



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 04:01 AM JST

PDB ID : 8JUT
EMDB ID : EMD-36663
Title : rat megalin RAP complex
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on : 2023-06-27
Resolution : 4.20 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

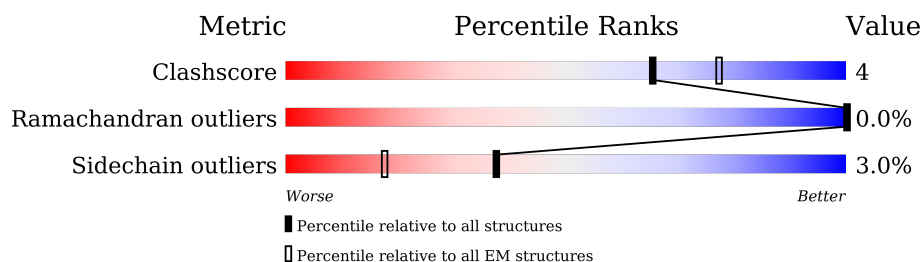
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.









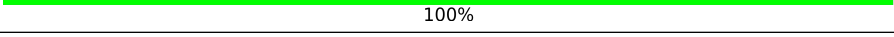
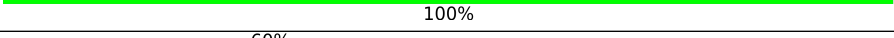
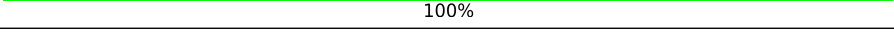
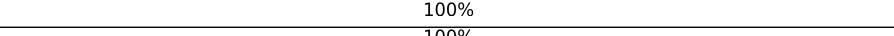
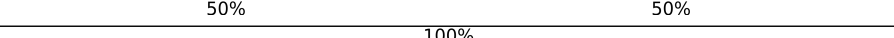
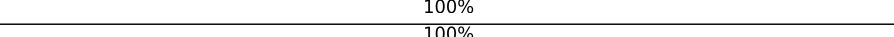

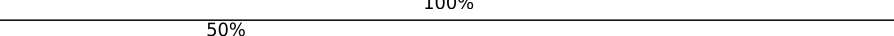
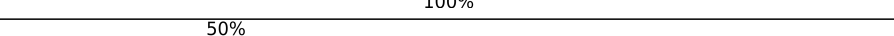
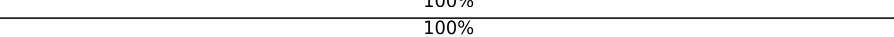
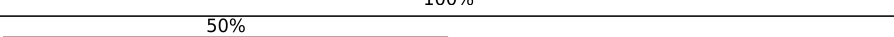
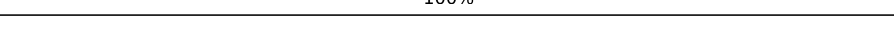







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4660	<div> <div>34%</div> <div>82% 10% 8%</div> </div>
1	B	4660	<div> <div>32%</div> <div>82% 10% 8%</div> </div>
2	C	360	<div> <div>47%</div> <div>39% 10% 51%</div> </div>
2	D	360	<div> <div>48%</div> <div>38% 11% 51%</div> </div>
3	G	6	<div> <div>100%</div> <div>100%</div> </div>
3	N	6	<div> <div>100%</div> <div>100%</div> </div>
4	H	5	<div> <div>20%</div> <div>100%</div> </div>
4	O	5	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	6	
5	P	6	
6	J	3	
6	Q	3	
7	K	5	
7	R	5	
8	L	5	
8	M	5	
8	S	5	
8	T	5	
9	E	2	
9	V	2	
9	X	2	
9	Y	2	
9	a	2	
9	d	2	
9	n	2	
9	q	2	
9	s	2	
9	t	2	
9	v	2	
9	x	2	
9	y	2	
10	1	5	
10	4	5	

