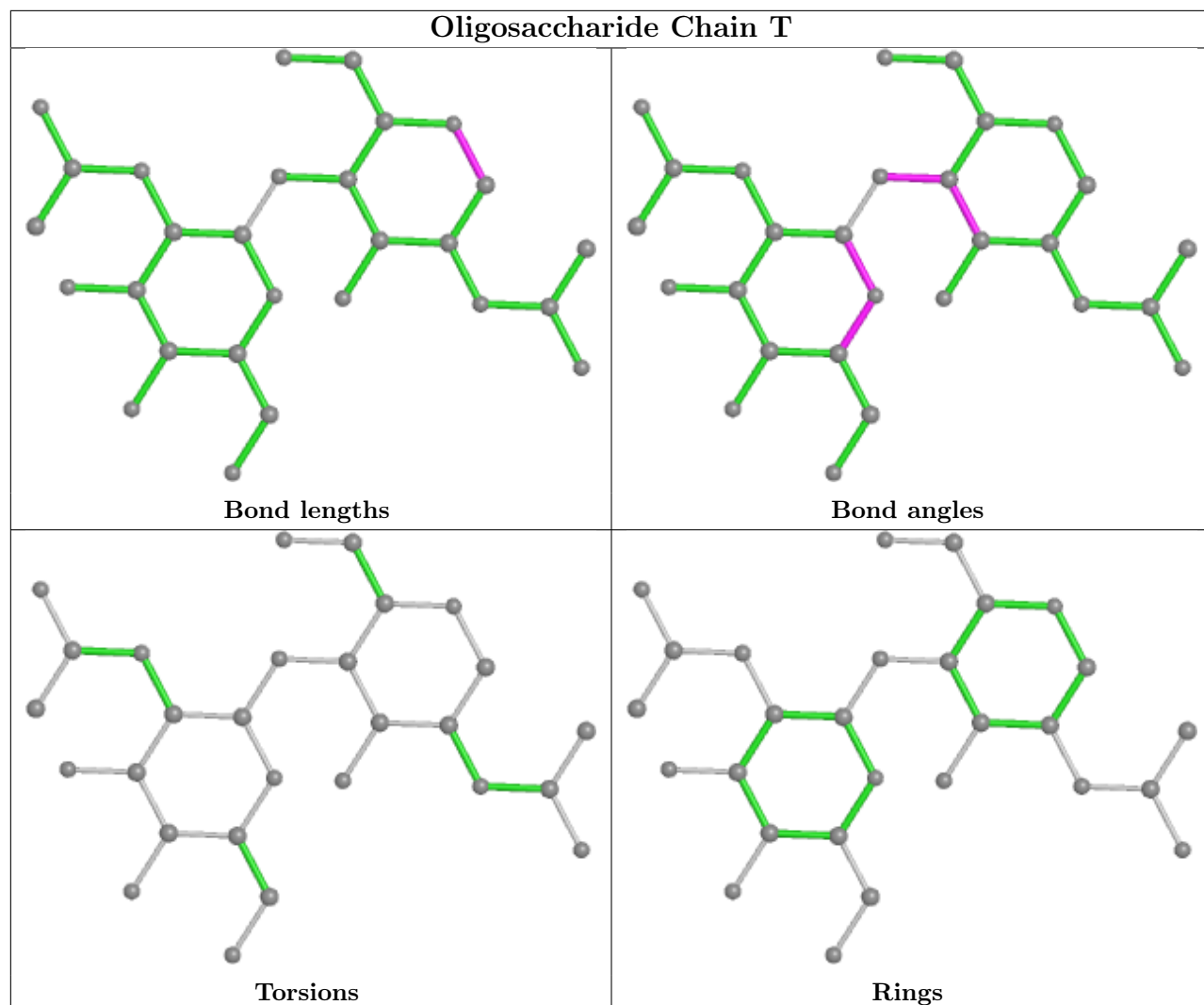


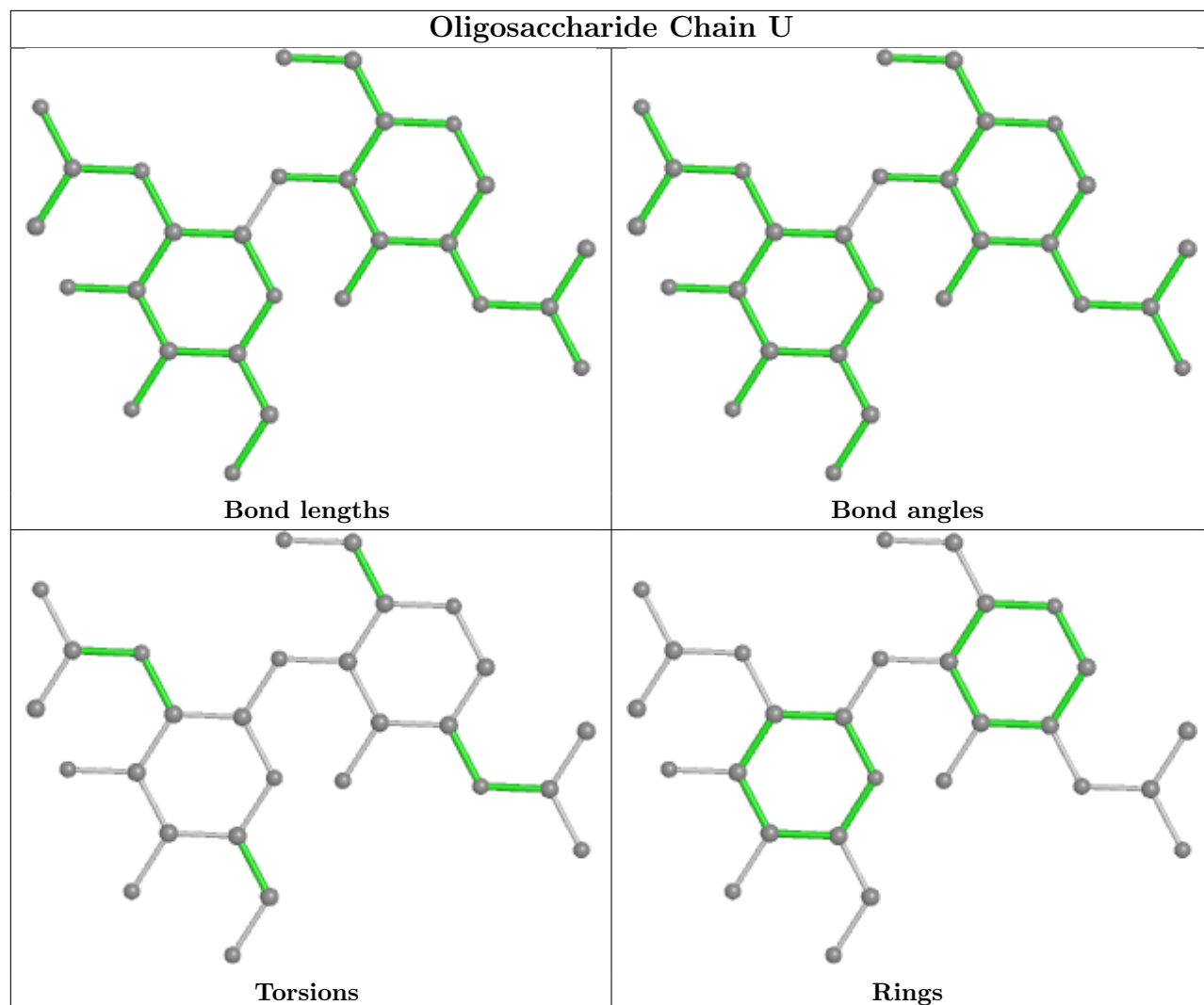


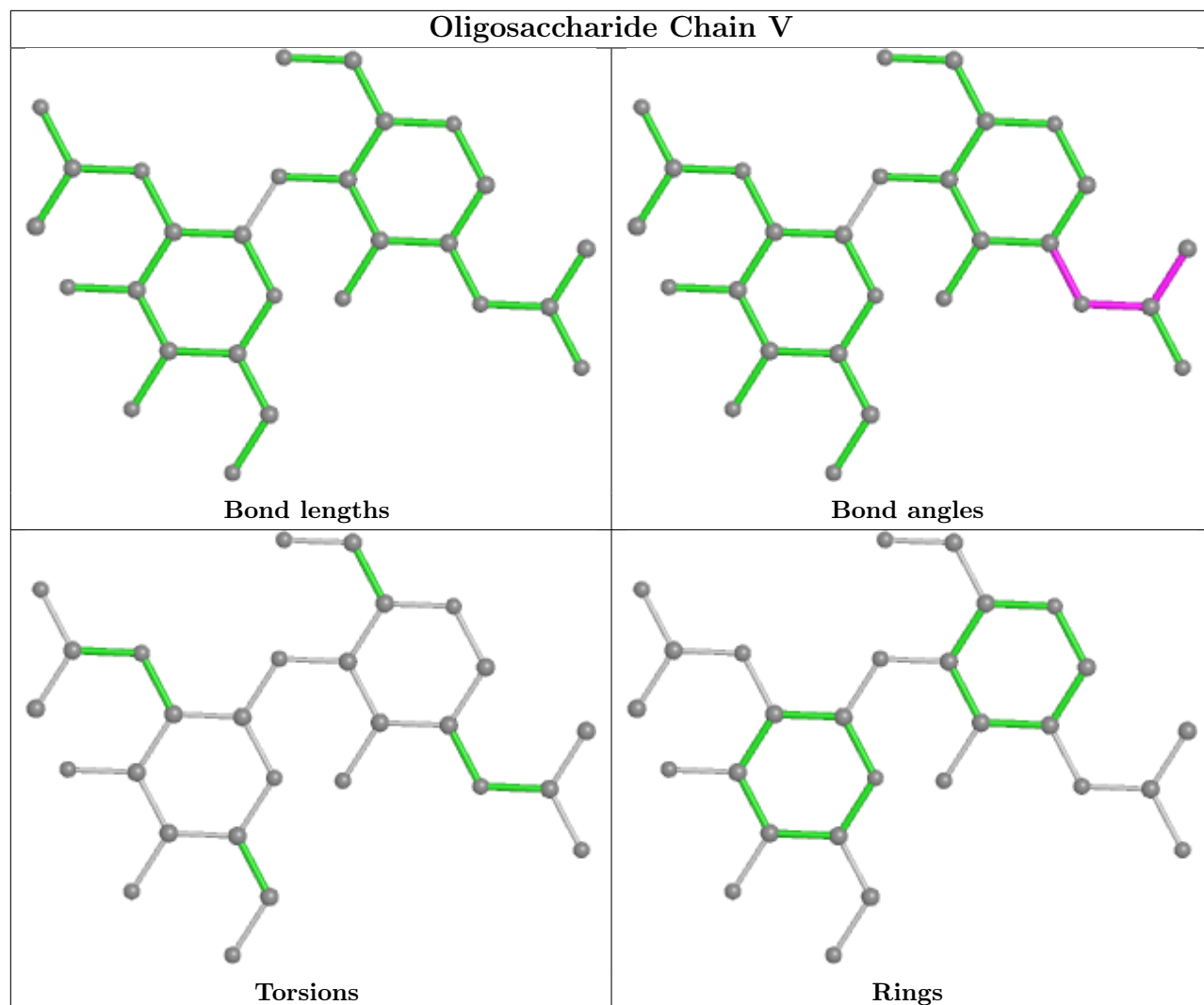


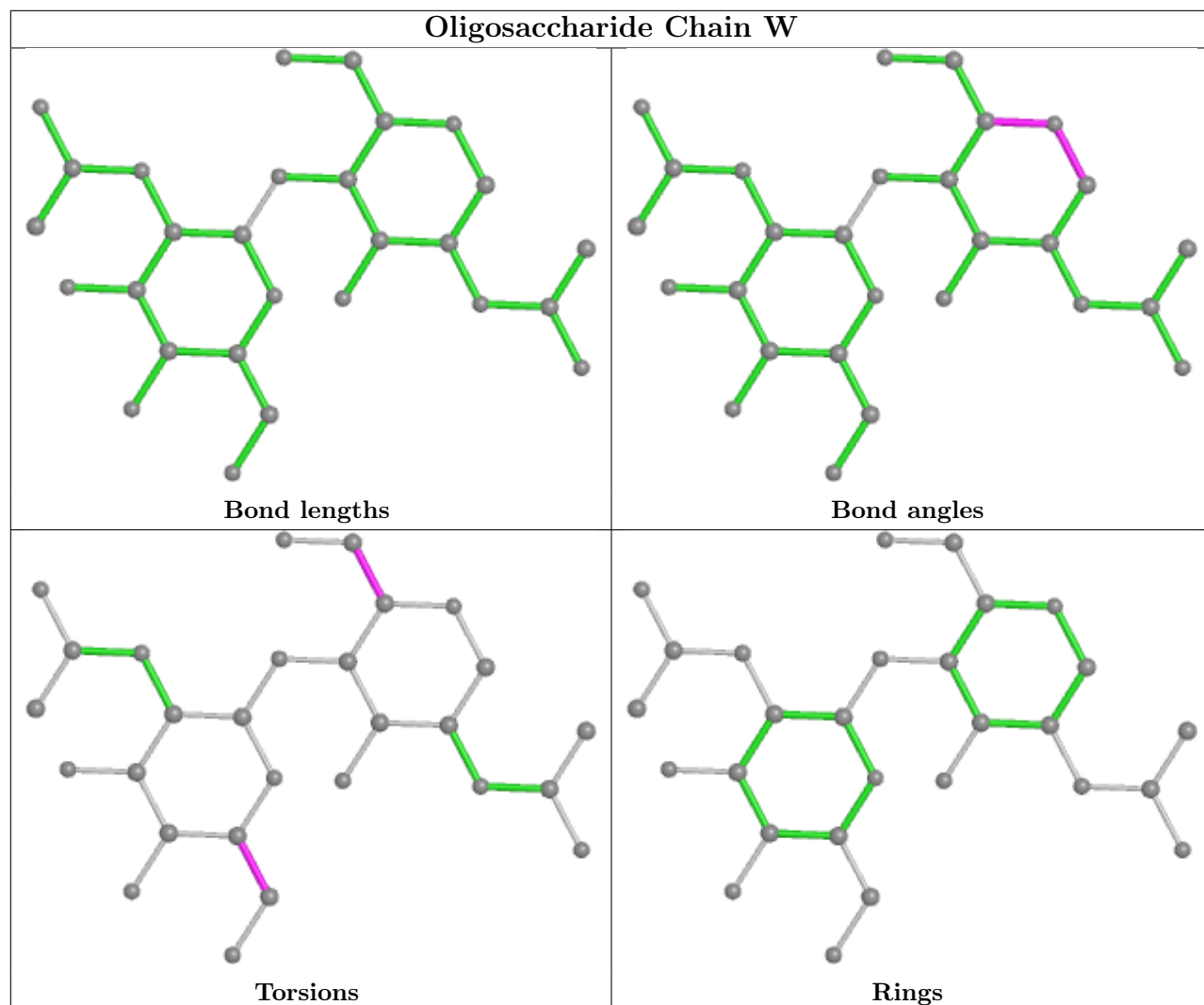


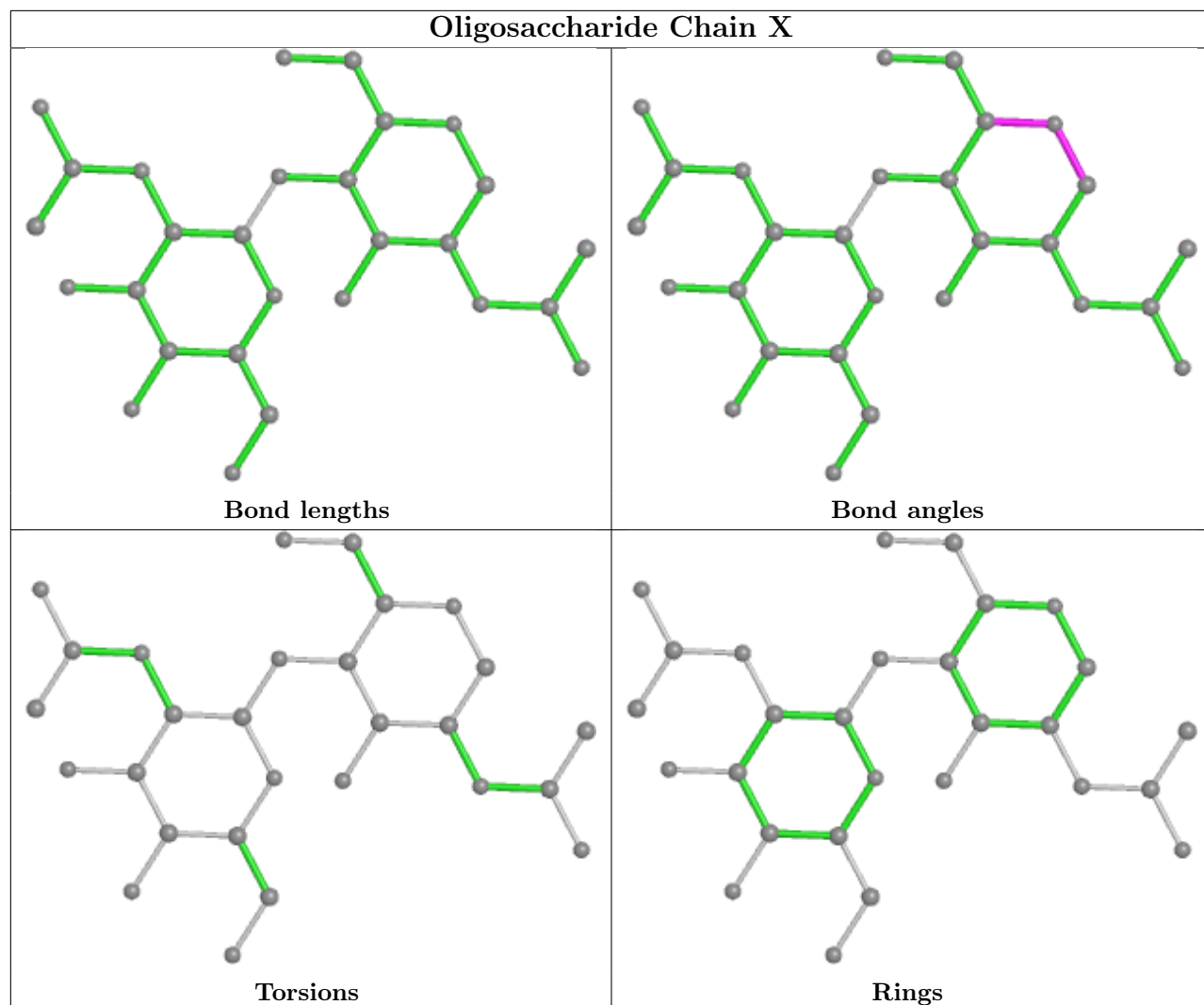


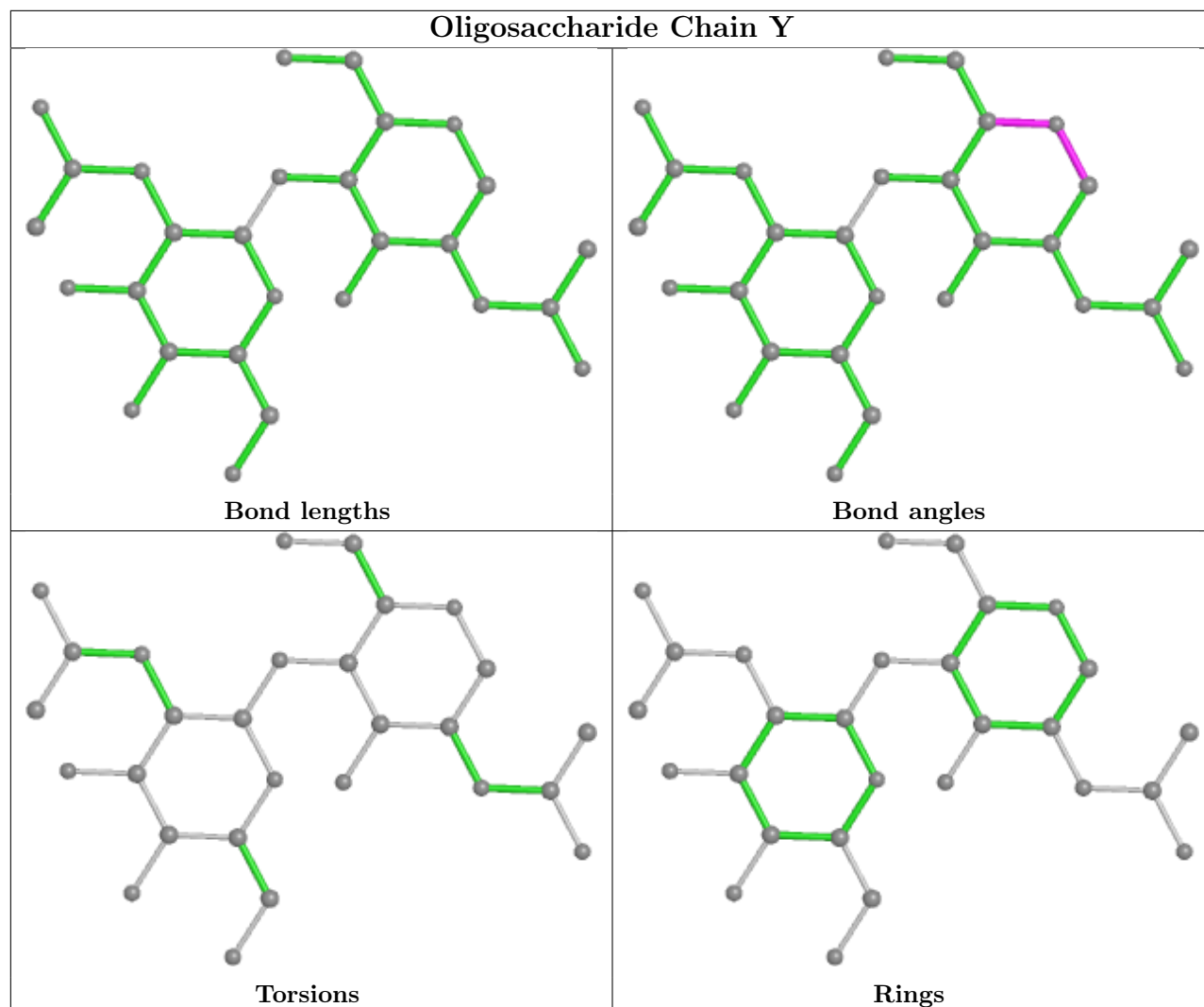


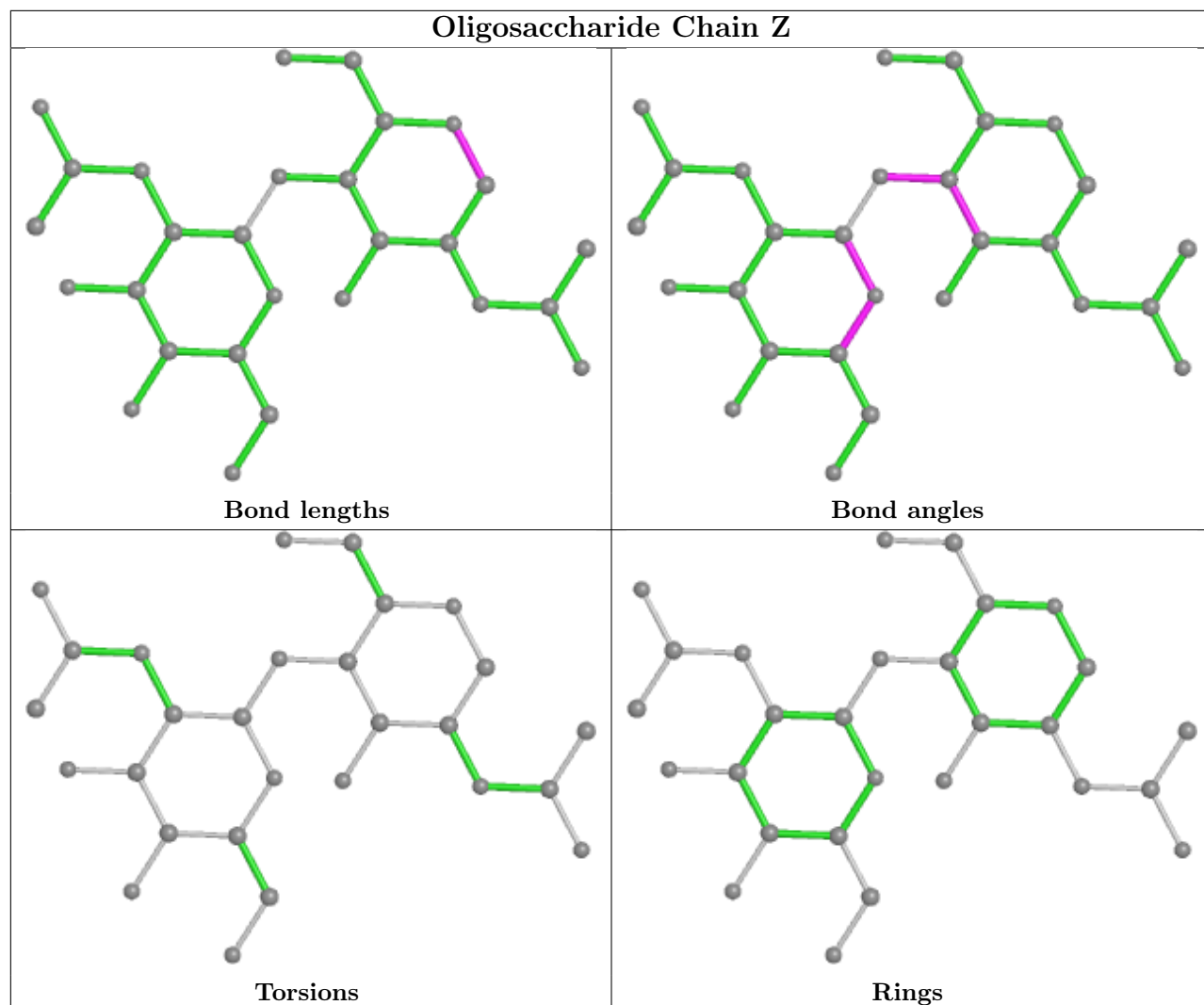


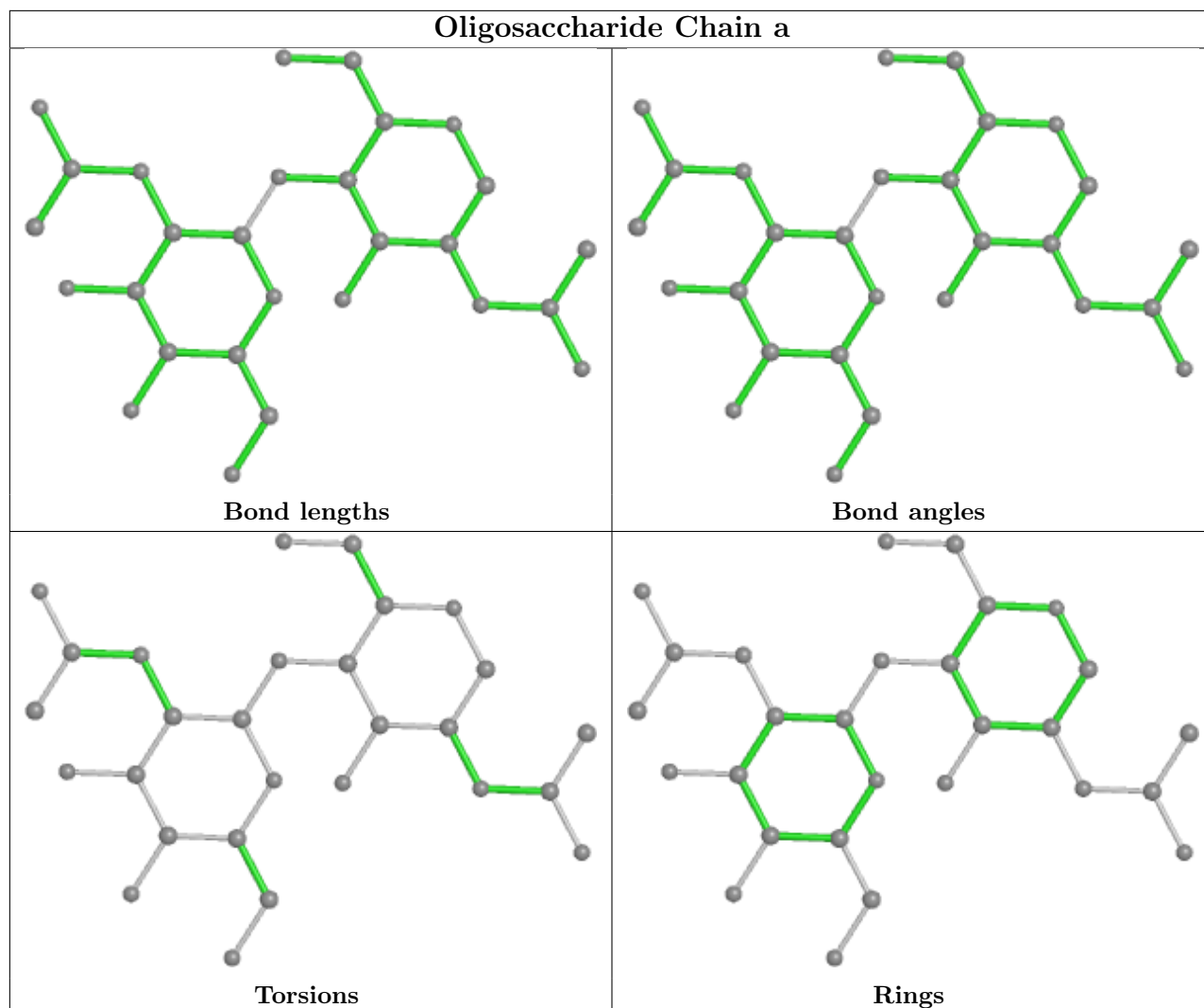












5.6 Ligand geometry [i](#)

33 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	C	1408	1	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	B	1404	1	14,14,15	0.25	0	17,19,21	0.58	0
5	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	C	1401	1	14,14,15	0.25	0	17,19,21	0.53	0
5	NAG	B	1401	1	14,14,15	0.25	0	17,19,21	0.54	0
5	NAG	C	1410	1	14,14,15	0.42	0	17,19,21	1.13	2 (11%)
5	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	A	1405	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	C	1405	1	14,14,15	0.29	0	17,19,21	0.44	0
5	NAG	B	1405	1	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	A	1403	1	14,14,15	0.31	0	17,19,21	0.43	0
5	NAG	B	1411	-	14,14,15	0.35	0	17,19,21	0.42	0
5	NAG	C	1403	1	14,14,15	0.31	0	17,19,21	0.43	0
5	NAG	B	1403	1	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	A	1409	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	A	1410	1	14,14,15	0.41	0	17,19,21	1.13	2 (11%)
5	NAG	B	1410	1	14,14,15	0.44	0	17,19,21	1.14	2 (11%)
5	NAG	C	1411	-	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
5	NAG	A	1404	1	14,14,15	0.24	0	17,19,21	0.58	0
5	NAG	A	1401	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	C	1406	1	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	C	1409	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	B	1409	1	14,14,15	0.31	0	17,19,21	0.41	0