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Mol	Chain	Length	Quality of chain
10	5	5	<div>80%</div> <div>60% 40%</div>
10	9	5	<div>100%</div> <div>80% 20%</div>
10	F	5	<div>100%</div> <div>80% 20%</div>
10	Z	5	<div>60%</div> <div>60% 40%</div>
10	b	5	<div>20%</div> <div>80% 20%</div>
10	g	5	<div>60%</div> <div>60% 40%</div>
10	j	5	<div>80%</div> <div>60% 40%</div>
10	k	5	<div>80%</div> <div>40% 60%</div>
10	l	5	<div>100%</div> <div>60% 40%</div>
10	u	5	<div>80%</div> <div>80% 20%</div>
11	U	5	<div>60%</div> <div>20% 60% 20%</div>
12	2	3	<div>67%</div> <div>100%</div>
12	3	3	<div>67%</div> <div>67% 33%</div>
12	W	3	<div>33%</div> <div>33% 33% 33%</div>
12	e	3	<div>100%</div> <div>67% 33%</div>
12	f	3	<div>67%</div> <div>67% 33%</div>
12	h	3	<div>100%</div> <div>100%</div>
12	i	3	<div>67%</div> <div>33% 67%</div>
12	m	3	<div>100%</div> <div>33% 67%</div>
12	p	3	<div>33%</div> <div>67% 33%</div>
12	r	3	<div>33%</div> <div>67% 33%</div>
13	8	2	<div>100%</div> <div>100%</div>
13	c	2	<div>50%</div> <div>100%</div>
13	o	2	<div>100%</div> <div>100%</div>
14	6	5	<div>100%</div> <div>40% 60%</div>

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Mol	Chain	Length	Quality of chain
14	w	5	<div><div></div><div>60%40%</div></div>
15	z	3	<div><div></div><div>33%100%67%</div></div>
16	0	3	<div><div></div><div>33%67%67%</div></div>
16	7	3	<div><div></div><div>100%100%</div></div>

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 73258 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 LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4308	Total	C	N	O	S	0	0
			33638	20708	5950	6605	375		
1	B	4308	Total	C	N	O	S	0	0
			33636	20706	5950	6605	375		

- Molecule 2 is a protein called Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		
2	D	177	Total	C	N	O	S	0	0
			1494	944	273	276	1		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	6	Total	C	N	O	0	0
			30	18	6	6		
3	N	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 4 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	5	Total	C	N	O	0	0
			28	16	6	6		
4	O	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 5 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	6	Total	C	N	O	0	0
			33	21	6	6		
5	P	6	Total	C	N	O	0	0
			33	21	6	6		

- Molecule 6 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	3	Total	C	N	O	S	0	0
			16	9	3	3	1		
6	Q	3	Total	C	N	O	S	0	0
			16	9	3	3	1		

- Molecule 7 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	5	Total	C	N	O	0	0
			33	19	5	9		
7	R	5	Total	C	N	O	0	0
			33	19	5	9		

- Molecule 8 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	5	Total	C	N	O	0	0
			28	16	6	6		
8	M	5	Total	C	N	O	0	0
			28	16	6	6		
8	S	5	Total	C	N	O	0	0
			28	16	6	6		
8	T	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



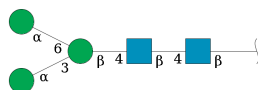
Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		
9	Y	2	Total	C	N	O	0	0
			28	16	2	10		
9	a	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		
9	n	2	Total	C	N	O	0	0
			28	16	2	10		
9	q	2	Total	C	N	O	0	0
			28	16	2	10		
9	s	2	Total	C	N	O	0	0
			28	16	2	10		
9	t	2	Total	C	N	O	0	0
			28	16	2	10		
9	v	2	Total	C	N	O	0	0
			28	16	2	10		
9	x	2	Total	C	N	O	0	0
			28	16	2	10		
9	y	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



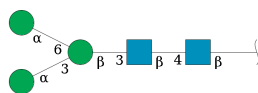
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	5	Total	C	N	O	0	0
			61	34	2	25		
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	b	5	Total	C	N	O	0	0
			61	34	2	25		
10	g	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	5	Total	C	N	O	0	0
			61	34	2	25		
10	k	5	Total	C	N	O	0	0
			61	34	2	25		
10	l	5	Total	C	N	O	0	0
			61	34	2	25		
10	u	5	Total	C	N	O	0	0
			61	34	2	25		
10	1	5	Total	C	N	O	0	0
			61	34	2	25		
10	4	5	Total	C	N	O	0	0
			61	34	2	25		
10	5	5	Total	C	N	O	0	0
			61	34	2	25		
10	9	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	3	Total	C	N	O	0	0
			39	22	2	15		
12	e	3	Total	C	N	O	0	0
			39	22	2	15		

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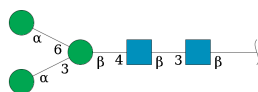
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	3	Total	C	N	O	0	0
			39	22	2	15		
12	h	3	Total	C	N	O	0	0
			39	22	2	15		
12	i	3	Total	C	N	O	0	0
			39	22	2	15		
12	m	3	Total	C	N	O	0	0
			39	22	2	15		
12	p	3	Total	C	N	O	0	0
			39	22	2	15		
12	r	3	Total	C	N	O	0	0
			39	22	2	15		
12	2	3	Total	C	N	O	0	0
			39	22	2	15		
12	3	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	2	Total	C	N	O	0	0
			28	16	2	10		
13	o	2	Total	C	N	O	0	0
			28	16	2	10		
13	8	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	w	5	Total	C	N	O	0	0
			61	34	2	25		
14	6	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 15 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



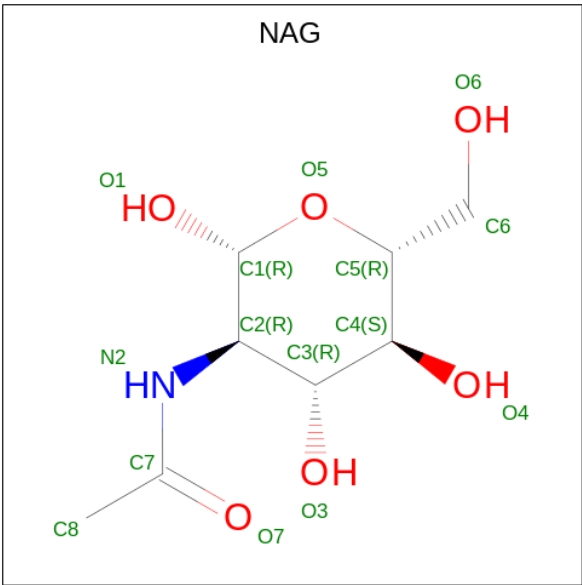
Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 16 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	3	Total	C	N	O	0	0
			39	22	2	15		
16	7	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



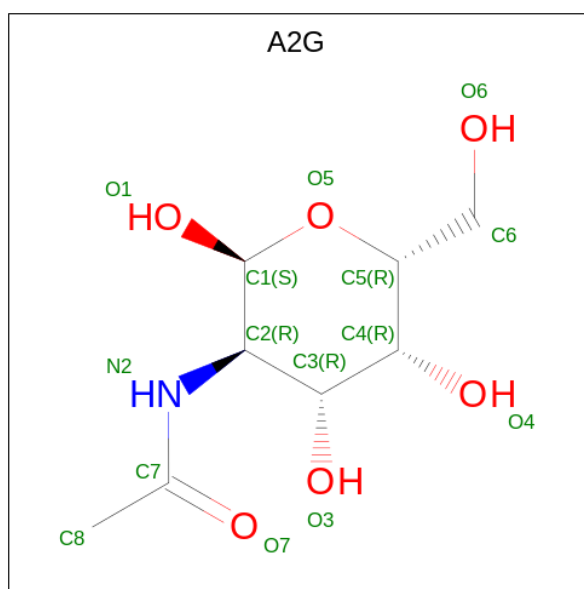
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14	8	1	5	
17	A	1	Total	C	N	O	0
			14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

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

- Molecule 18 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	A	44	Total 44	Ca 44	0
19	B	44	Total 44	Ca 44	0