5	NAG	A	1411	-	14,14,15	0.37	0	17,19,21	0.41	0
5	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.66	1 (5%)
5	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
5	NAG	C	1404	1	14,14,15	0.22	0	17,19,21	0.58	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	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	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	1404	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1402	NAG	C1-O5-C5	2.39	115.43	112.19
5	C	1402	NAG	C1-O5-C5	2.35	115.38	112.19
5	B	1402	NAG	C1-O5-C5	2.35	115.37	112.19
5	C	1410	NAG	C8-C7-N2	2.21	119.84	116.10
5	A	1410	NAG	C8-C7-N2	2.21	119.83	116.10
5	B	1410	NAG	C8-C7-N2	2.20	119.83	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1410	NAG	C2-N2-C7	-2.09	119.92	122.90
5	C	1410	NAG	C2-N2-C7	-2.07	119.95	122.90
5	A	1410	NAG	C2-N2-C7	-2.06	119.96	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 21 short contacts:

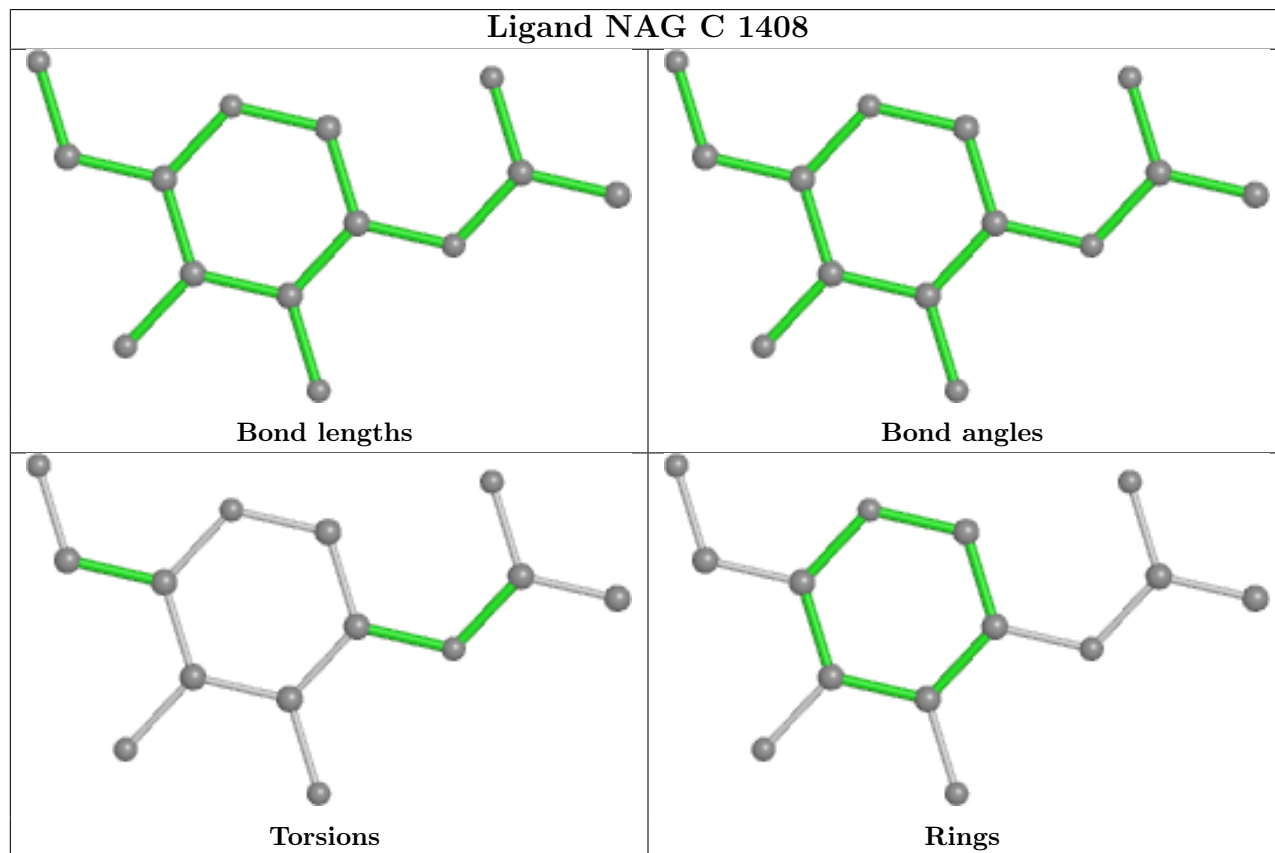
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1410	NAG	5	0
5	B	1411	NAG	4	0
5	A	1410	NAG	6	0
5	B	1410	NAG	6	0

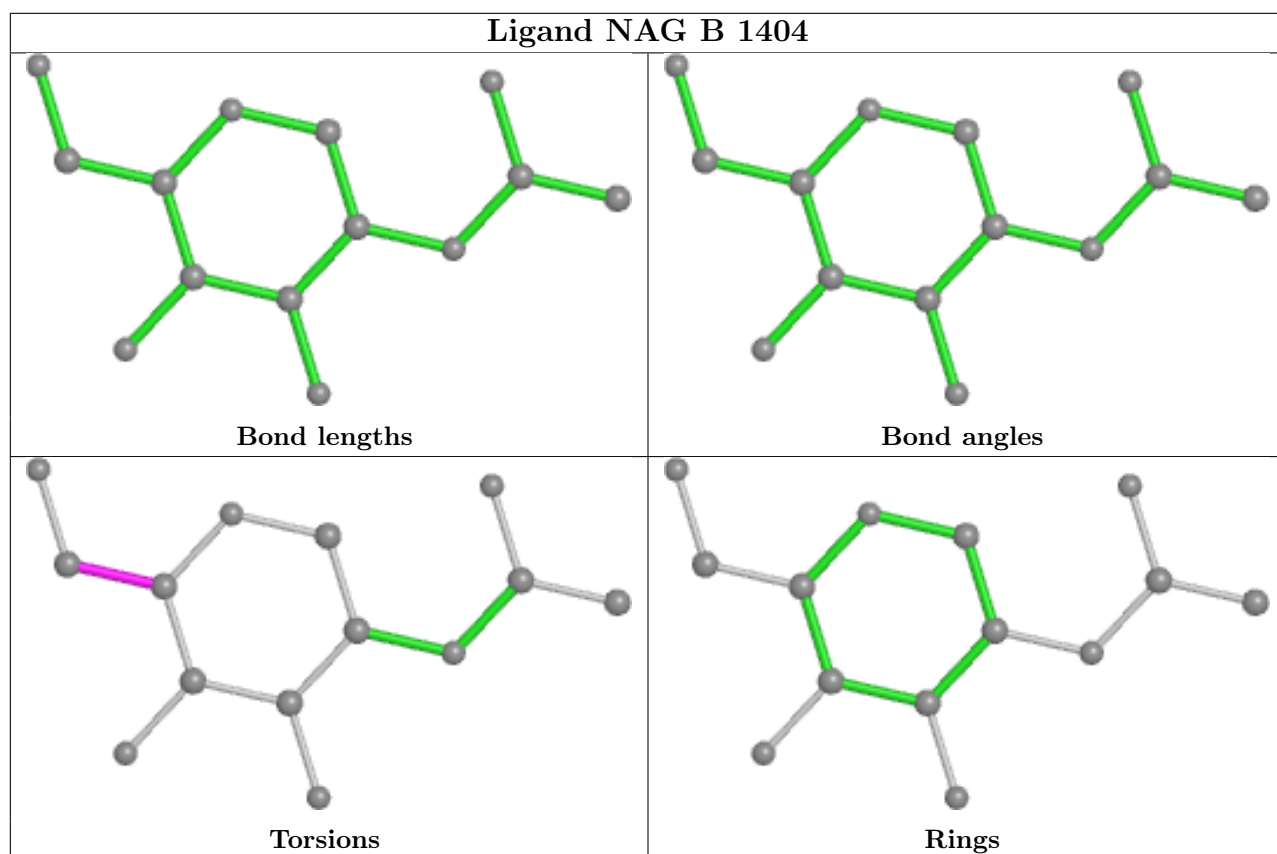
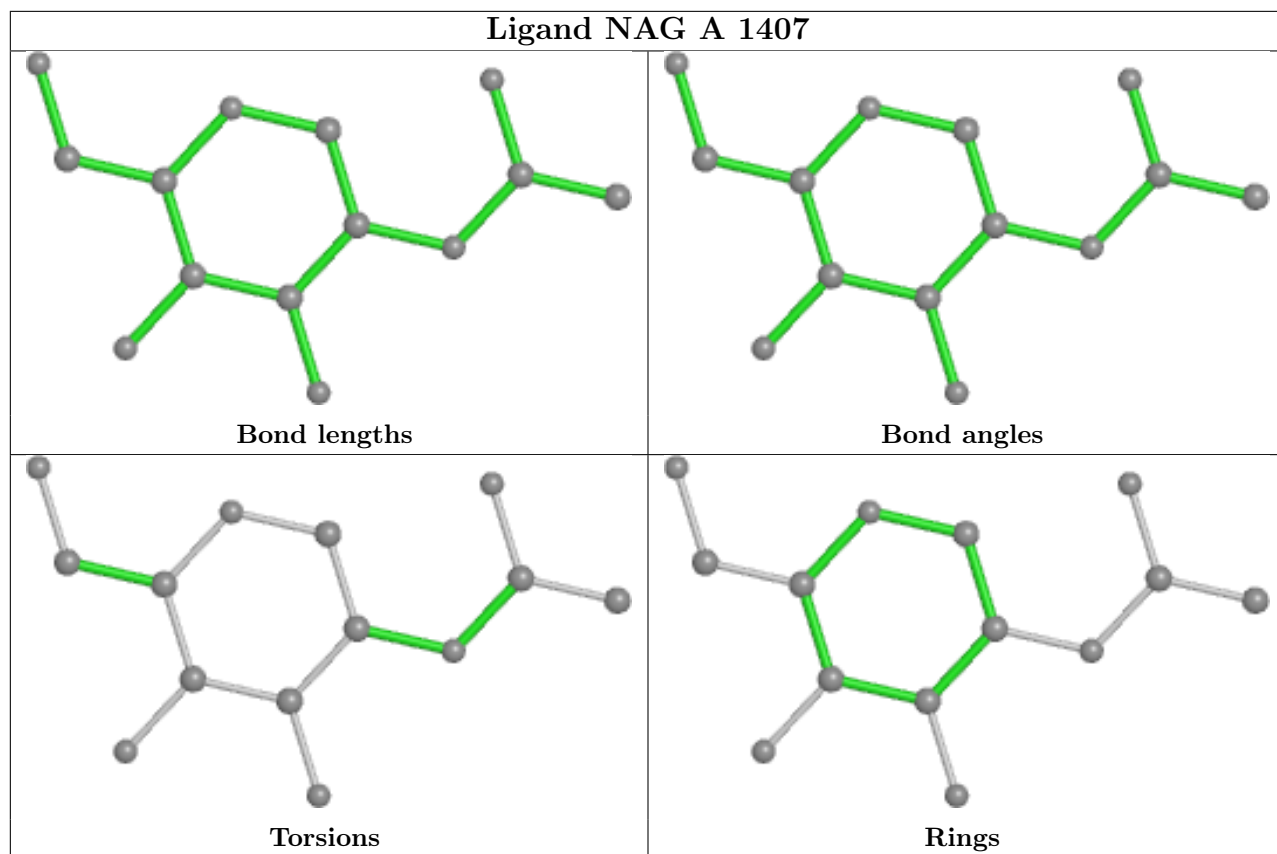
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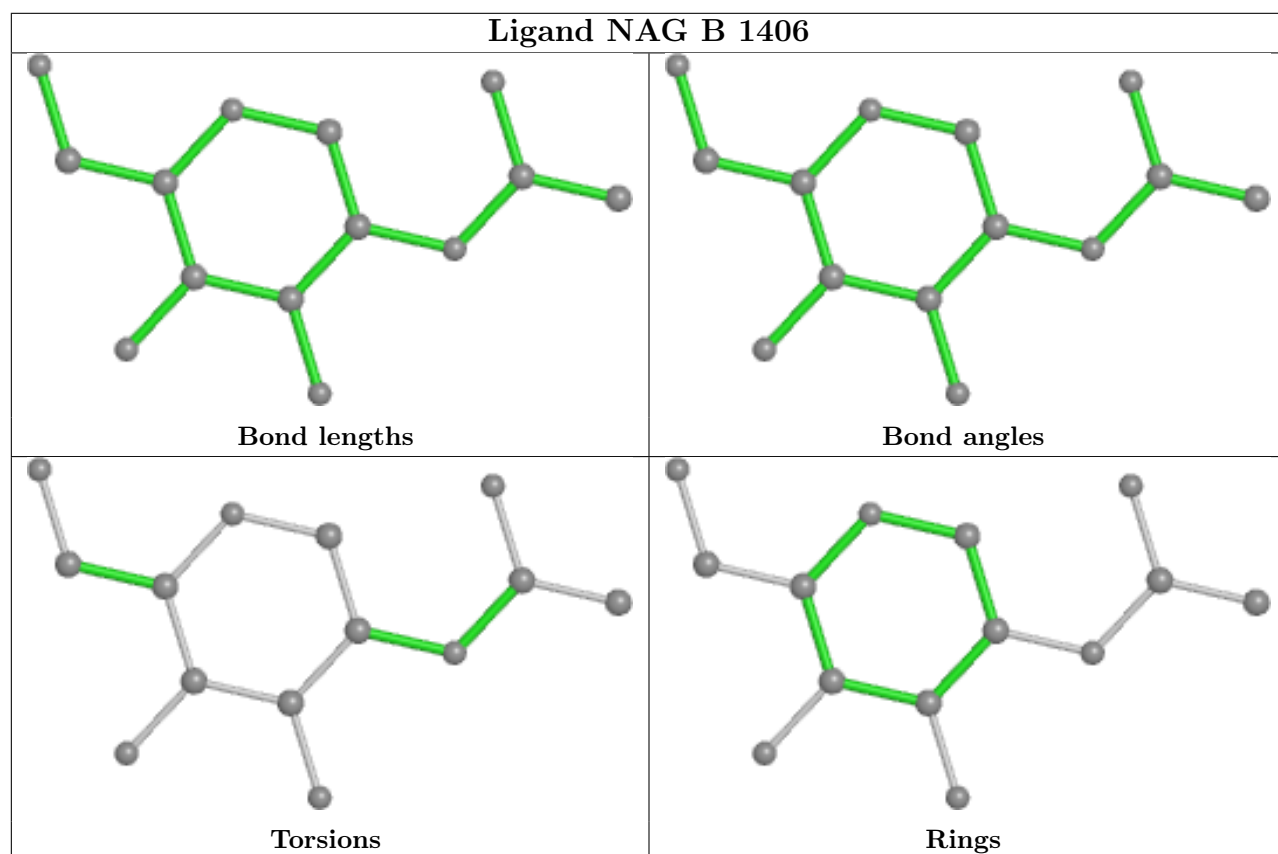
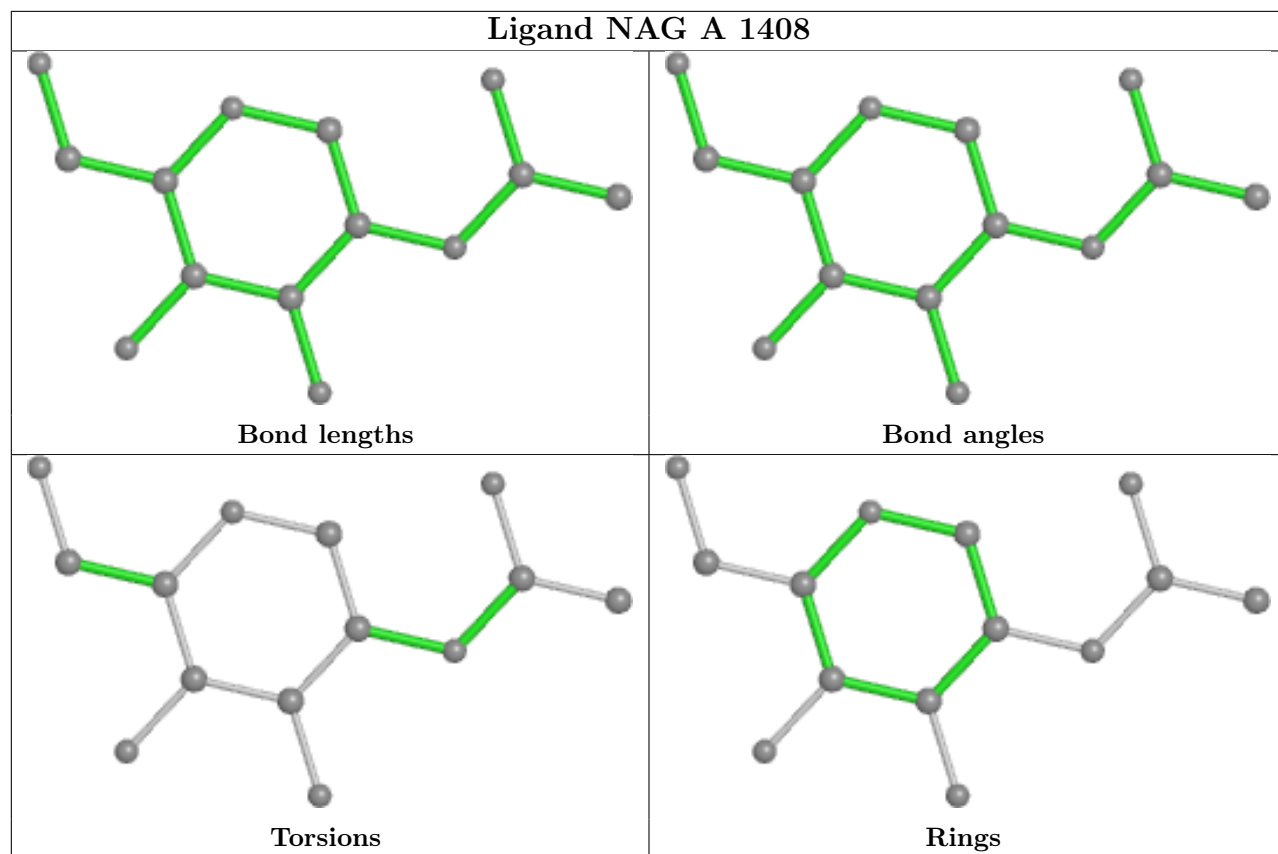
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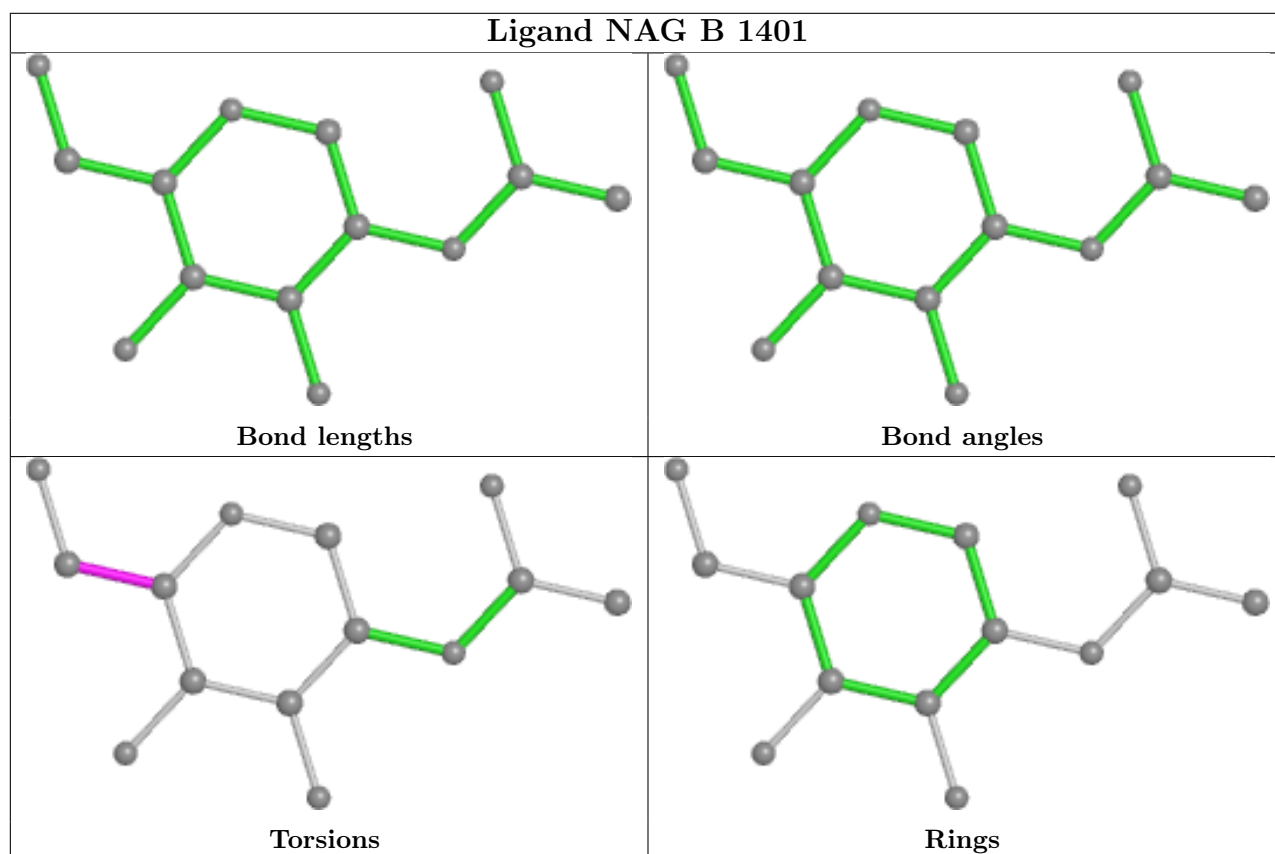
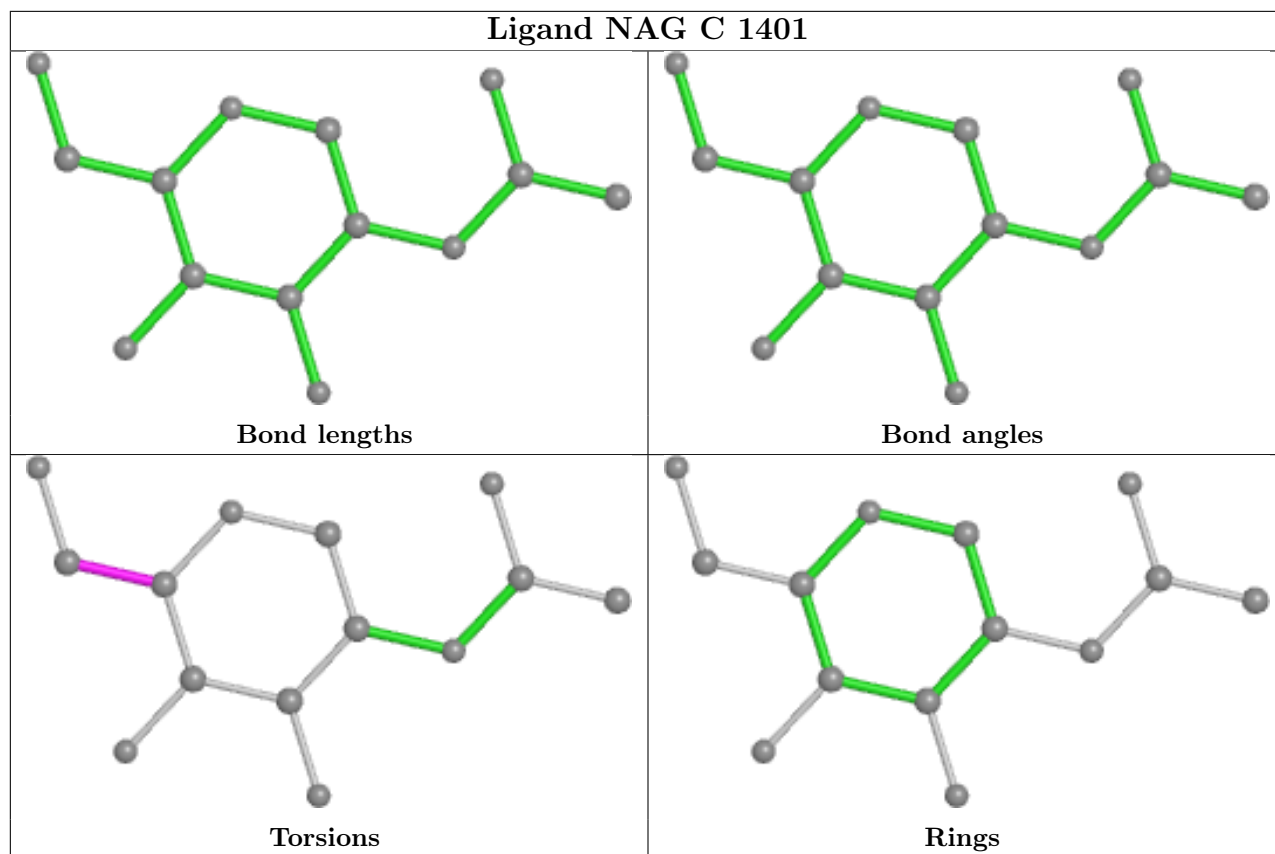
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1411	NAG	3	0
5	C	1402	NAG	1	0
5	A	1404	NAG	1	0
5	A	1411	NAG	4	0
5	A	1402	NAG	1	0
5	B	1402	NAG	1	0