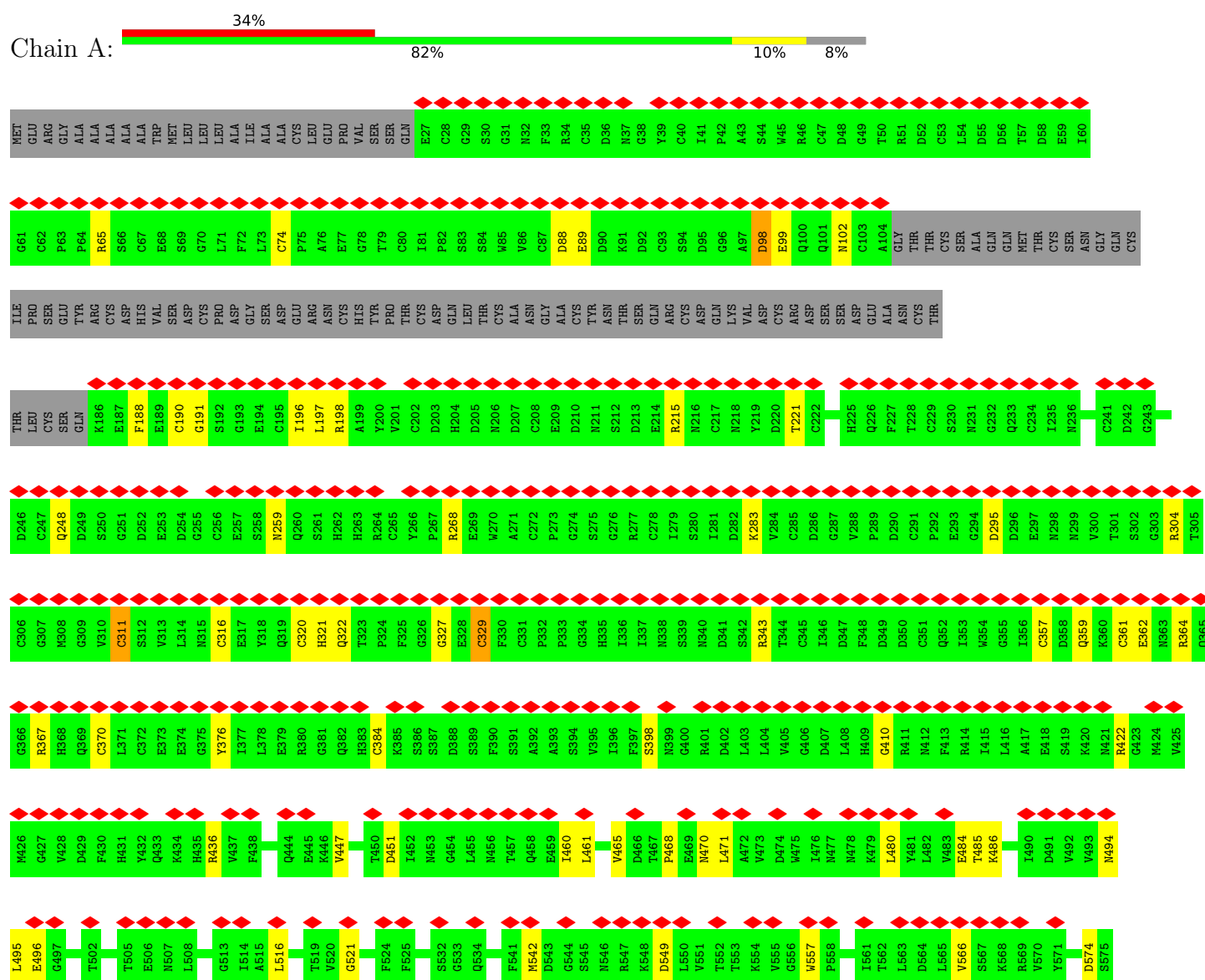
- Molecule 20 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

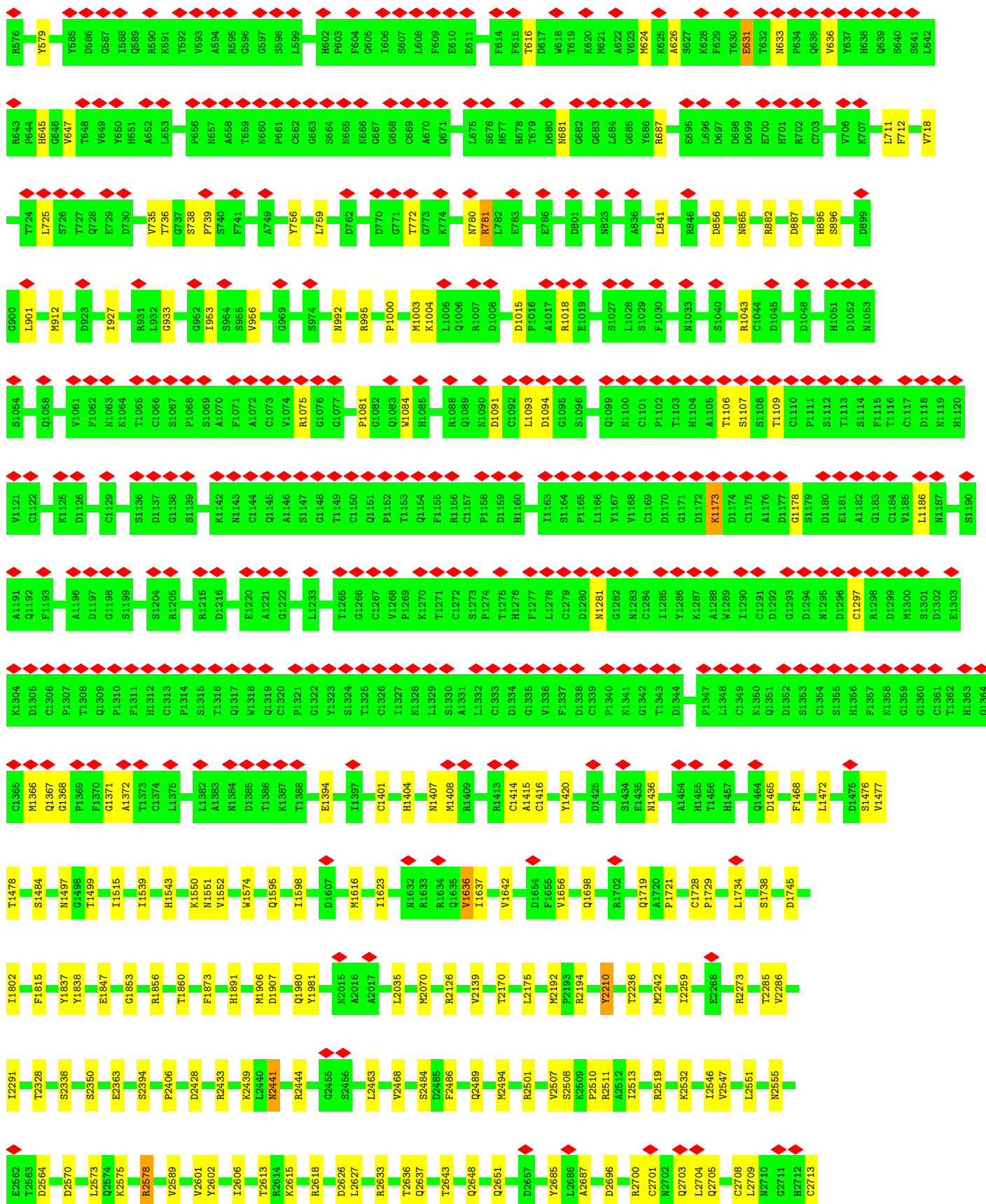
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Ni 1	0
20	B	1	Total 1	Ni 1	0

3 Residue-property plots

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

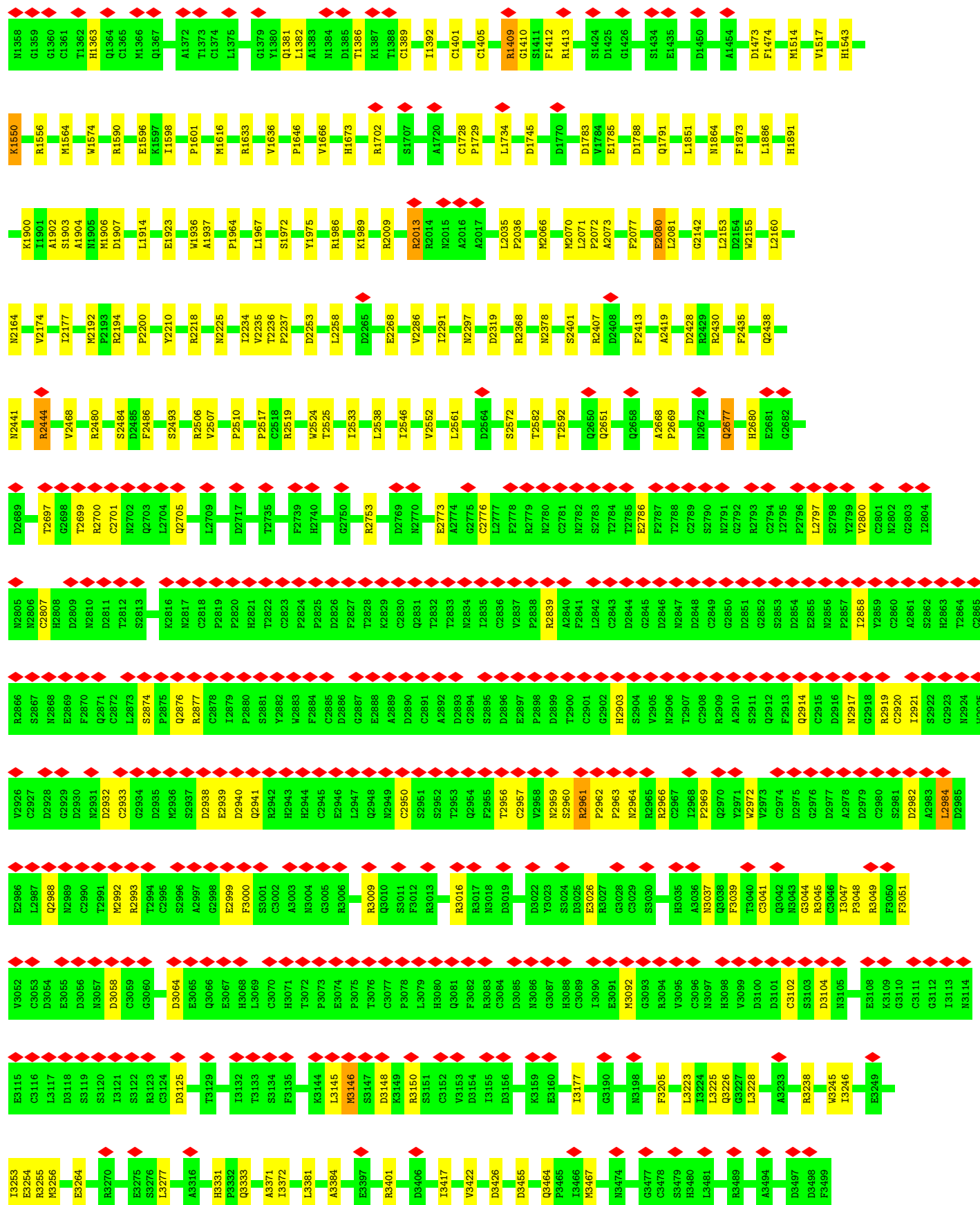
- Molecule 1: LDL receptor related protein 2