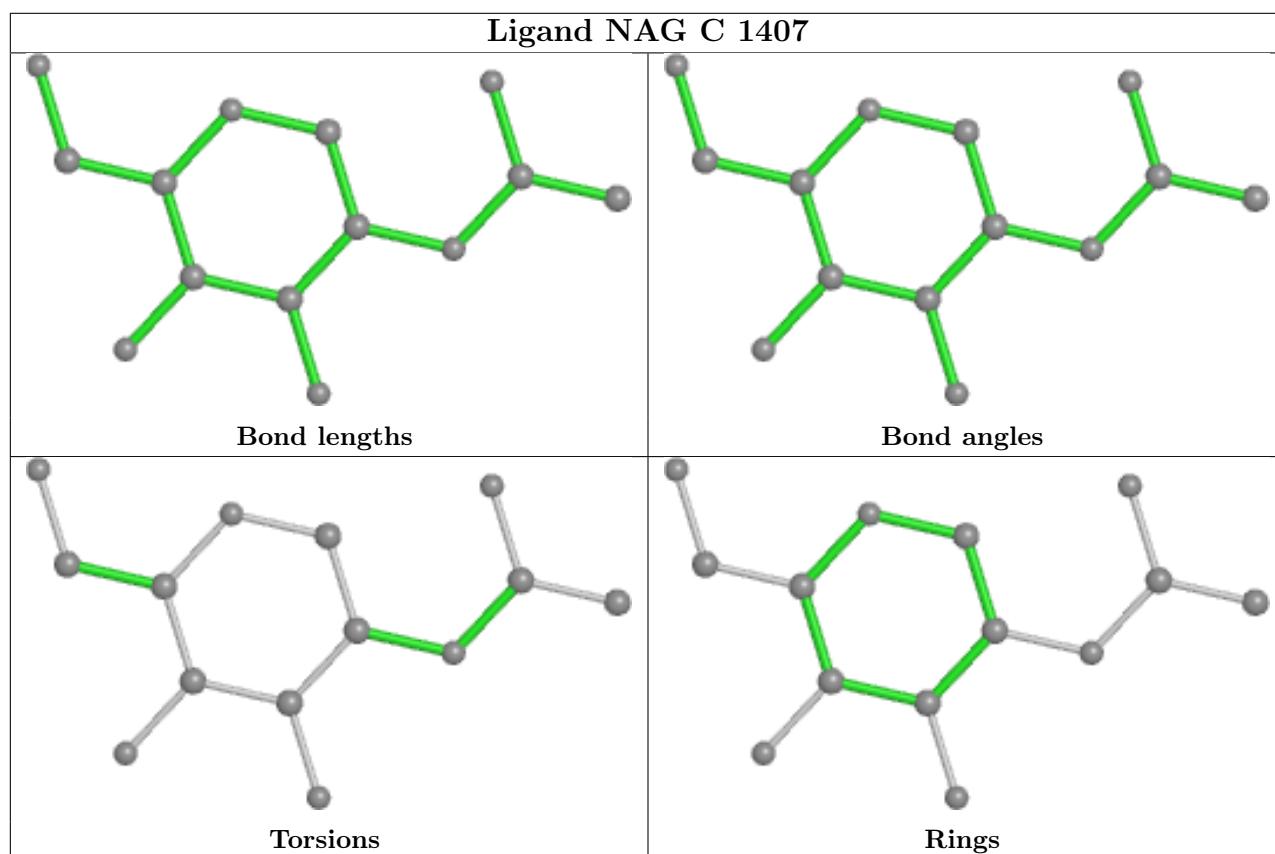
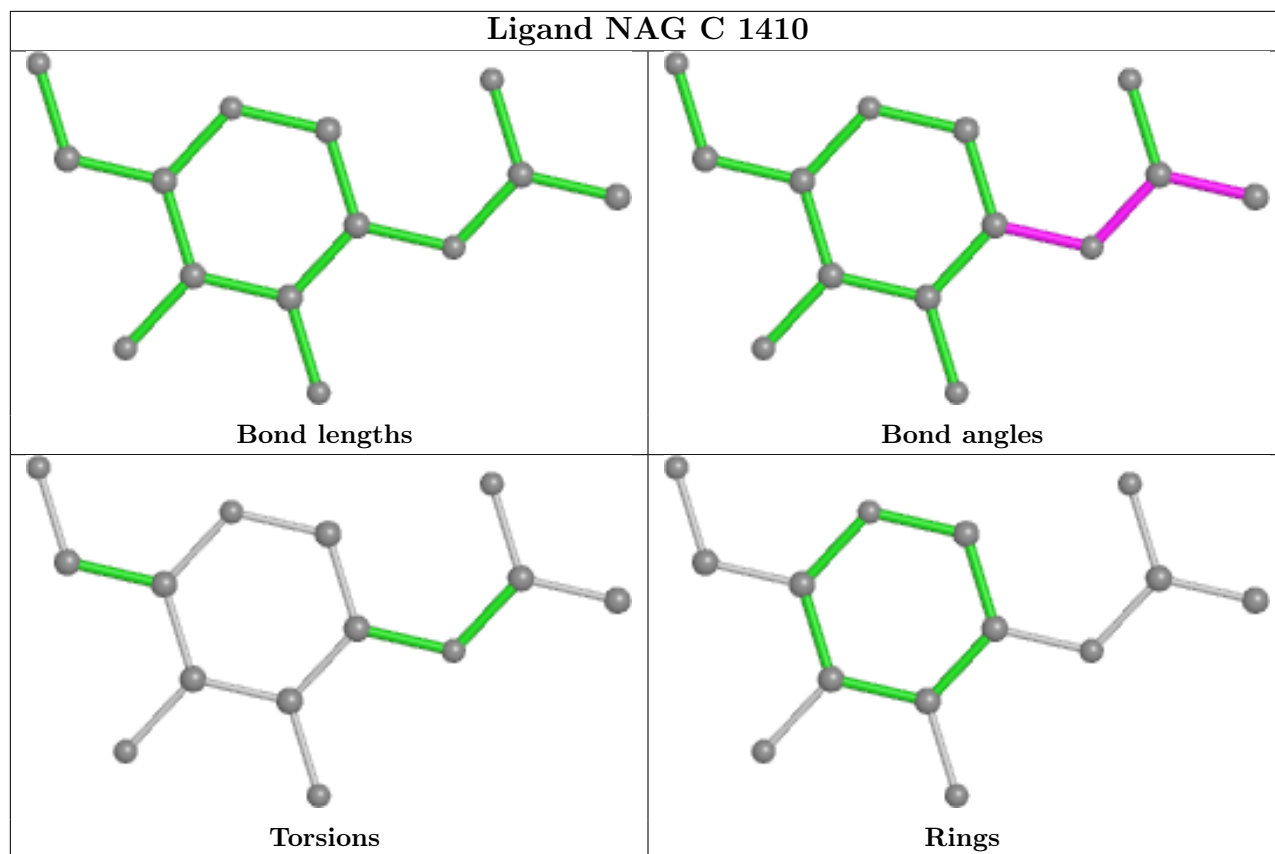
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

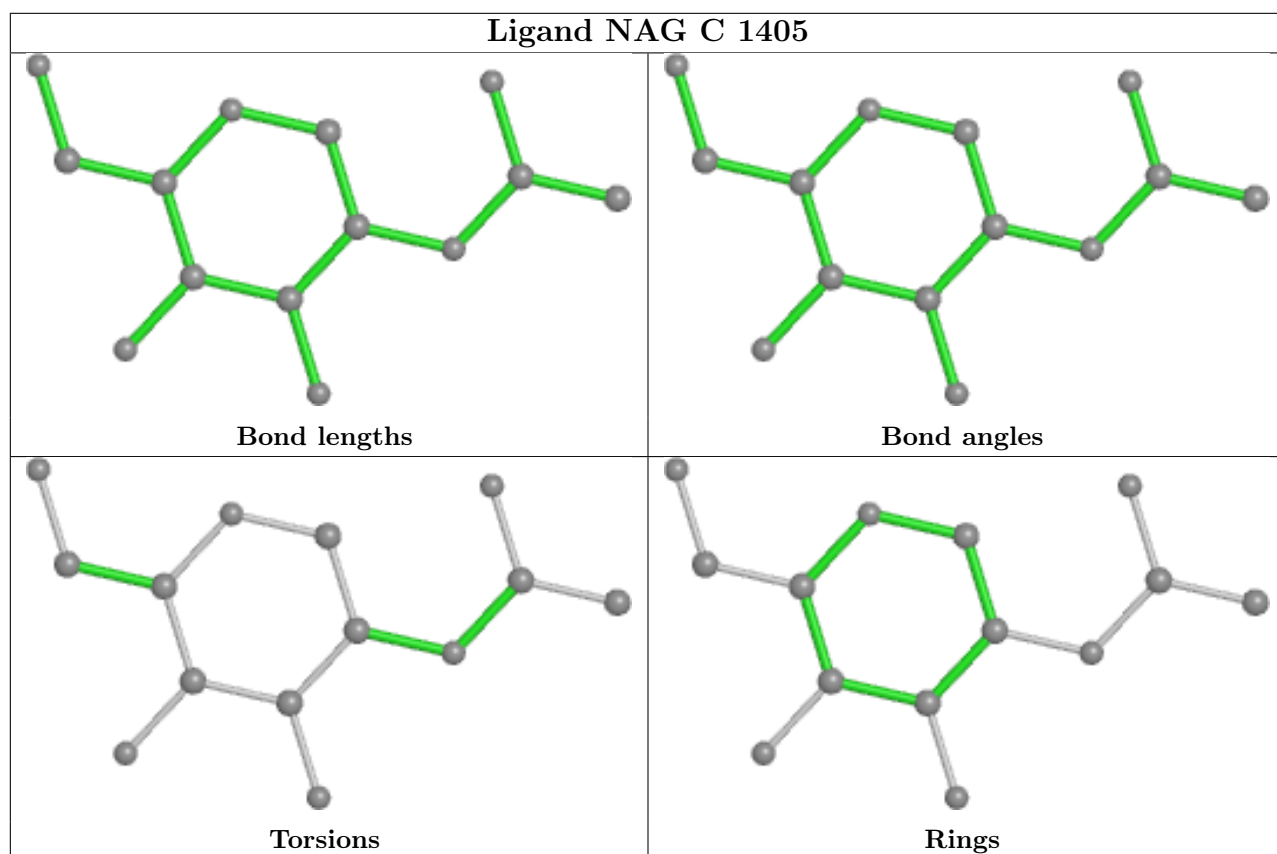
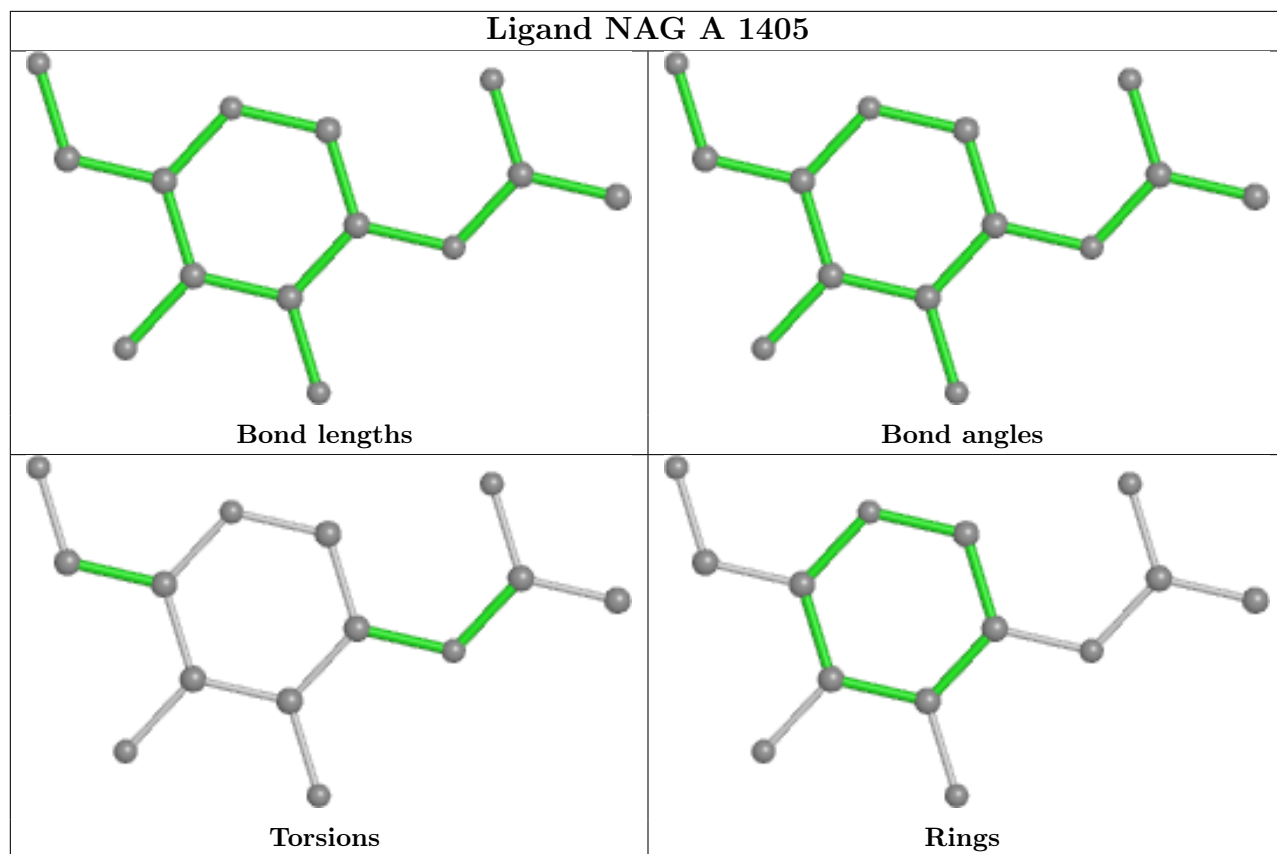