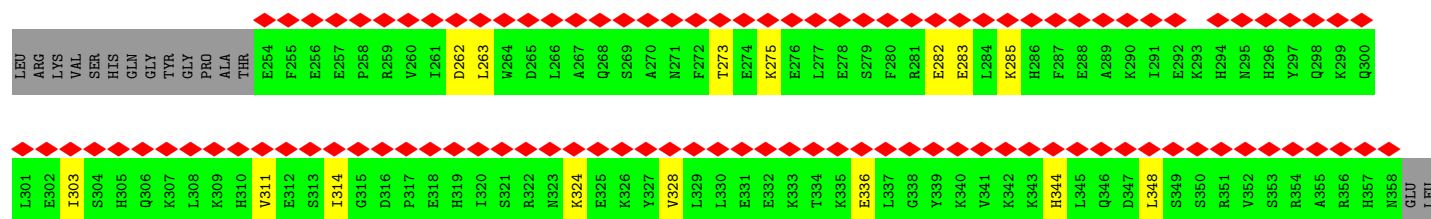




THR	LEU	CYS	SER	GLN	K186	E187	F188	E189	C190	G191	S192	G193	E194	C195	I196	L197	R198	A199	Y200	V201	H204	D205	N206	D207	C208	E209	D210	N211	S212	D213	E214	R215	N216	C217	N218	Y219	D220	T221	C222	G223	G224	H225	Q226	F227	T228	C229	S230	Q233	C234	N238	W239	V240	G243	D244	D245				
D246	C247	Q248	D249	S250	E253	D254	G255	C256	E257	S258	N259	Q260	S261	H262	H263	R264	C265	Y266	P267	R268	E269	W270	A271	C272	P273	G274	S275	G276	R277	C278	I279	N280	I281	D282	K283	V284	C285	D286	G287	V288	P289	D290	C291	P292	E293	G294	D295	D296	E297	N298	N299	V300	T301	S302	G303	R304	T305	C306	
G307	K308	G309	V310	C311	S312	V313	L314	N315	C316	E317	Y318	Q319	C320	H321	Q322	T323	P324	F325	G326	G327	E328	C329	F330	C331	P332	S333	G334	H335	I336	I337	N338	S339	N340	D341	S342	R343	T344	C345	I346	D347	F348	D349	C350	Q351	Q352	I353	W354	G355	I356	C357	D358	Q359	K360	E361	E362	N363	R364	Q365	G366
R367	H368	Q369	C370	L371	C372	E373	E374	G375	Y376	I377	L378	E379	R380	G381	Q382	H383	C384	K385	S386	S387	D388	S389	F390	S391	A392	A393	S394	G395	I396	F397	S398	R401	D402	L403	L404	G405	D407	L408	H409	G410	R411	N412	F413	R414	I415	A416	A417	E418	N421	G427	V428	D429	F430	H431	Y432				
Q433	K434	F438	W439	T440	D441	P442	M443	Q444	E445	K446	V447	F448	S449	T450	D451	I452	M453	L455	M456	T457	Q458	L461	S464	V465	D466	T467	P468	E469	N470	L471	V473	D474	N475	I476	N477	M478	K479	L480	Y481	K486	V487	M488	R489	I490	D491	V492	V493	E496	G497	M498	Q499	R500							
L503	I504	L508	R512	G513	I514	A515	L516	D517	P518	T519	F525	S526	D527	S530	L531	S532	C588	G533	Q534	V537	G544	D549	L550	V551	T552	T553	K554	A559	G560	I561	T562	L563	D564	L565	V566	S567	K568	Y571	D574	Y577	I580	S586	G587	I588	Q589														
T592	V593	A594	R595	S598	L599	V600	F604	G605	I606	S607	L608	F609	E610	F611	H612	V613	F614	F615	T616	T619	K620	V623	M624	K625	A626	D627	K628	F629	T630	E631	T632	N633	P634	Q635	V636	Y637	H638	Q639	S640	S641	L642	R643	P644	H645	G646	V647	T648	V649	R654	T659	N660	P661	C662						
G663	S664	N665	N666	G667	C668	A670	Q671	L675	R678	T679	D680	N681	G682	G683	L684	R687	C688	K689	C690	E691	E695	L696	D697	D698	D699	E700	H701	R702	C703	V704	A705	V706	K707	L725	V735	T736	G737	S738	F739	S740	F741	F742	D746	Y756	S757	K766	G771												
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C1110	P1111	S1112	T1113	F1115	D1118	M1119	H1120	V1121	C1122	I1123	P1124	K1125	D1126	C1129	D1134	C1135	S1136	D1137	G1138	S1139	D1140	E1141	K1142	M1143	C1144	Q1145	A1146	S1147	G1148	T1149	C1150	Q1151	P1152	T1153	Q1154	F1155	R1156	C1157	P1158	D1159	H1160	R1161	C1162	S1164	P1165	L1166	C1169	D1170	G1171	D1172	K1173	A1176							
D1177	G1178	S1179	E1180	E1181	A1182	G1183	V1185	L1186	N1187	C1188	T1189	S1190	A1191	K1194	C1195	A1196	D1197	G1198	S1199	S1200	C1201	R1215	D1216	N1217	C1223	L1233	E1250	T1265	G1266	C1267	K1270	T1271	C1272	S1273	P1274	T1275	H1276	F1277	L1278	C1279	D1280	N1281	G1282	N1283	C1284	I1285	Y1286	K1287	D1292	G1293									
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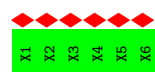




- Molecule 3: unclear peptide



- Molecule 3: unclear peptide



- Molecule 4: unclear peptide

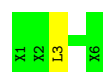
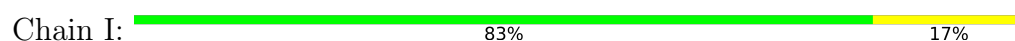


- Molecule 4: unclear peptide

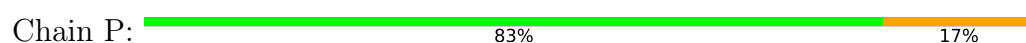


There are no outlier residues recorded for this chain.

- Molecule 5: unclear peptide



- Molecule 5: unclear peptide



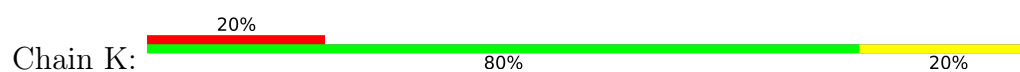
- Molecule 6: unclear peptide



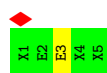
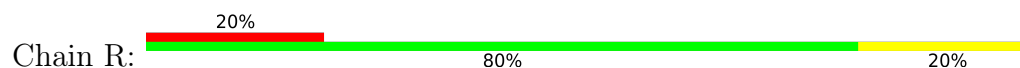
- Molecule 6: unclear peptide



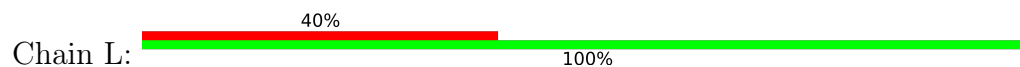
- Molecule 7: unclear peptide



- Molecule 7: unclear peptide



- Molecule 8: unclear peptide



- Molecule 8: unclear peptide



There are no outlier residues recorded for this chain.

- Molecule 8: unclear peptide



- Molecule 8: unclear peptide

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%
100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50%
100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50%
100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



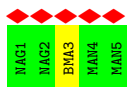
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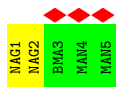
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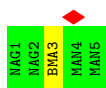
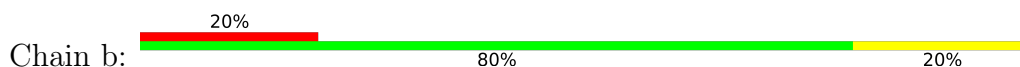
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

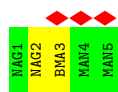


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

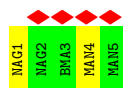
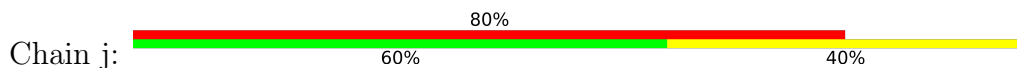