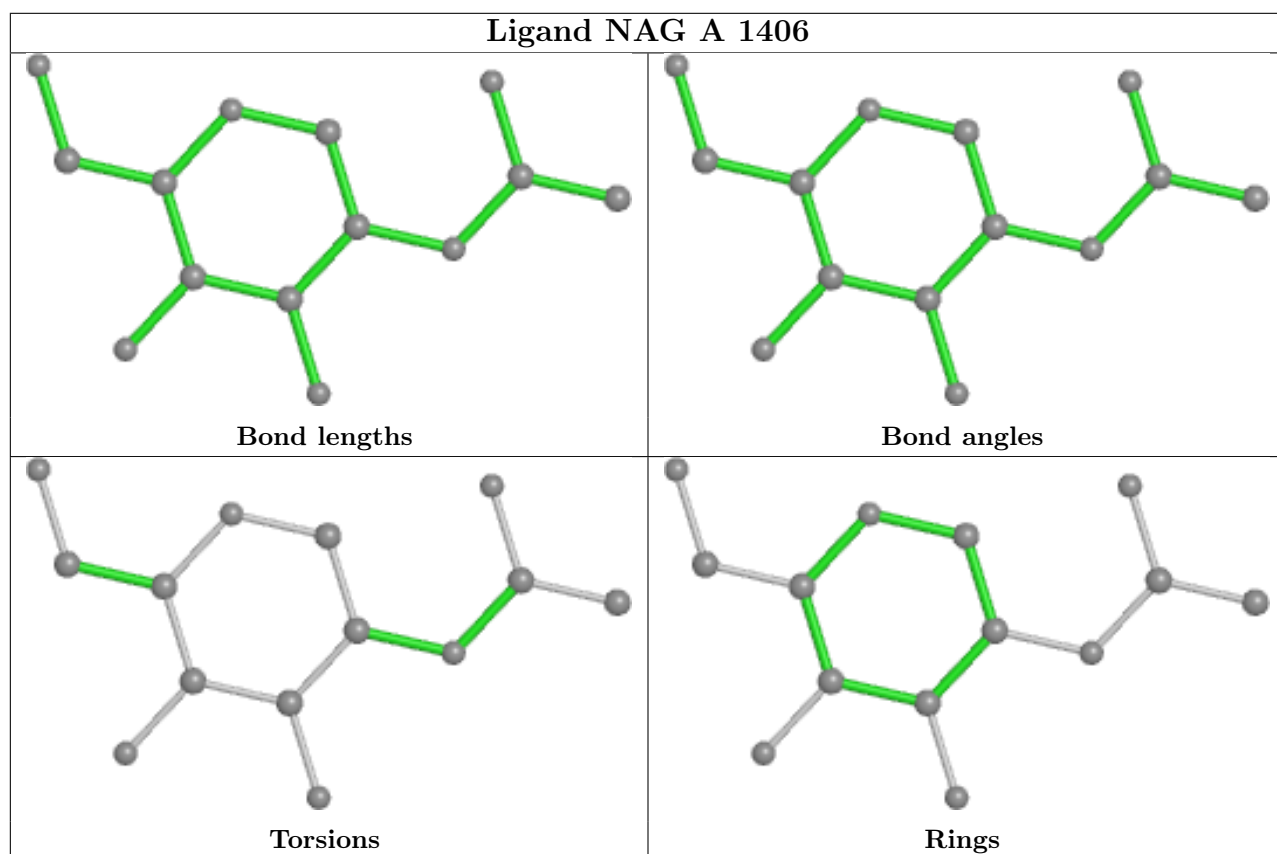
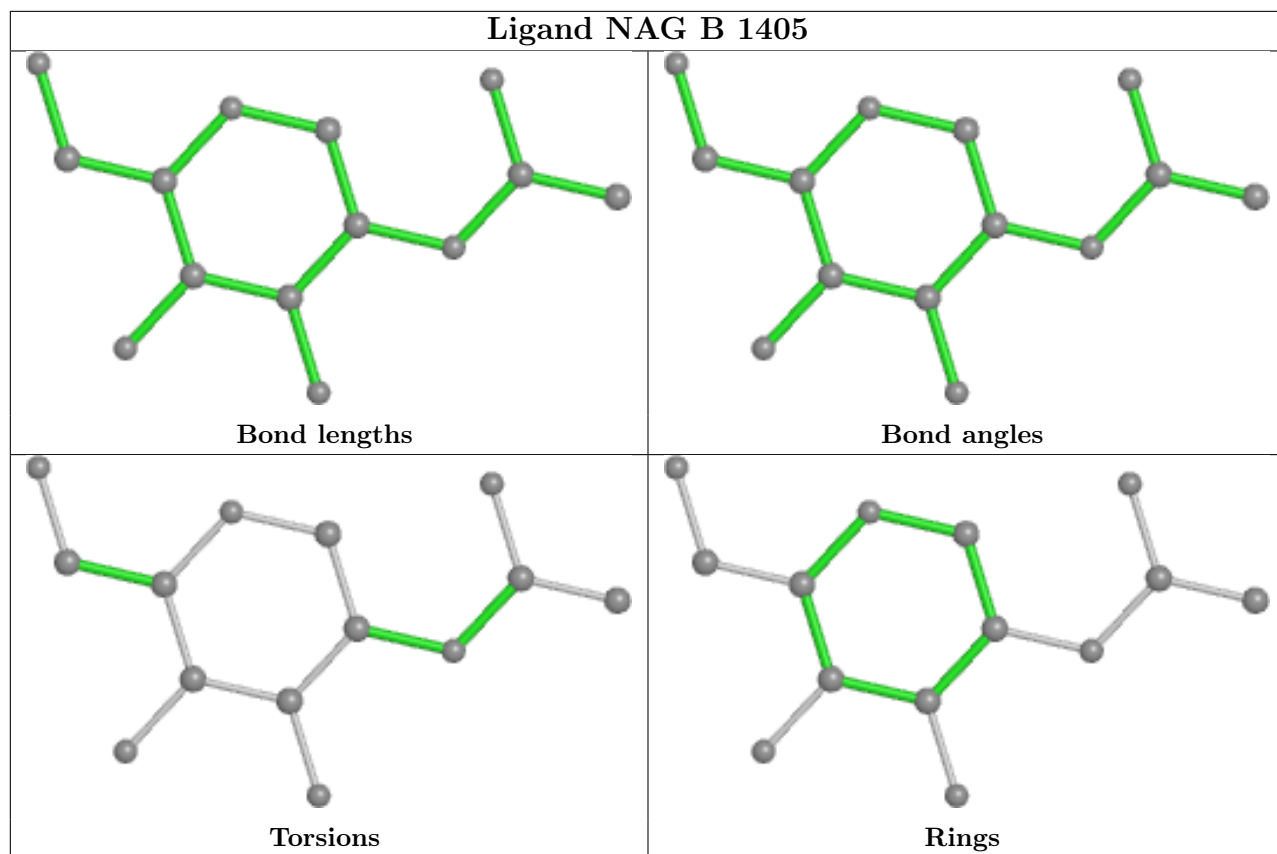


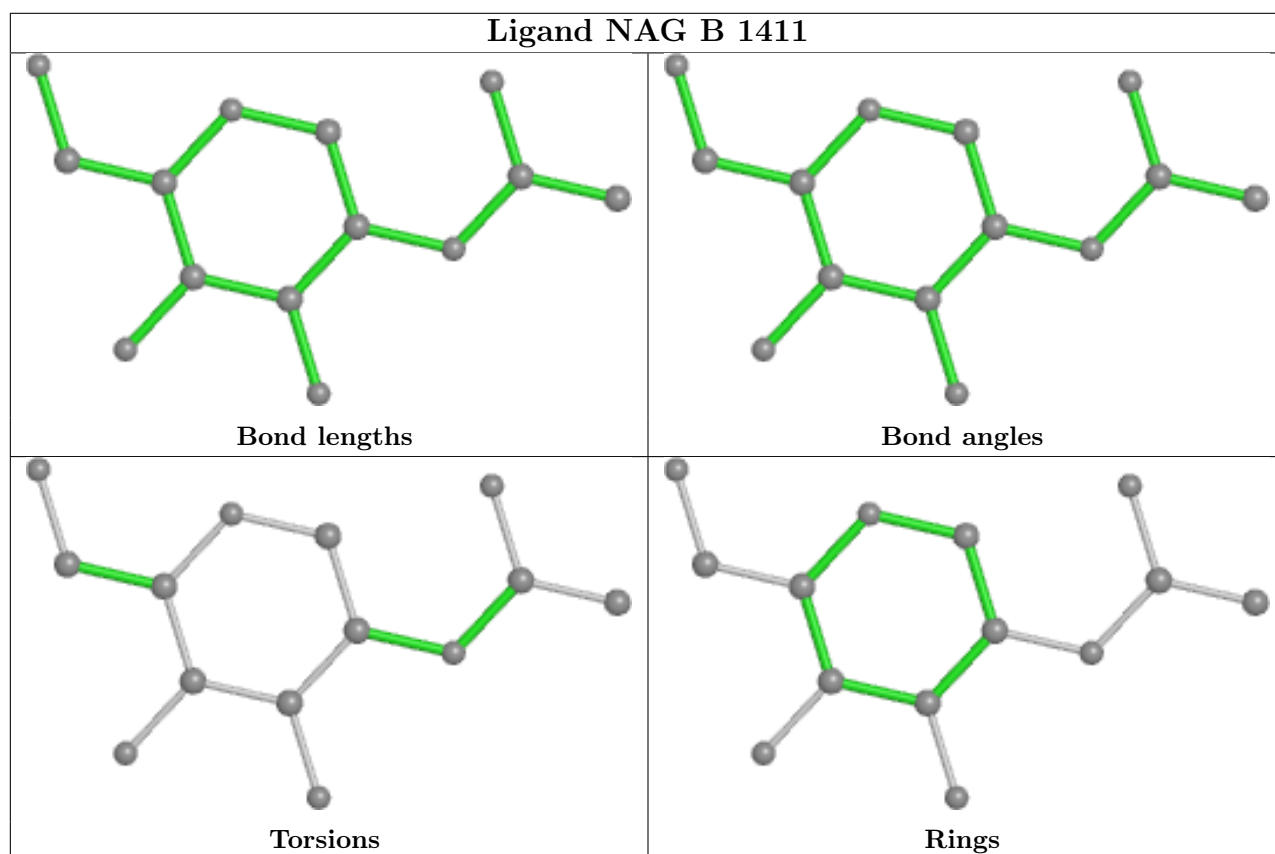
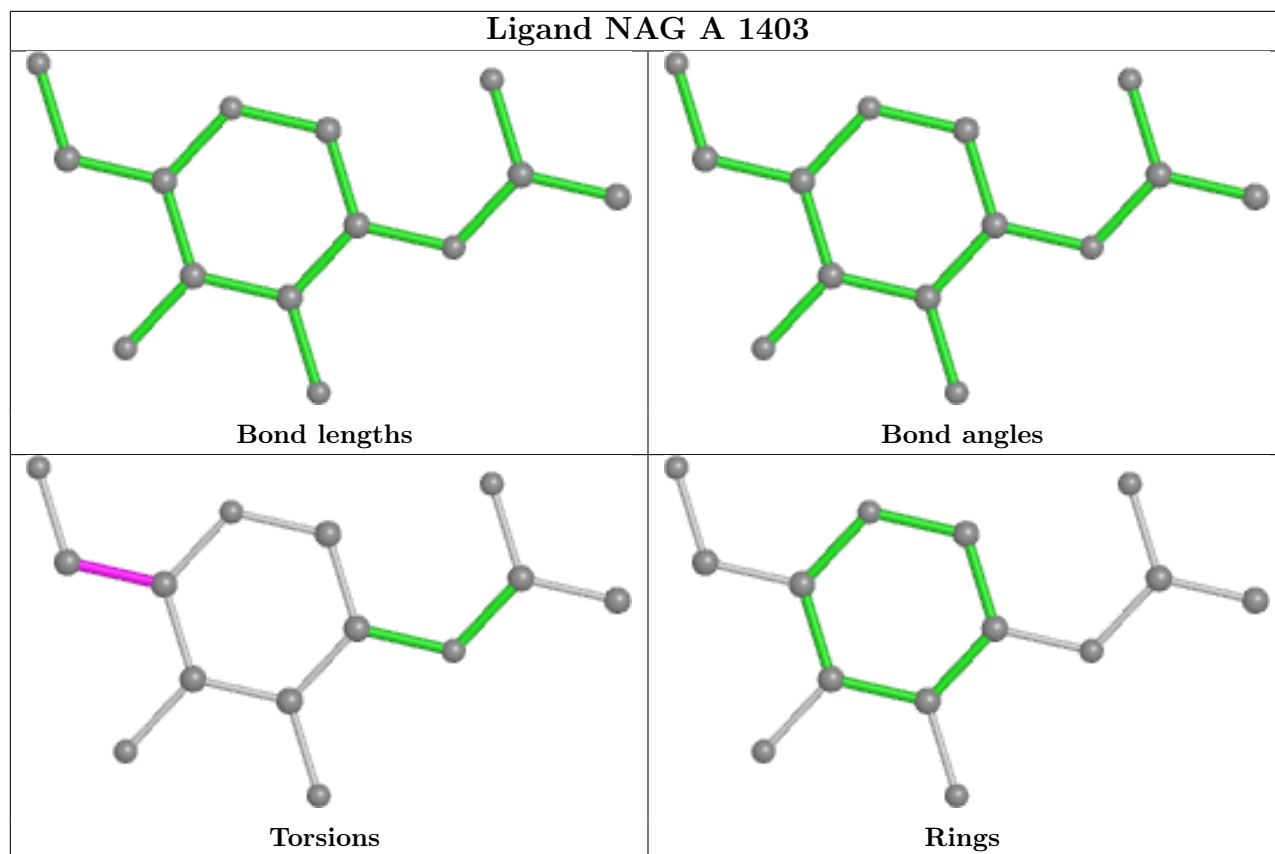


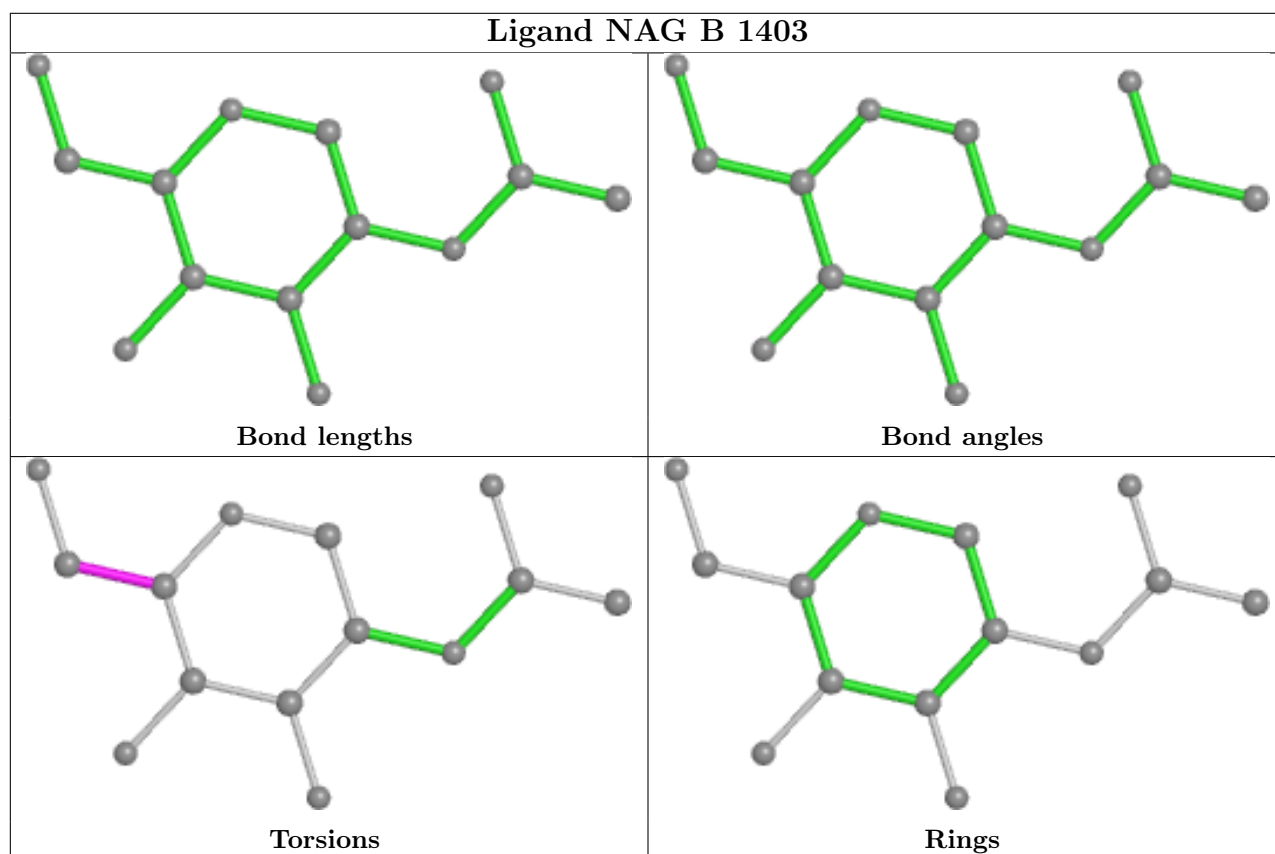
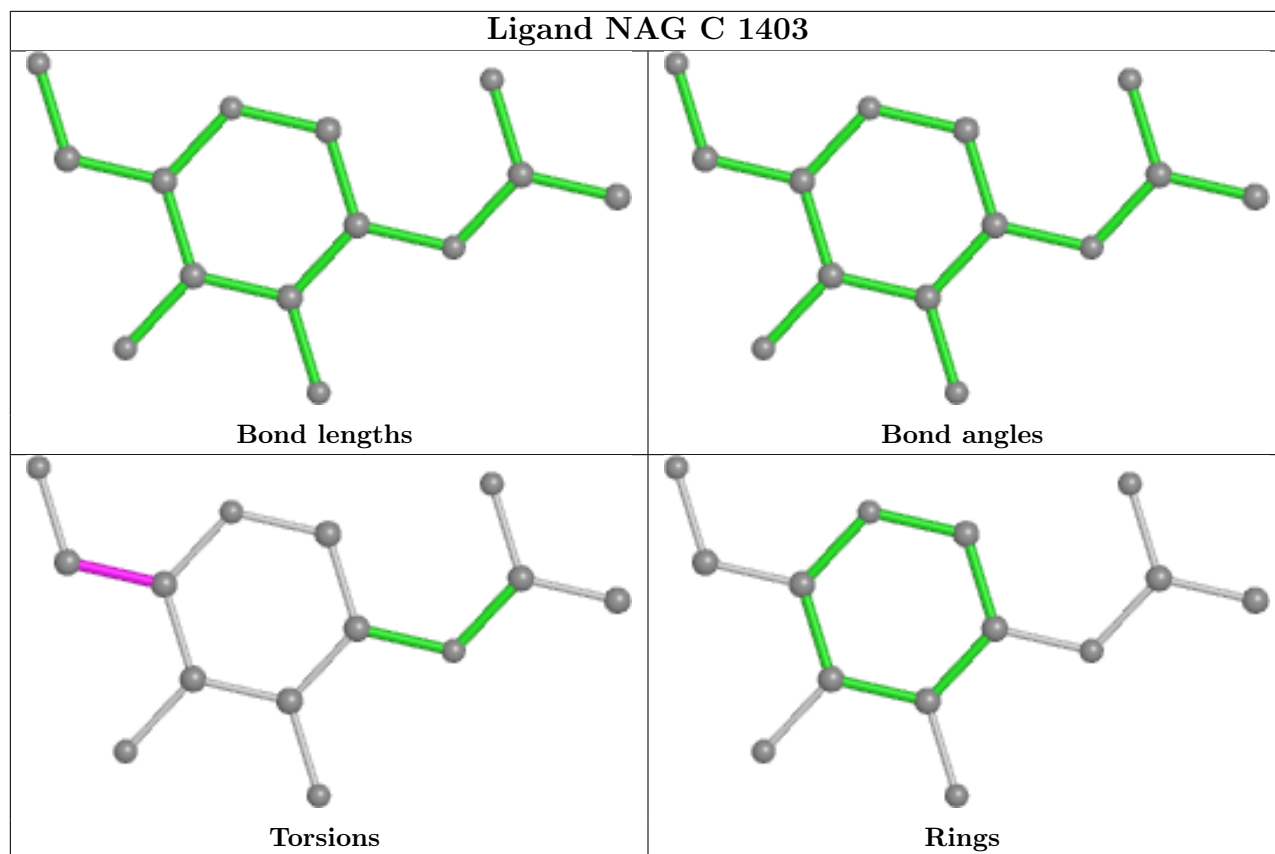


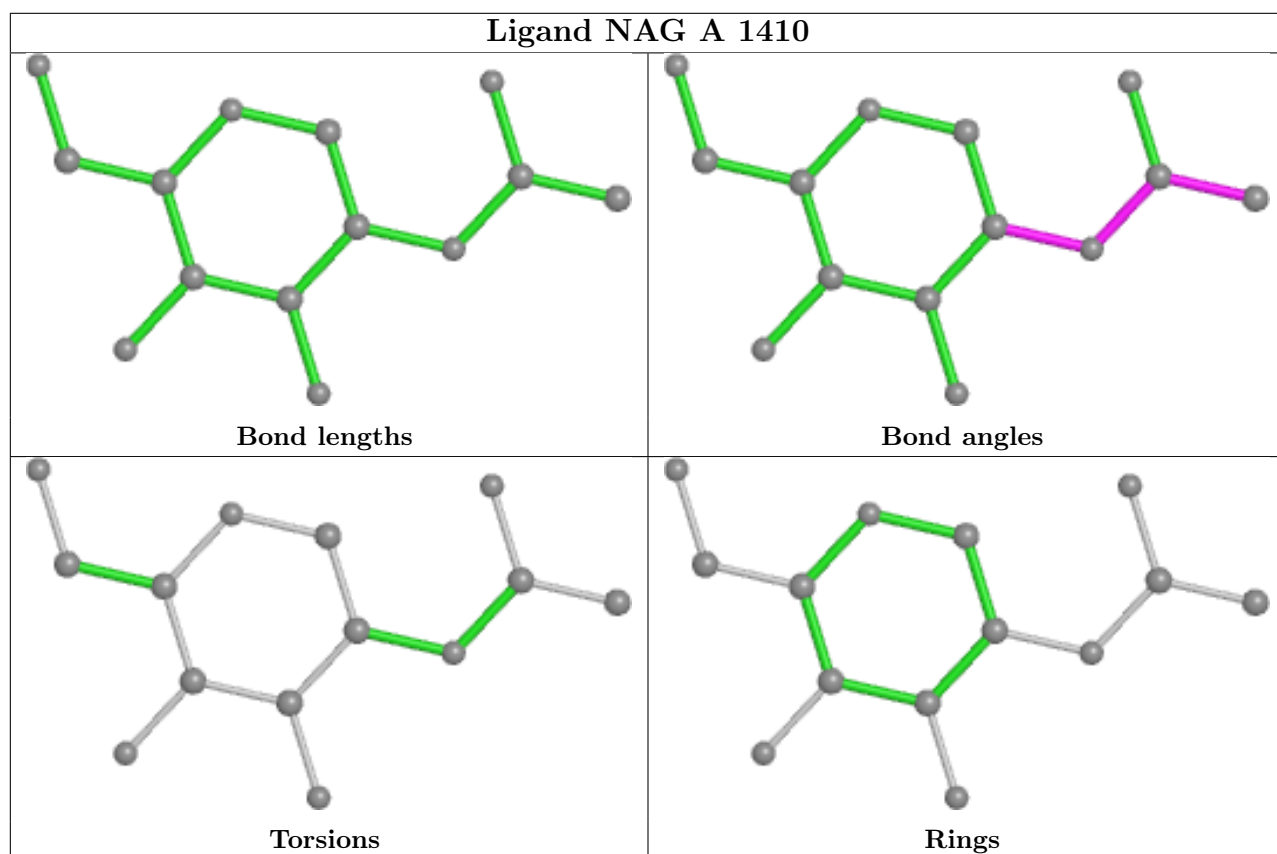
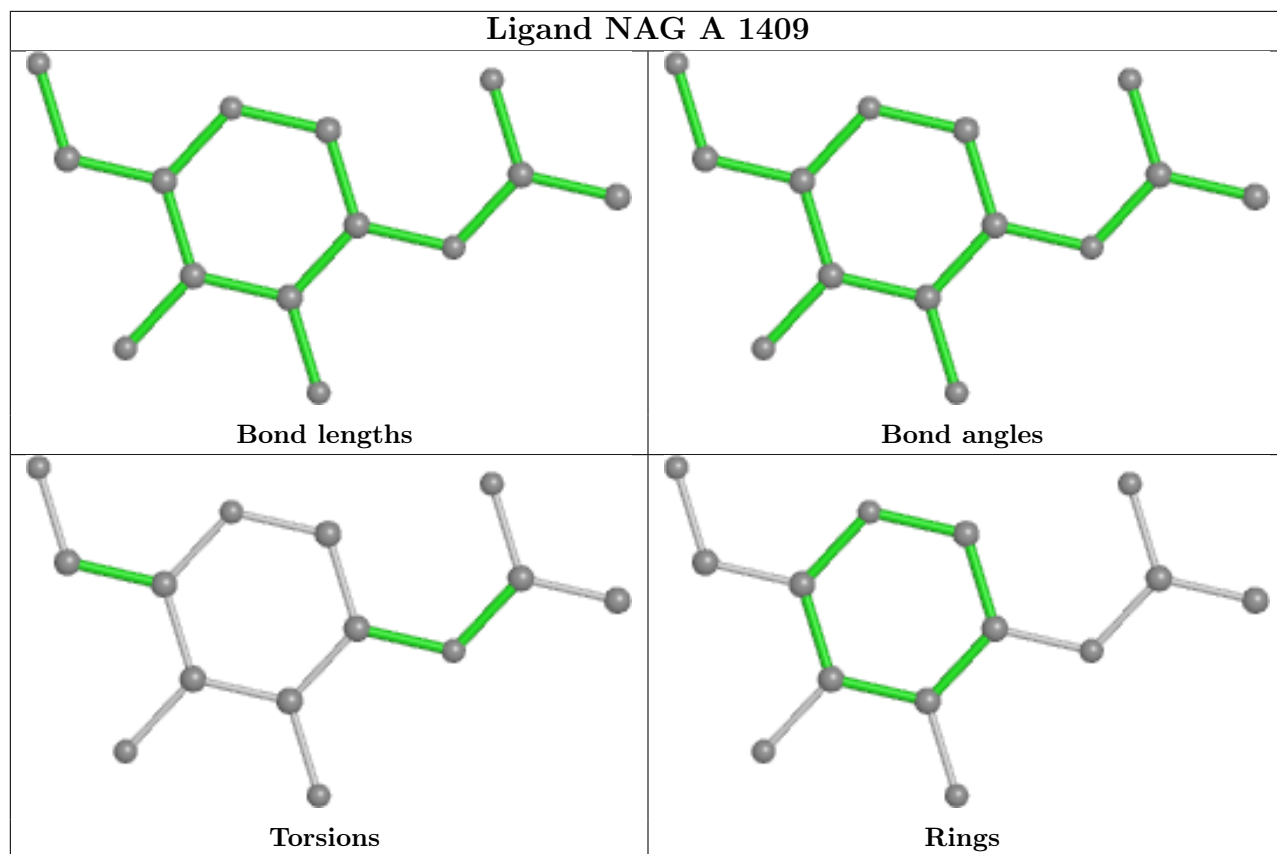


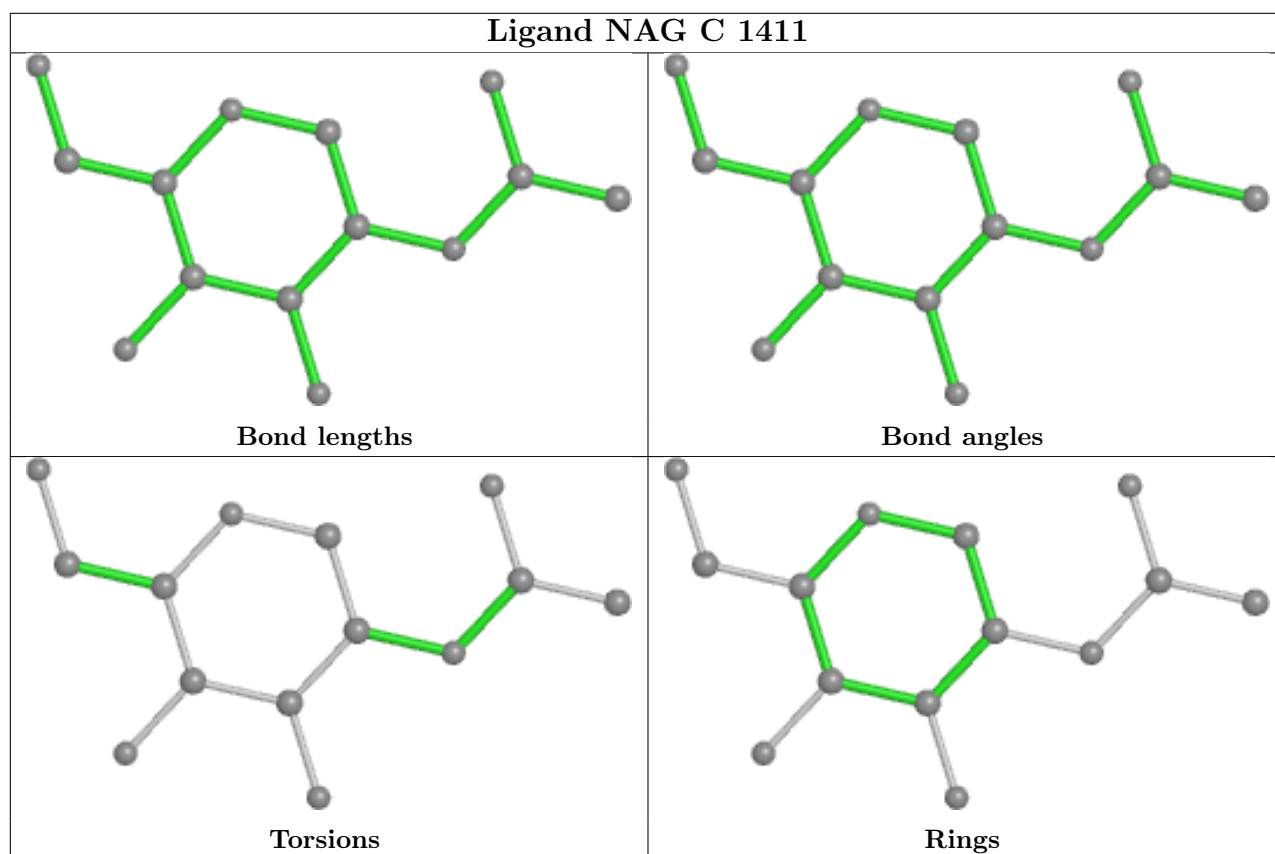
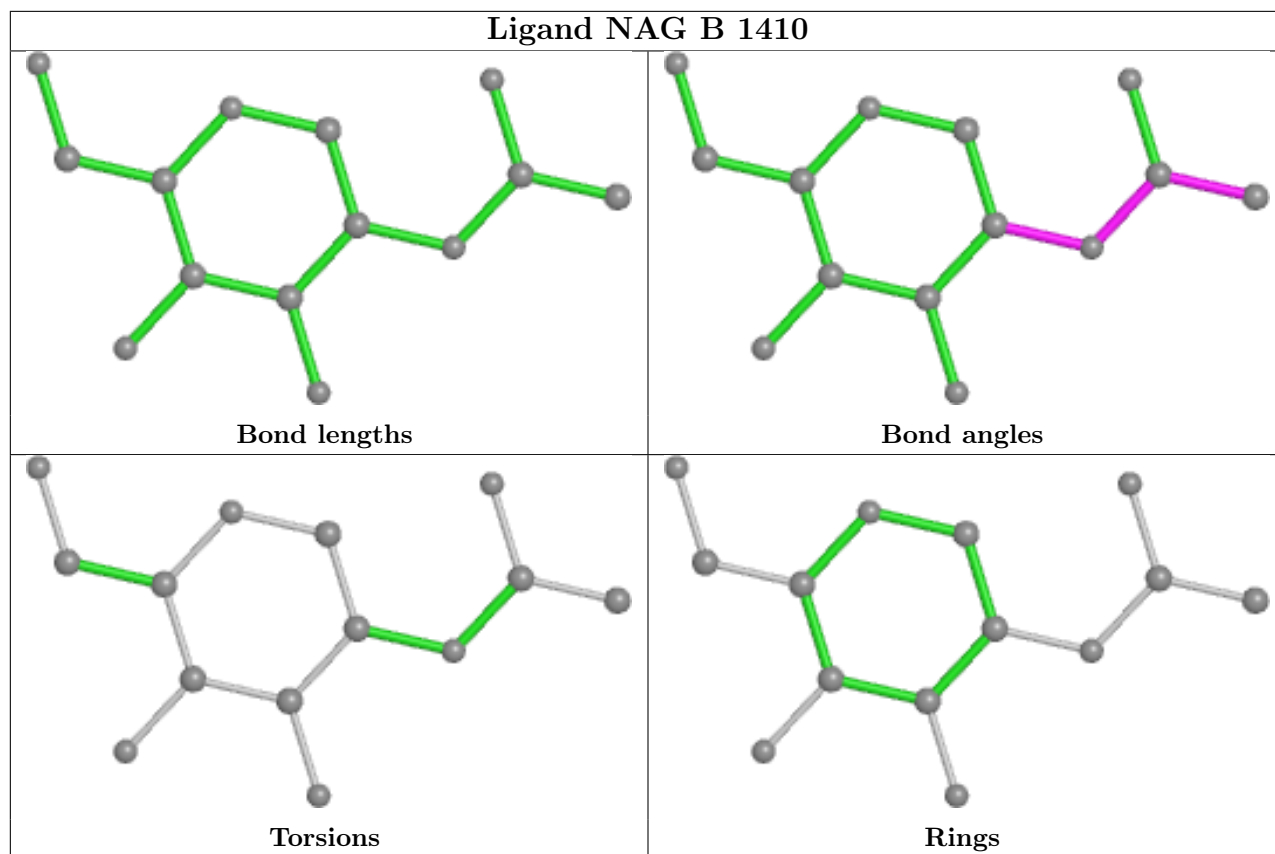


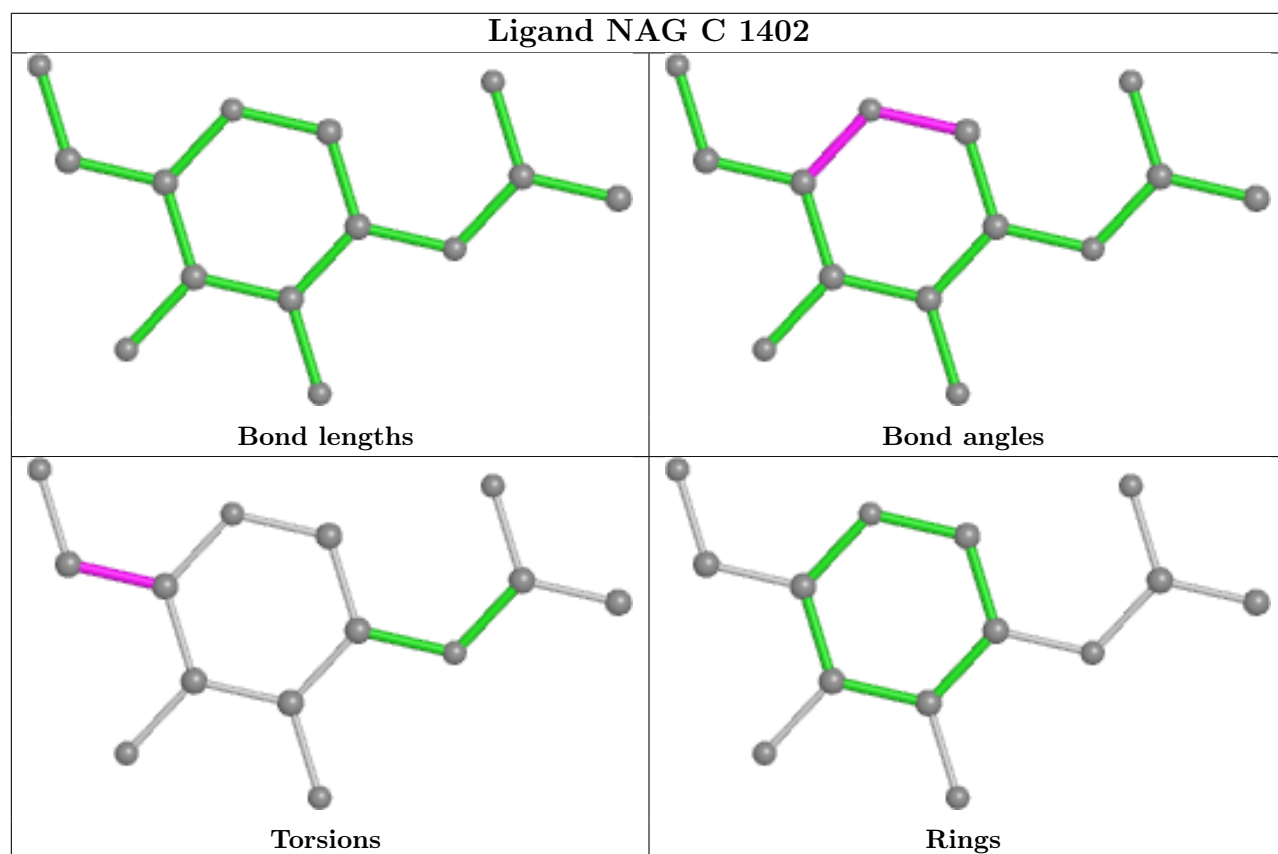
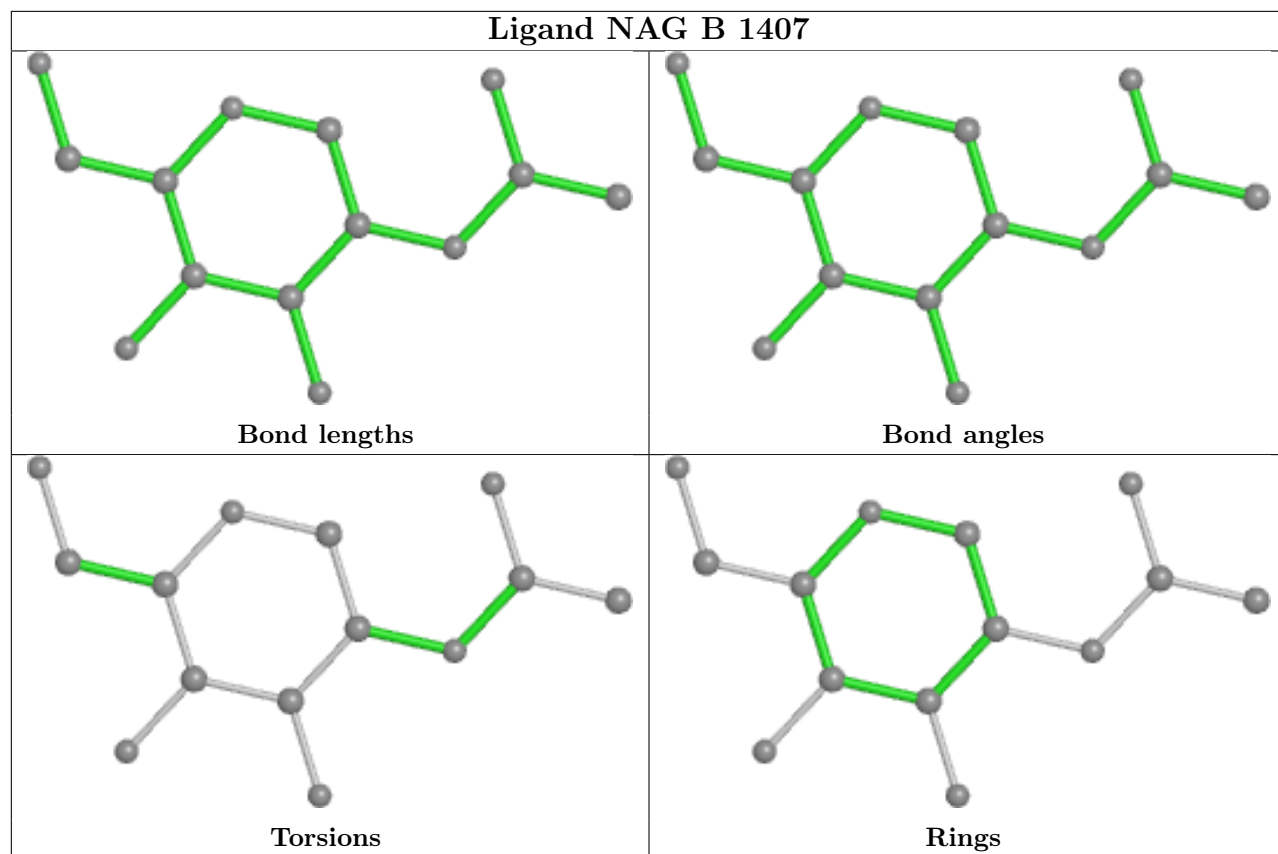


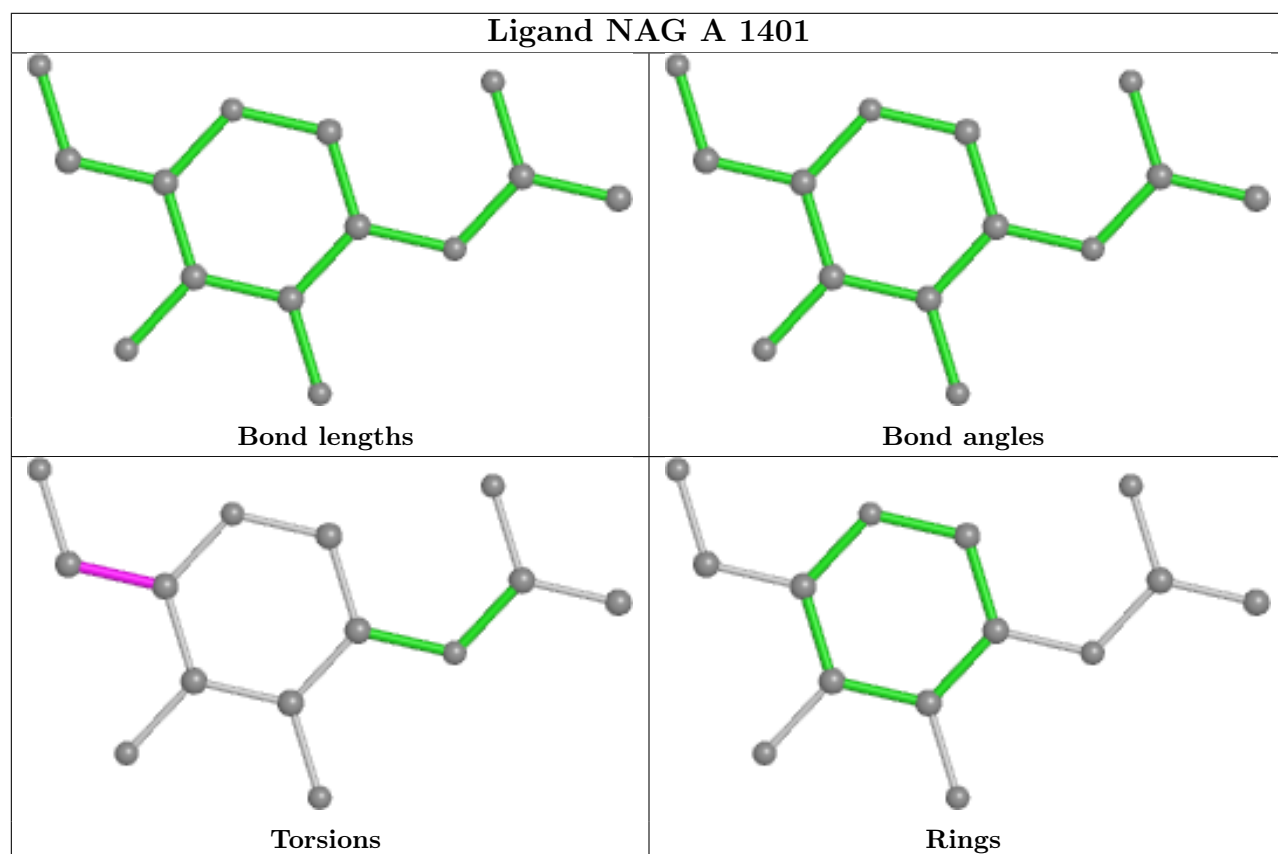
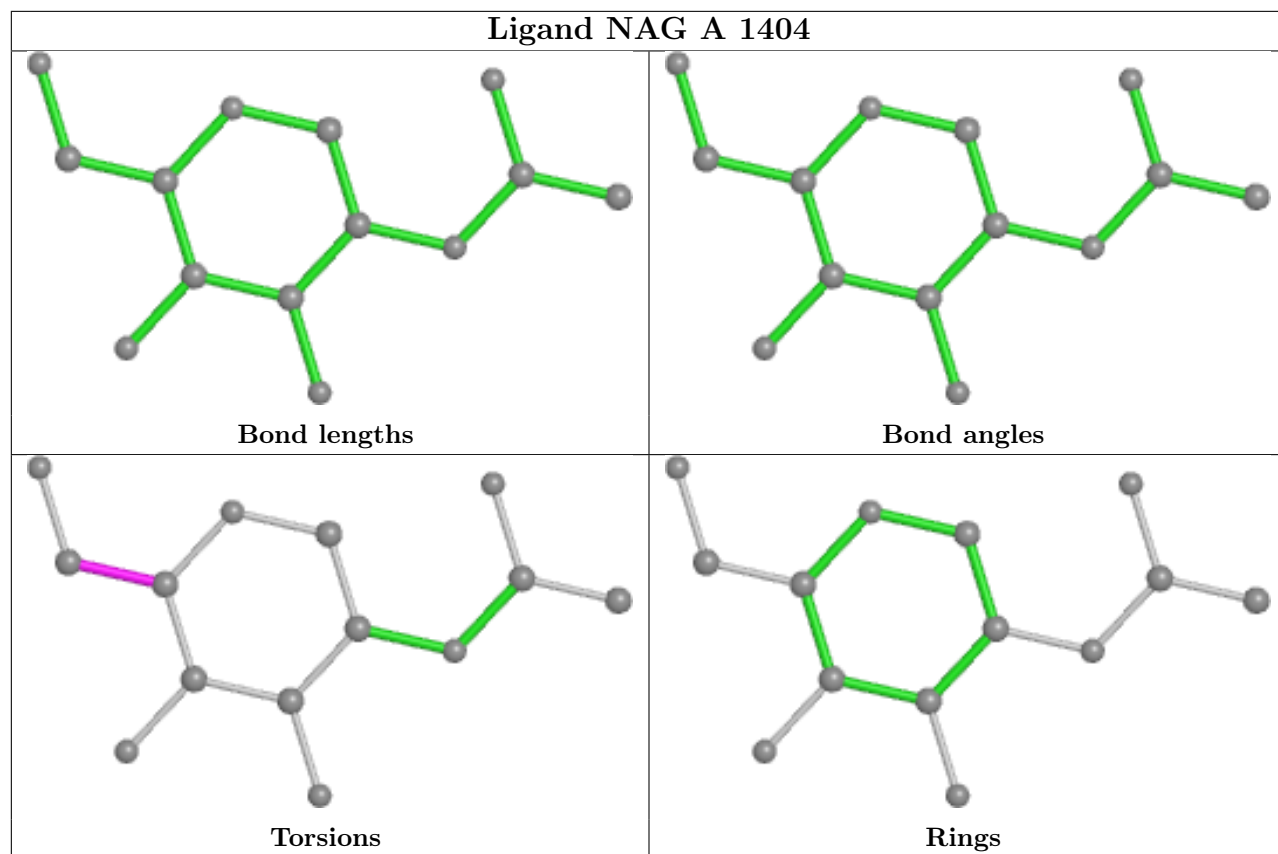


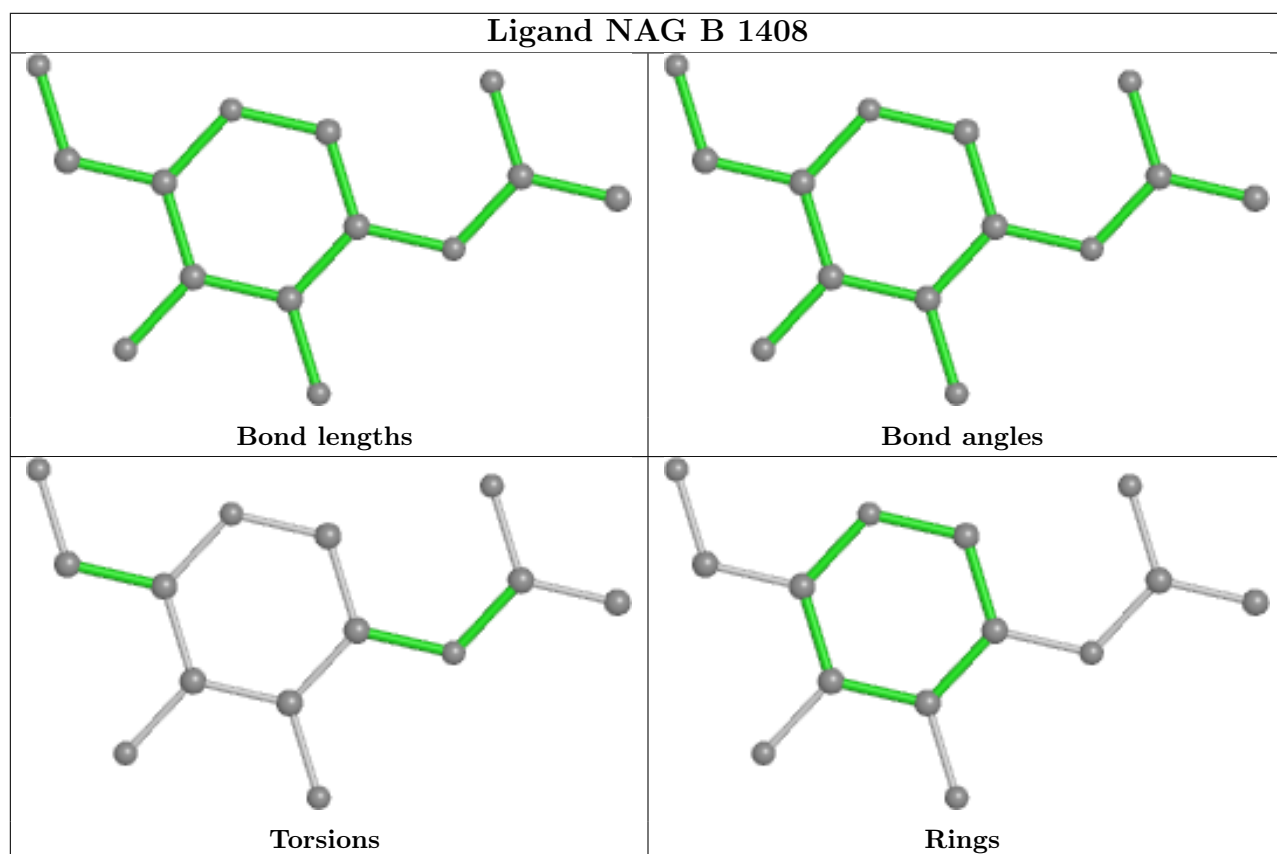
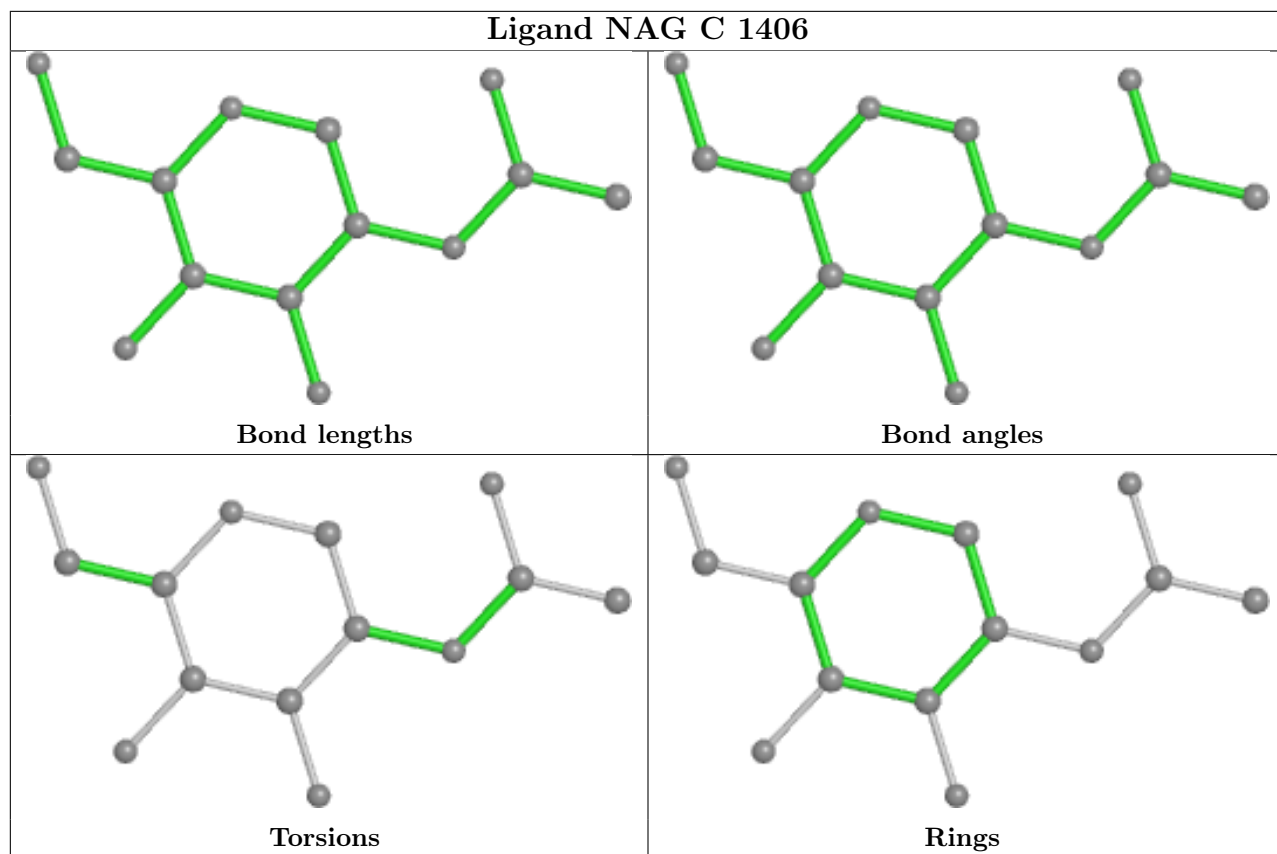


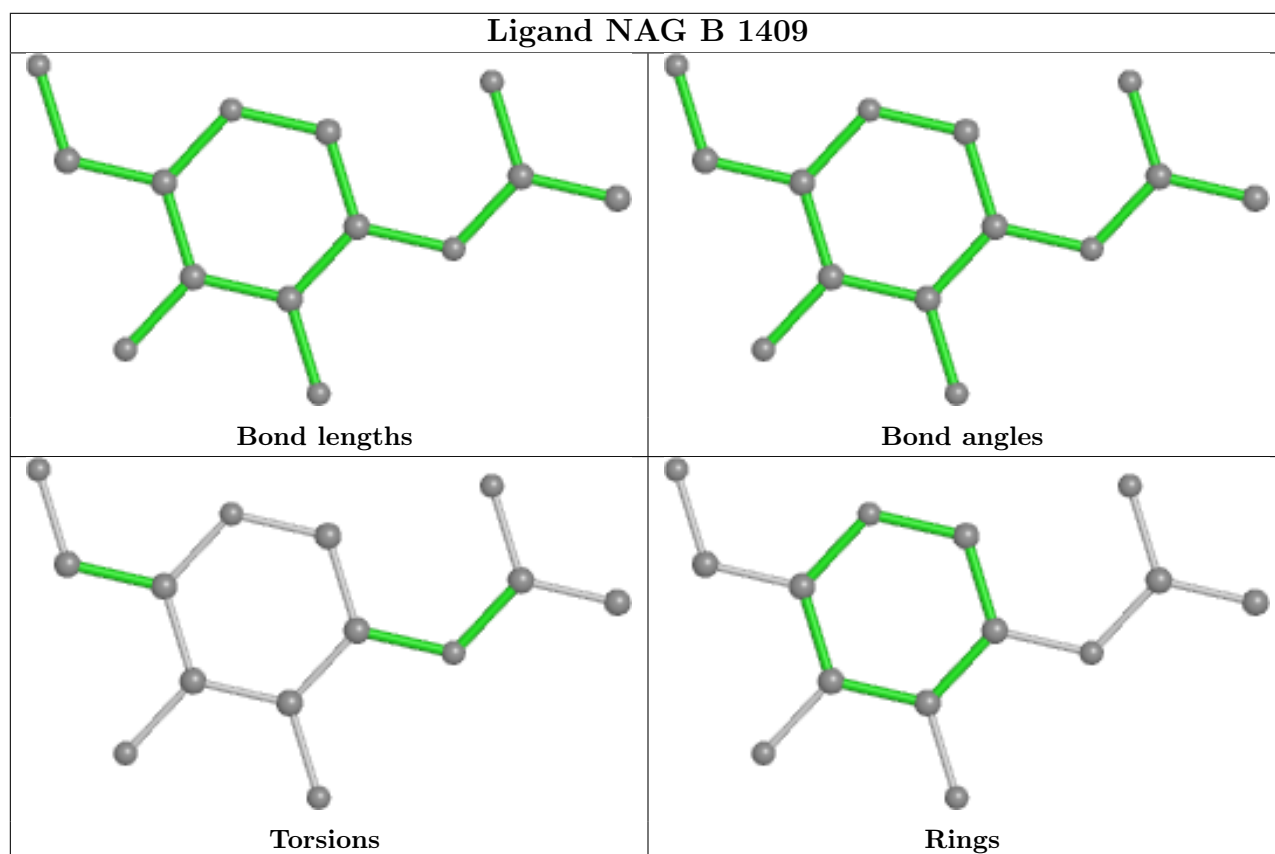
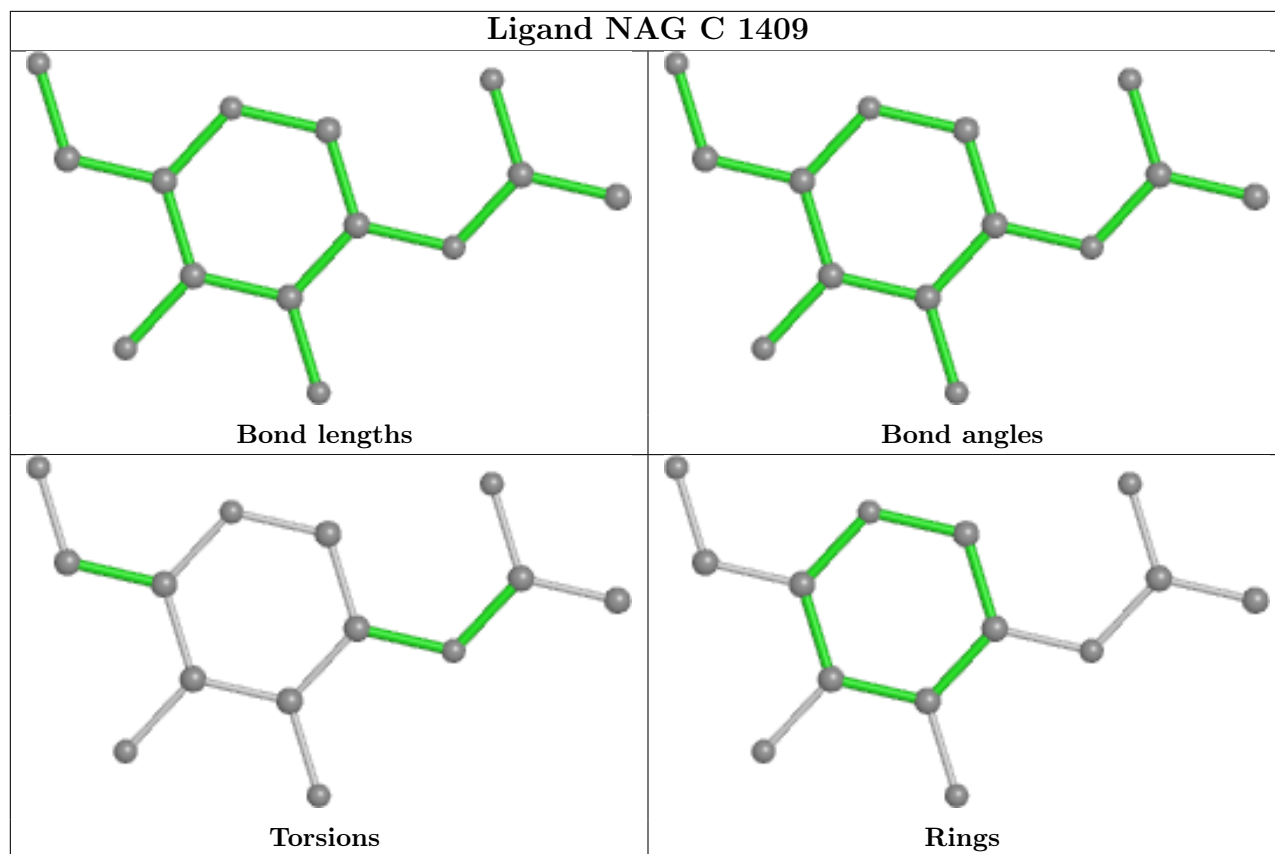


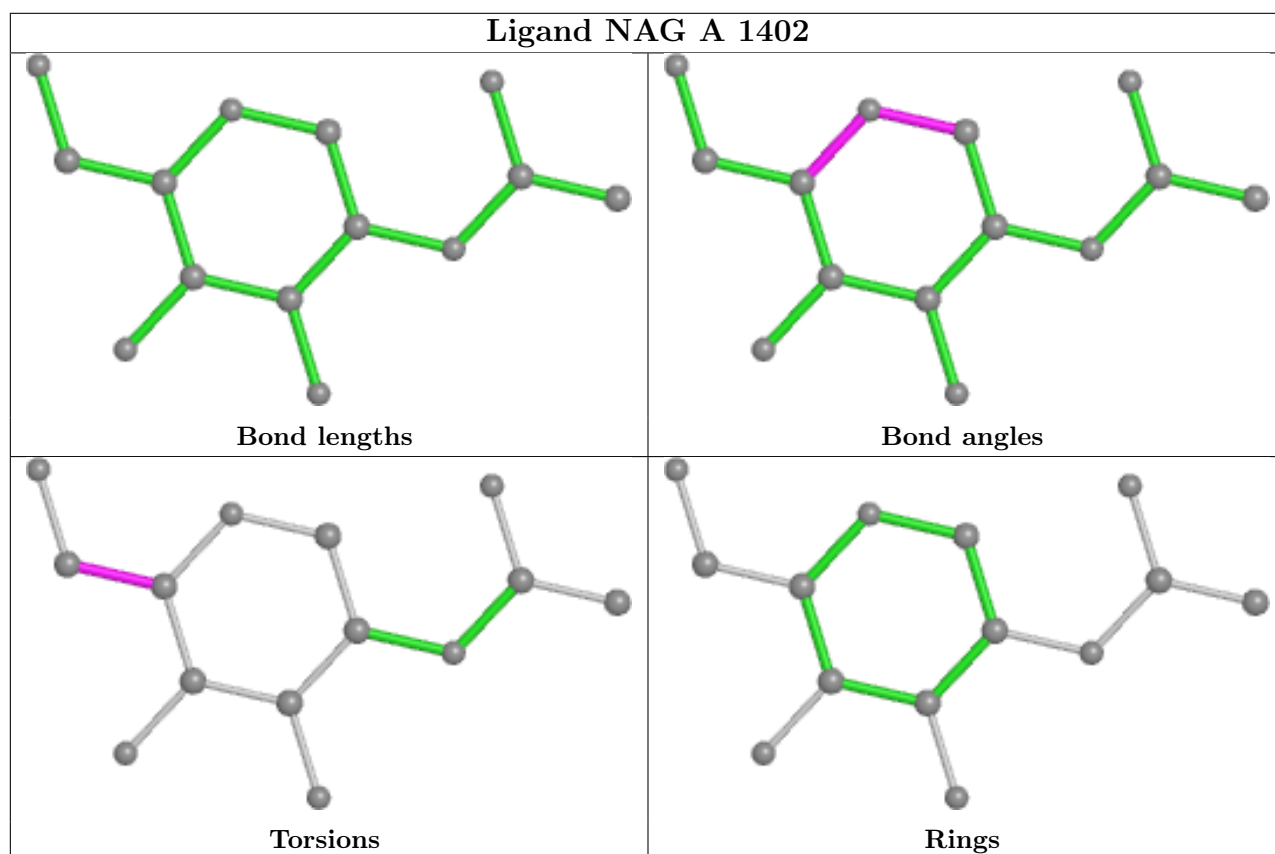
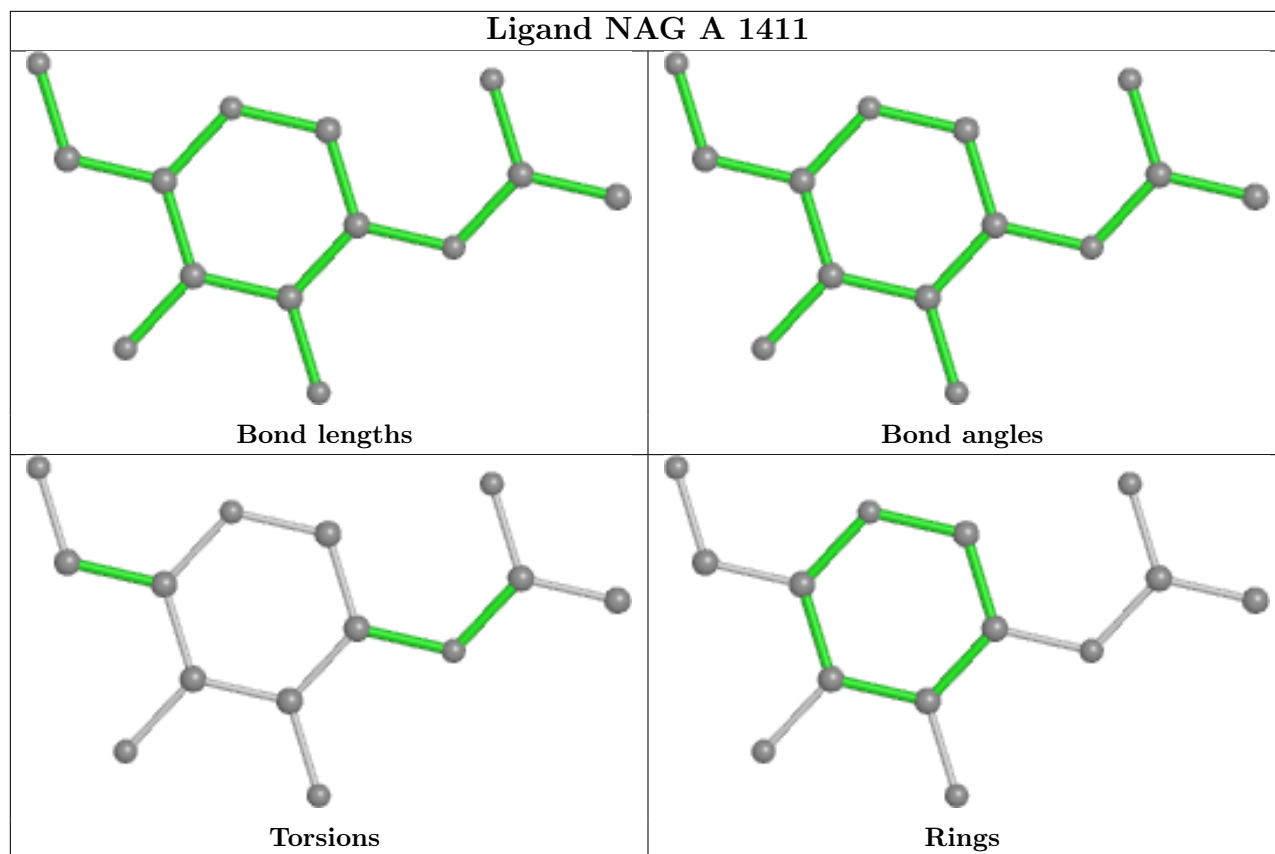


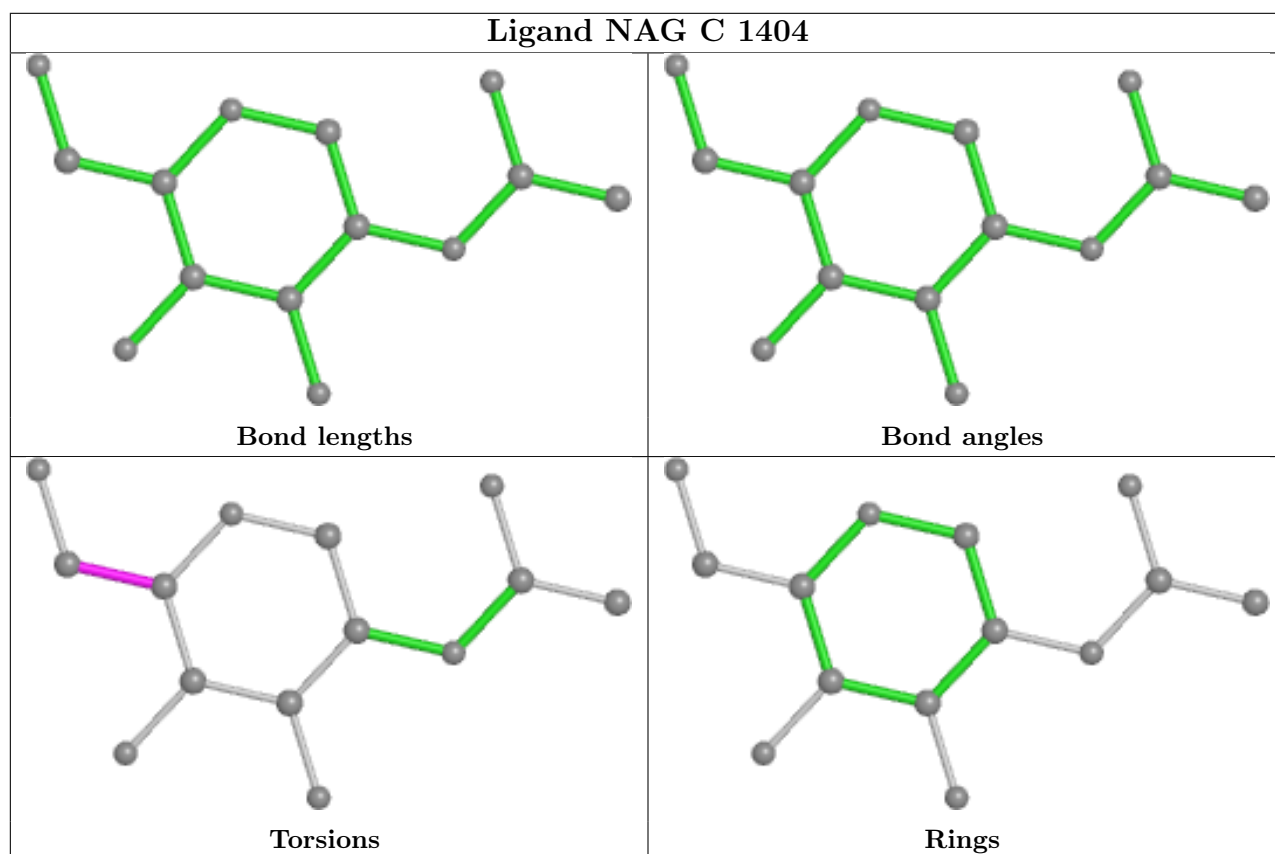
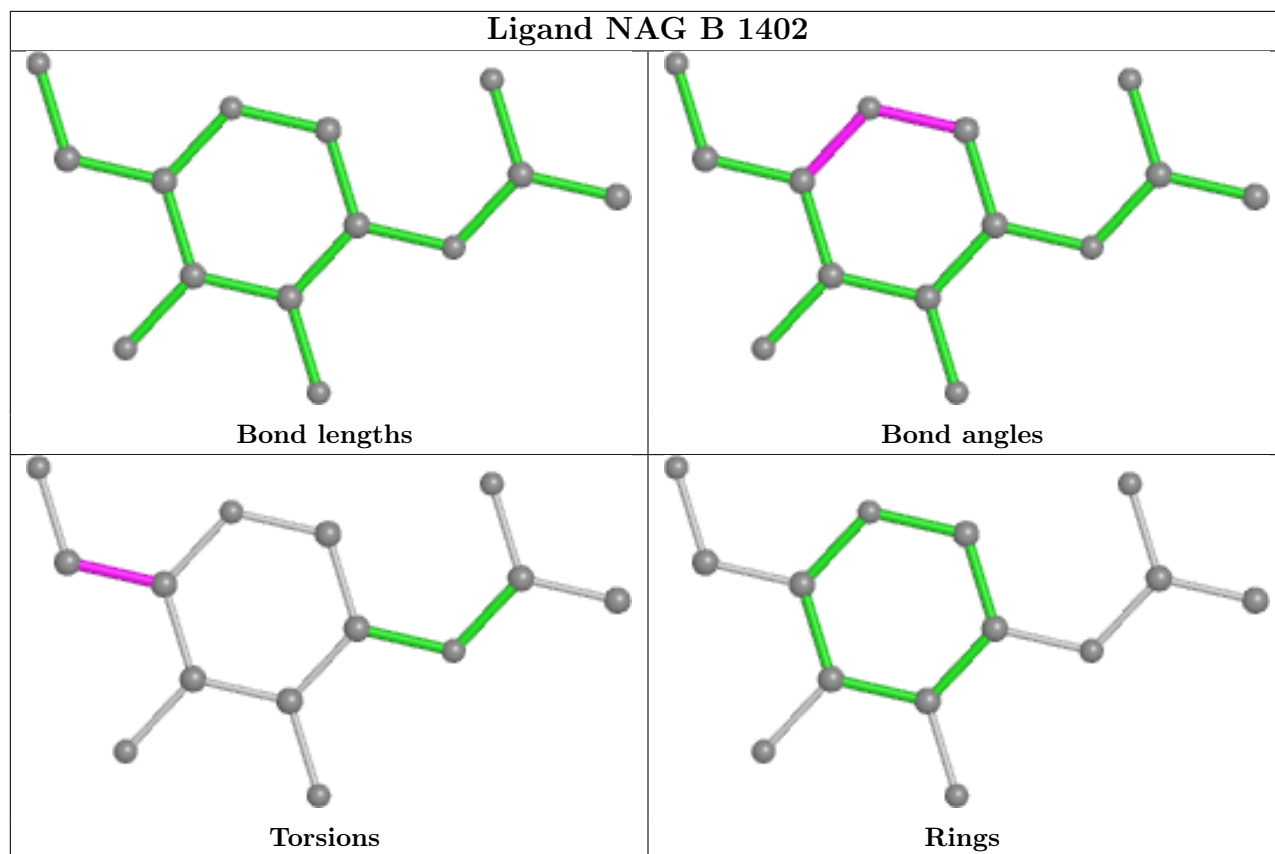












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

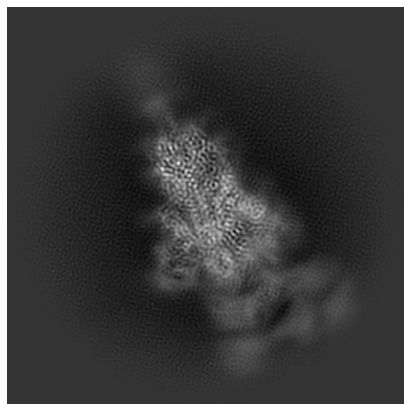
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34259. These allow visual inspection of the internal detail of the map and identification of artifacts.

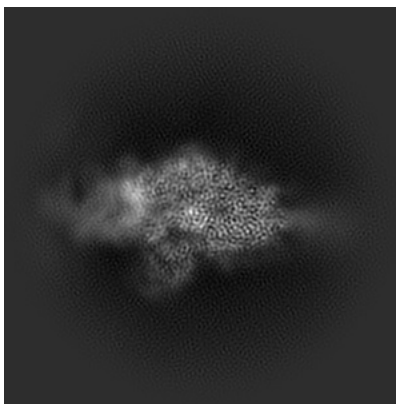
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

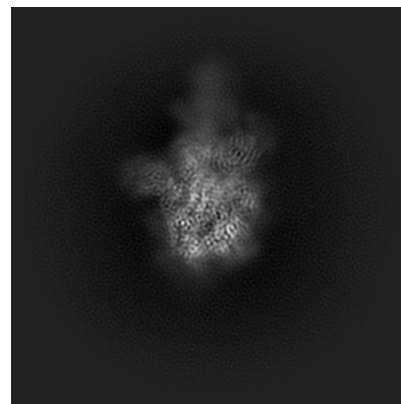
6.1.1 Primary map



X

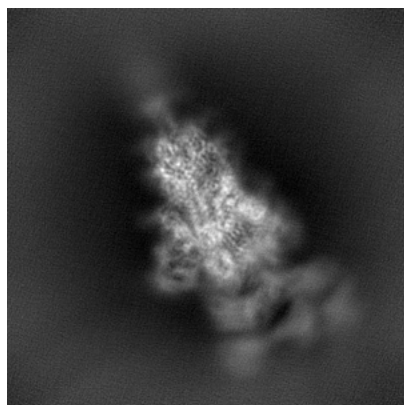


Y

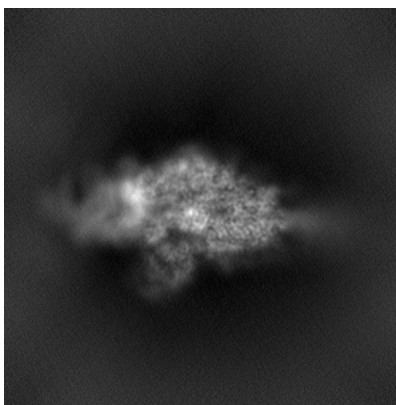


Z

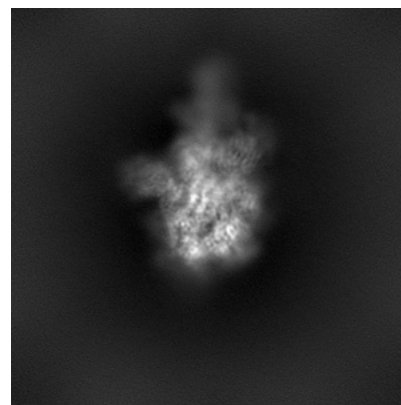
6.1.2 Raw map



X



Y

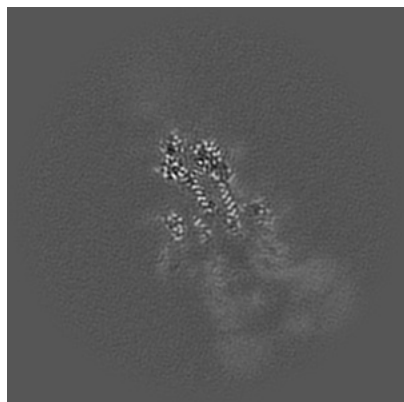


Z

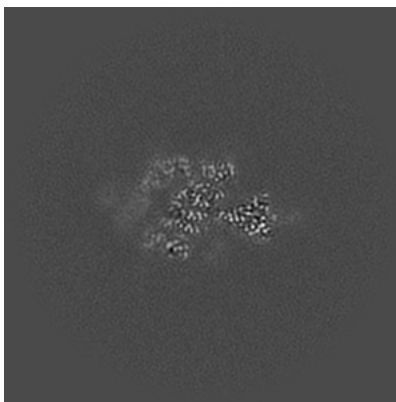
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

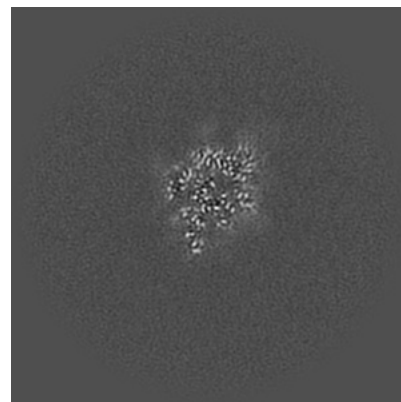
6.2.1 Primary map



X Index: 160

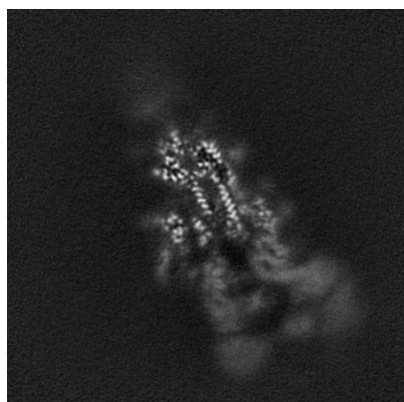


Y Index: 160

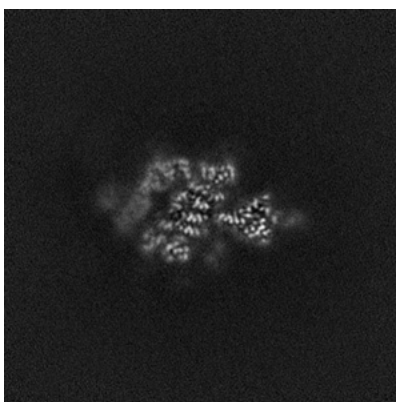


Z Index: 160

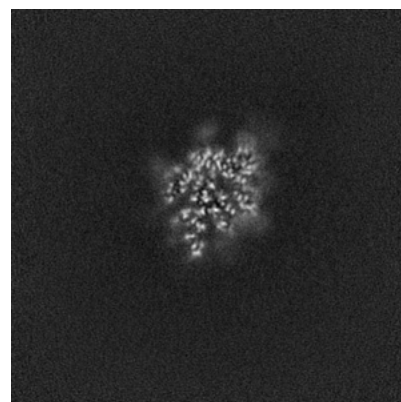
6.2.2 Raw map



X Index: 160



Y Index: 160

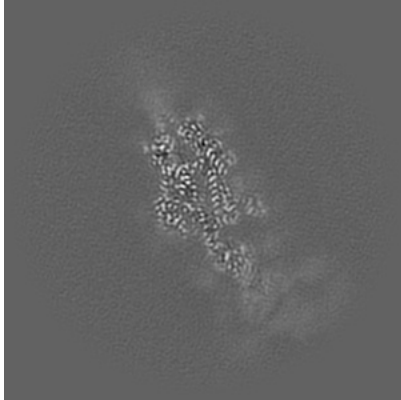


Z Index: 160

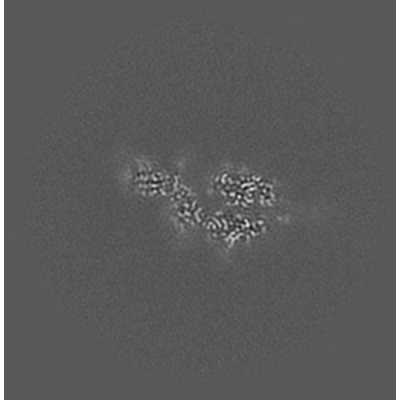
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

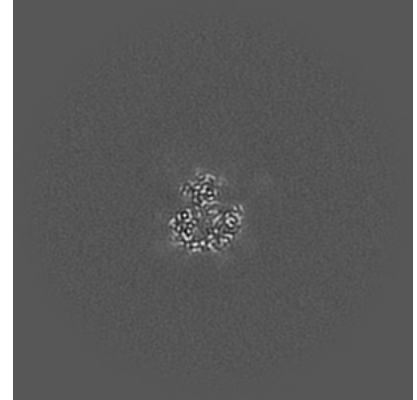
6.3.1 Primary map



X Index: 147

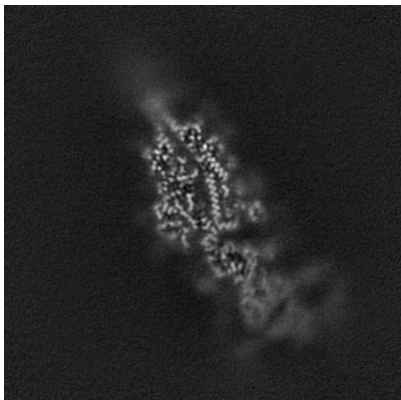


Y Index: 136

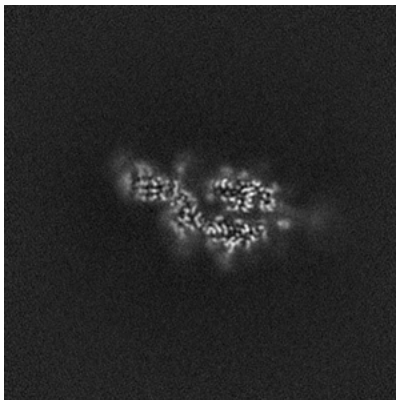


Z Index: 189

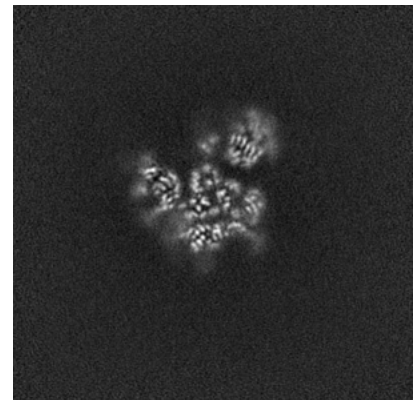
6.3.2 Raw map



X Index: 145



Y Index: 136

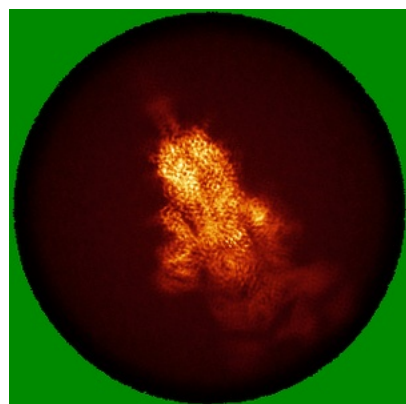


Z Index: 143

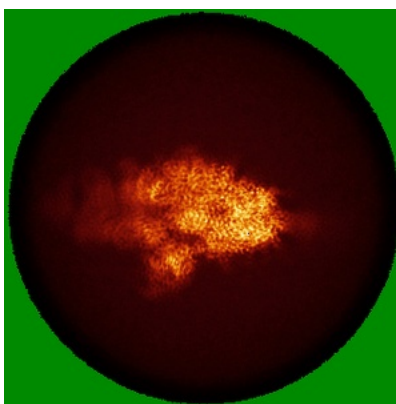
The images above show the largest variance slices of the map in three orthogonal directions.

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

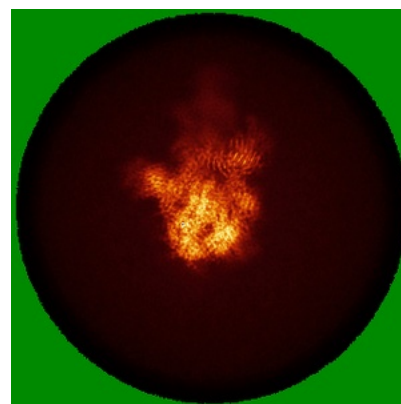
6.4.1 Primary map



X

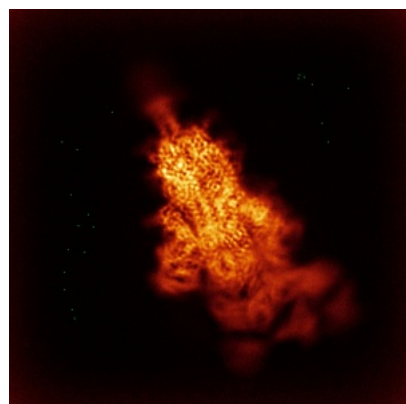


Y

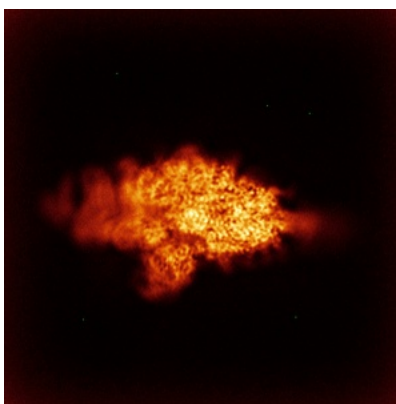


Z

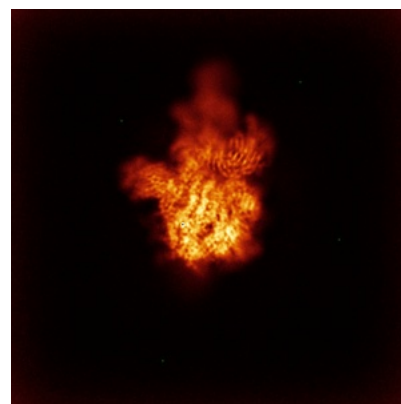
6.4.2 Raw map



X



Y

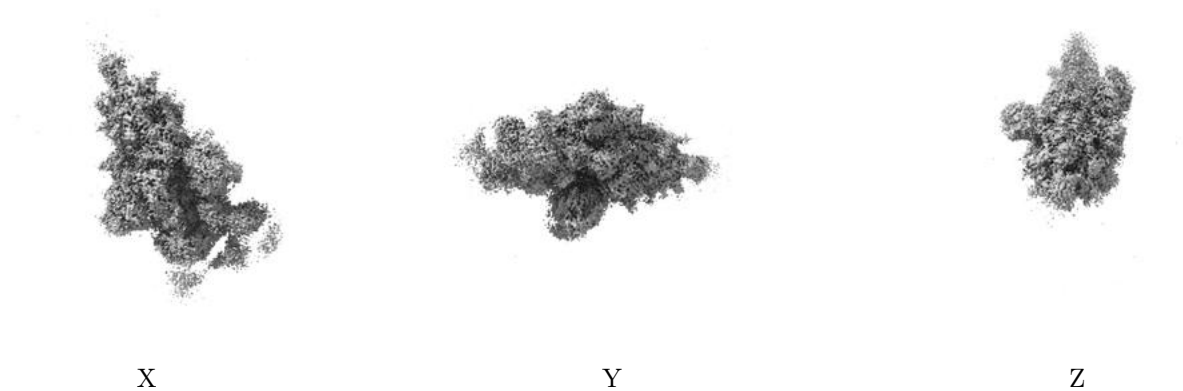


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

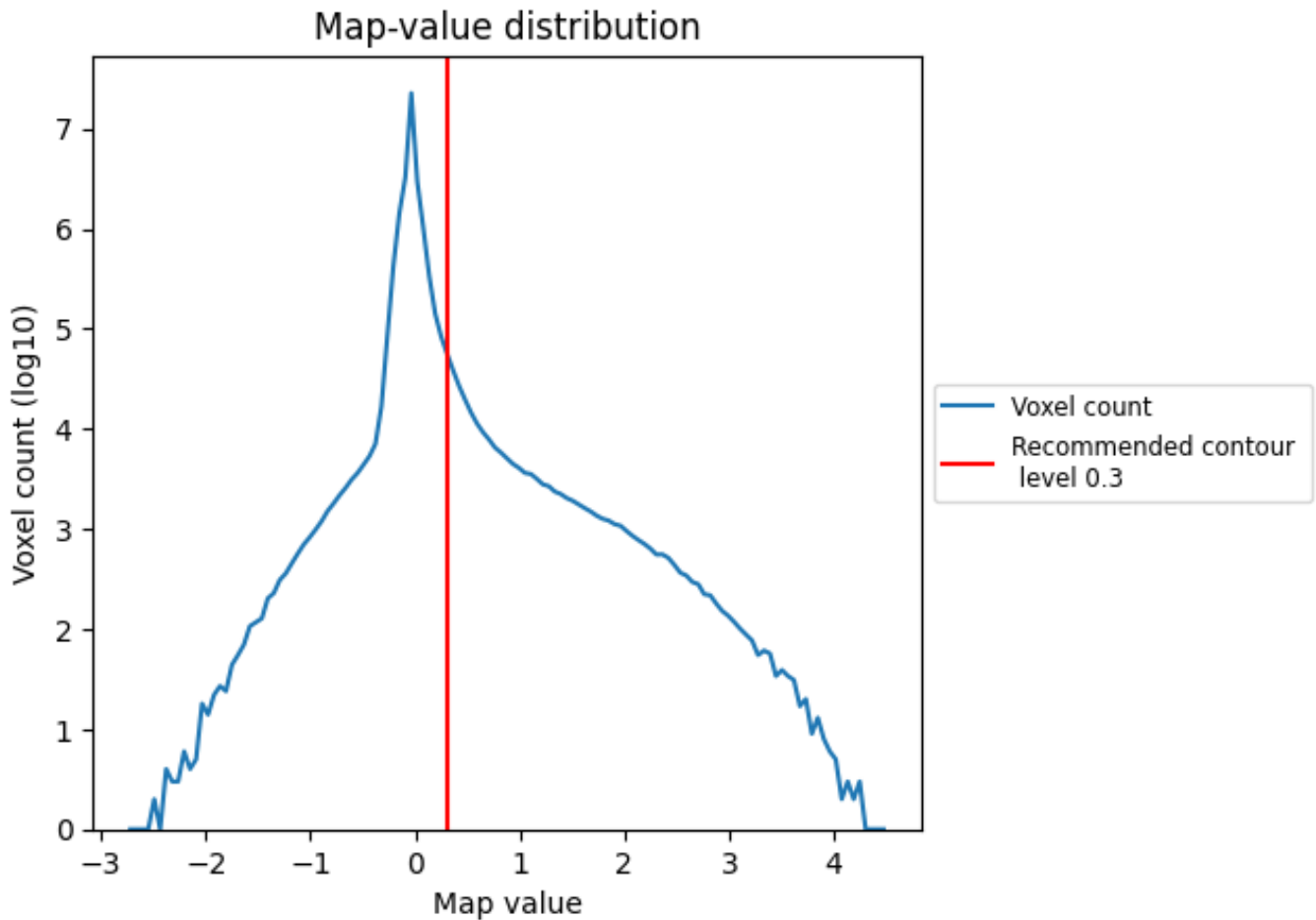
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

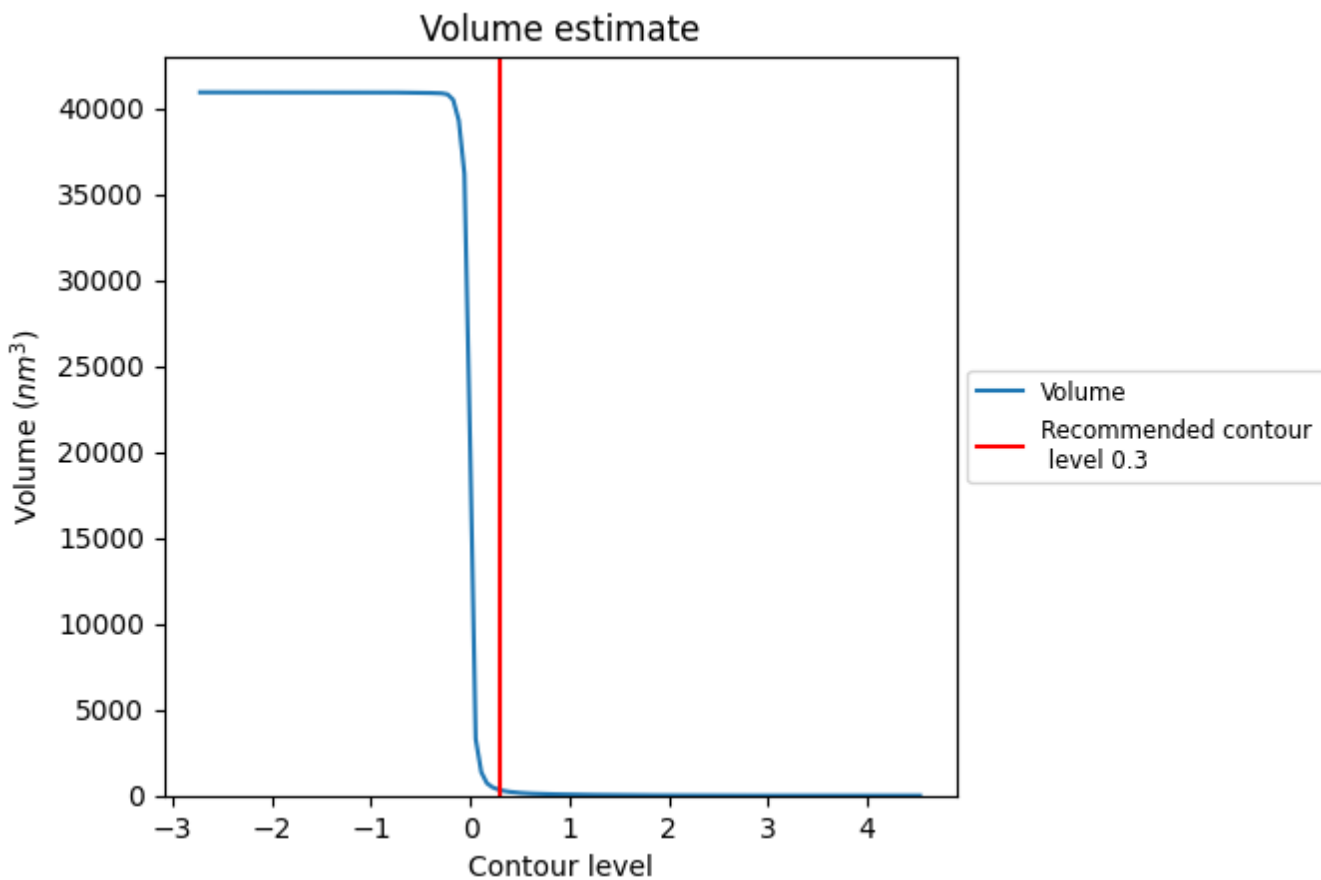
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

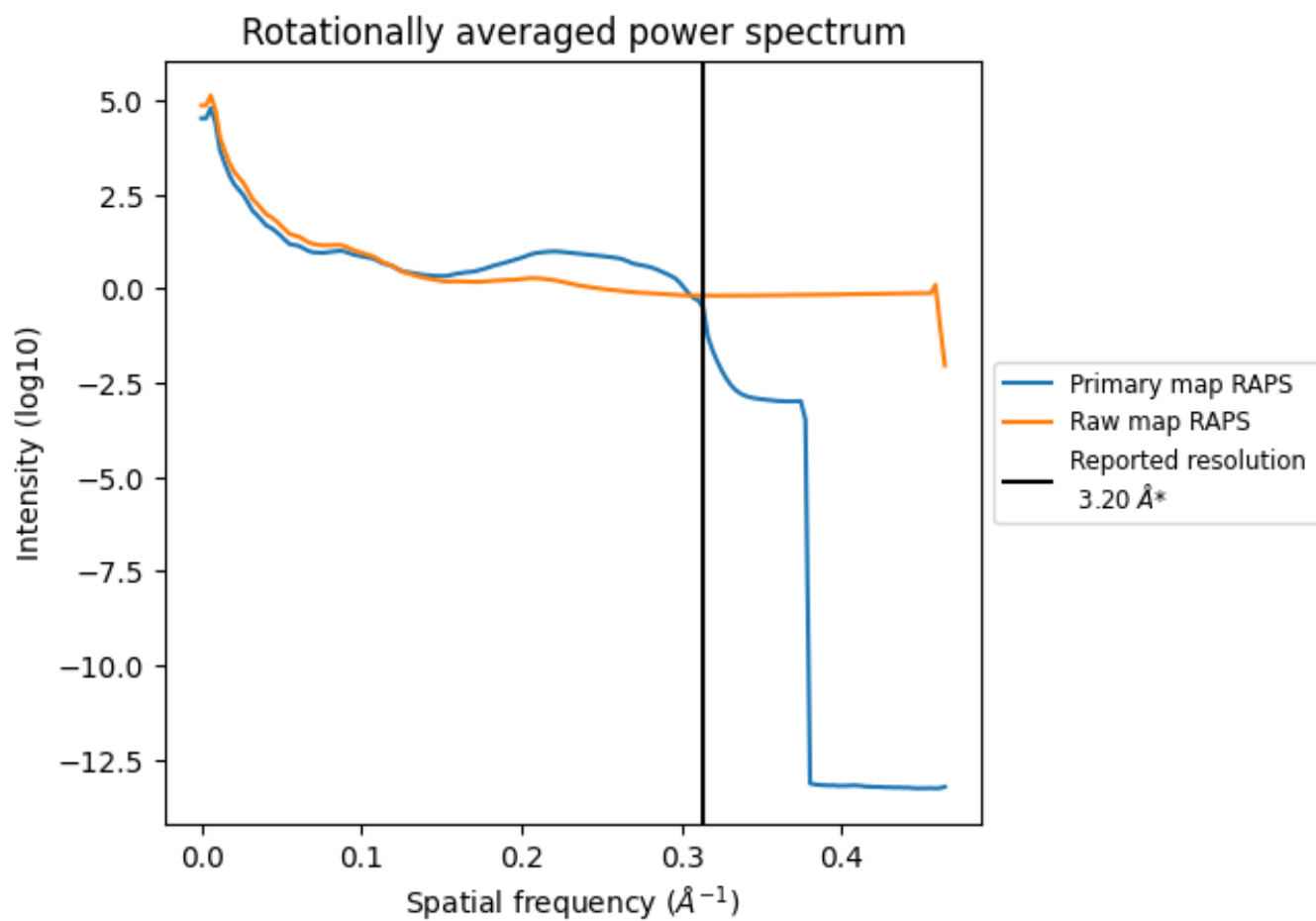
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 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](#)

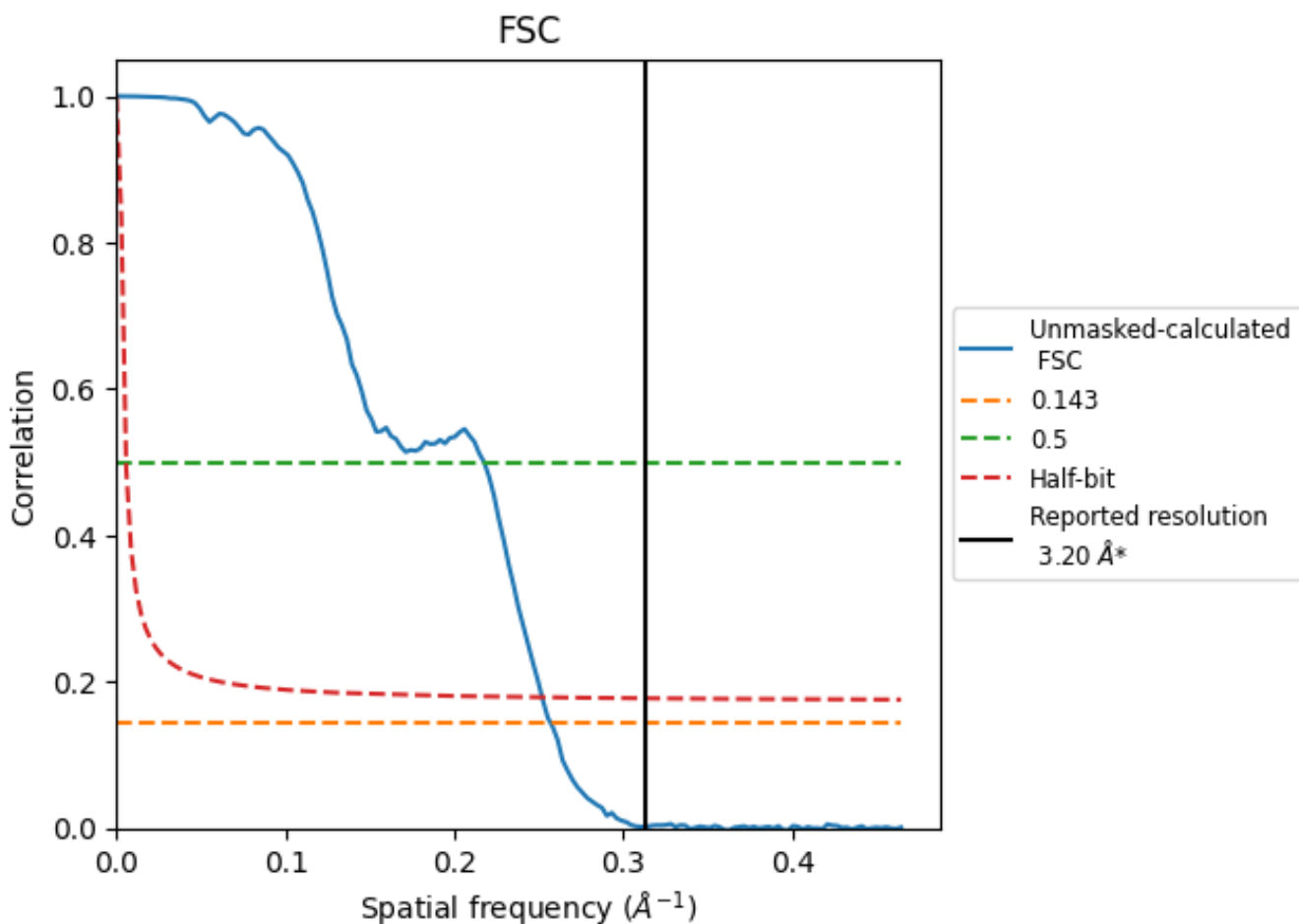


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312\AA^{-1}

8.2 Resolution estimates [i](#)

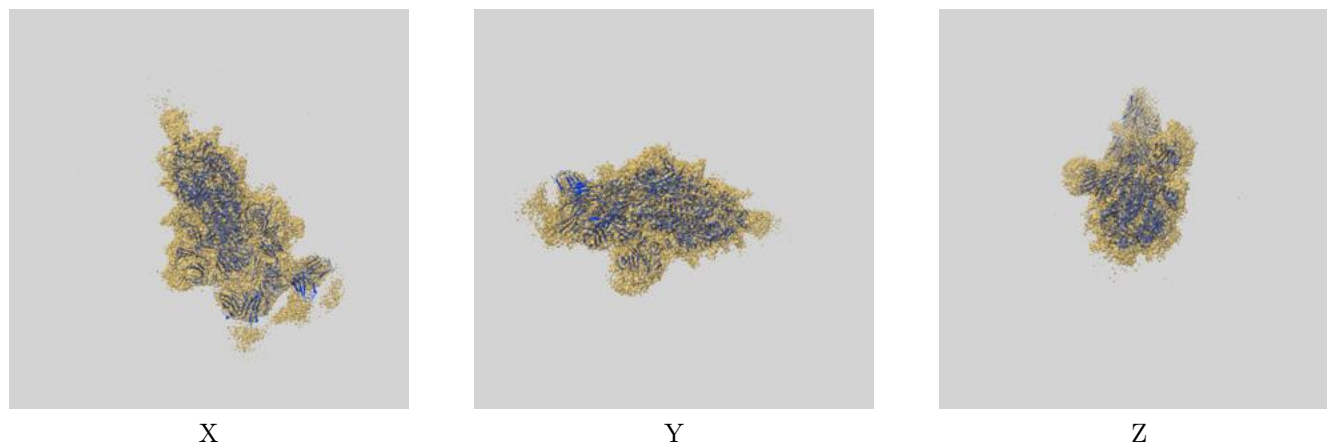
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	4.60	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

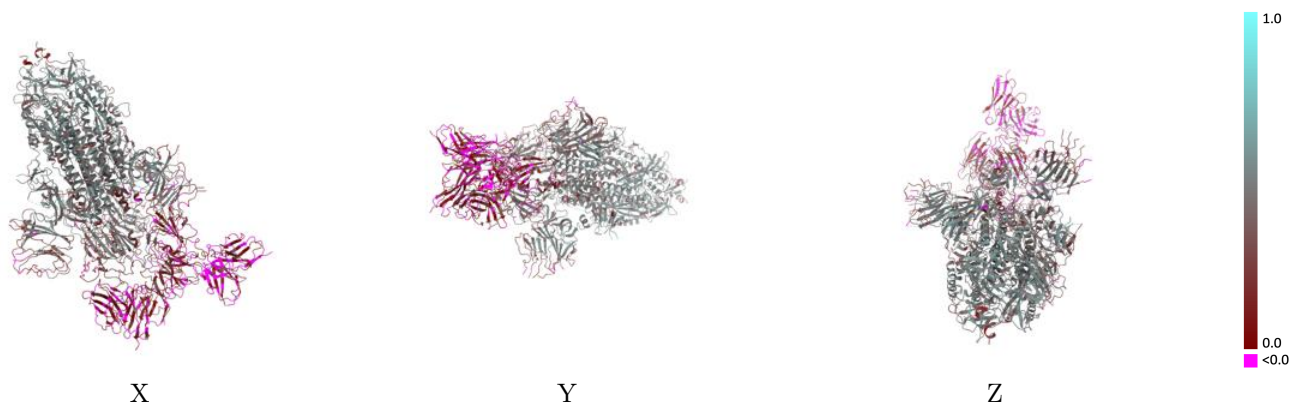
This section contains information regarding the fit between EMDB map EMD-34259 and PDB model 8GTO. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



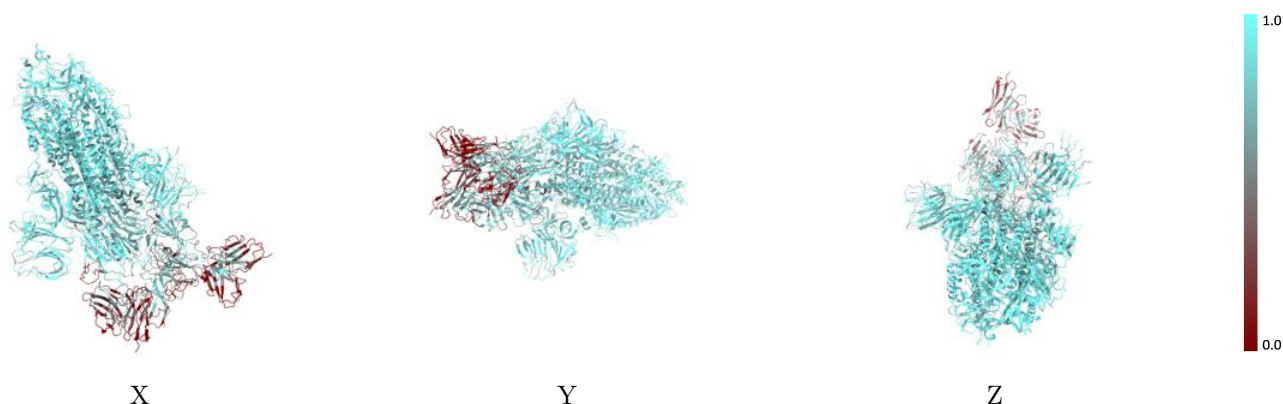
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



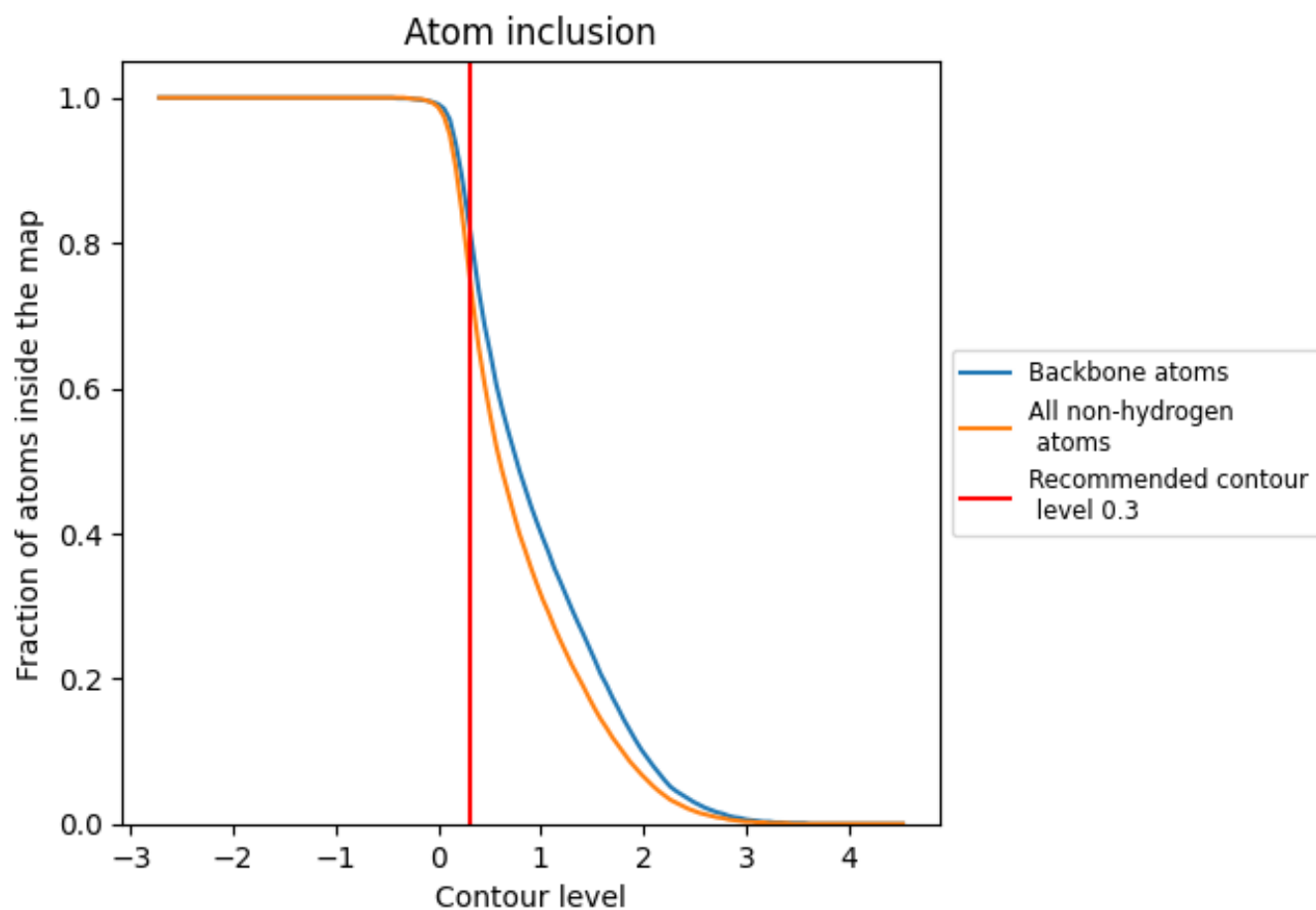
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.3420
A	 0.8680	 0.4140
B	 0.8220	 0.3860
C	 0.8450	 0.3950
D	 0.4640	 0.2360
E	 0.5360	 0.1280
F	 0.7500	 0.2600
G	 0.8210	 0.2740
H	 0.6050	 0.1580
I	 0.3230	 0.0310
J	 0.2970	 0.0540
K	 0.7500	 0.2960
L	 0.5090	 0.1050
M	 0.2730	 0.0480
N	 0.2090	 0.0710
O	 0.8570	 0.3530
P	 0.6430	 0.2530
Q	 0.3930	 0.1920
R	 0.6790	 0.2440
S	 0.8210	 0.3270
T	 0.8210	 0.2650
U	 0.8210	 0.3660
V	 0.4290	 0.1070
W	 0.3570	 -0.0500
X	 0.7140	 0.2660
Y	 0.8210	 0.3390
Z	 0.8570	 0.3060
a	 0.8570	 0.4000