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

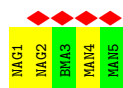
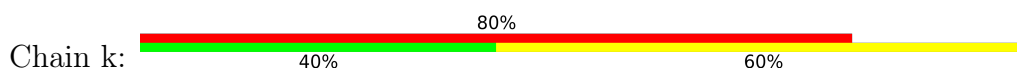




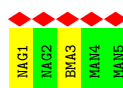
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



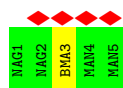
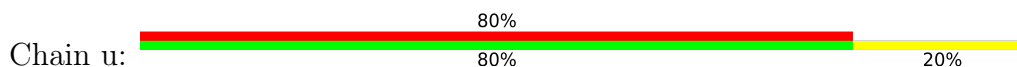
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

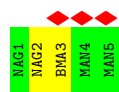


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

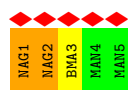


- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

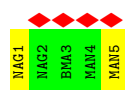
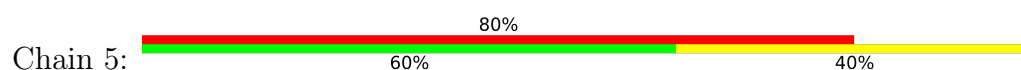




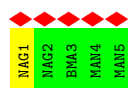
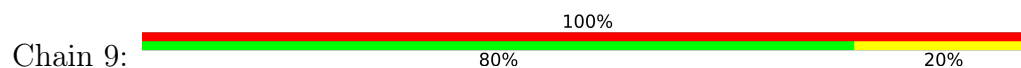
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



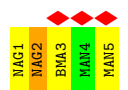
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



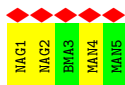
- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: beta-D-mannopyranose-(1-3)-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, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0242	Depositor
Map size (\AA)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.411, 1.411, 1.411	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NI, BMA, NAG, MAN, A2G

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	0.32	0/34456	0.58	5/46804 (0.0%)
1	B	0.63	0/34454	0.67	5/46801 (0.0%)
2	C	0.64	0/1521	0.60	0/2033
2	D	0.63	0/1521	0.62	0/2033
4	H	0.68	0/7	0.49	0/8
4	O	0.82	0/7	0.68	0/8
5	I	0.67	0/7	0.63	0/8
5	P	0.68	0/7	0.88	0/8
6	J	1.03	0/5	0.57	0/5
6	Q	1.03	0/5	0.38	0/5
7	K	0.95	0/17	0.64	0/21
7	R	0.65	0/17	0.48	0/21
8	L	0.57	0/7	0.62	0/8
8	M	0.64	0/7	0.52	0/8
8	S	0.93	0/7	0.59	0/8
8	T	0.58	0/7	0.54	0/8
All	All	0.51	0/72052	0.63	10/97787 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4327	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	3693	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	B	2218	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	364	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	2919	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	4245	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	2919	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	4327	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	4245	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	2368	ARG	NE-CZ-NH2	5.14	122.87	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1043	ARG	Sidechain
1	A	3212	ARG	Sidechain
1	A	4321	ARG	Sidechain
1	A	781	ARG	Sidechain
1	B	2877	ARG	Sidechain
1	B	3693	ARG	Sidechain

5.2 Too-close contacts

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	33638	0	31021	237	0
1	B	33636	0	31021	245	0
2	C	1494	0	1505	22	0
2	D	1494	0	1505	26	0
3	G	30	0	8	0	0
3	N	30	0	8	0	0
4	H	28	0	12	0	0
4	O	28	0	12	0	0
5	I	33	0	18	5	0
5	P	33	0	18	1	0
6	J	16	0	8	0	0
6	Q	16	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	33	0	18	1	0
7	R	33	0	17	0	0
8	L	28	0	12	0	0
8	M	28	0	12	0	0
8	S	28	0	12	0	0
8	T	28	0	12	0	0
9	E	28	0	25	0	0
9	V	28	0	25	0	0
9	X	28	0	25	1	0
9	Y	28	0	25	0	0
9	a	28	0	25	0	0
9	d	28	0	25	0	0
9	n	28	0	25	0	0
9	q	28	0	25	0	0
9	s	28	0	25	0	0
9	t	28	0	25	0	0
9	v	28	0	25	0	0
9	x	28	0	25	0	0
9	y	28	0	25	0	0
10	1	61	0	52	0	0
10	4	61	0	52	1	0
10	5	61	0	52	0	0
10	9	61	0	52	0	0
10	F	61	0	52	0	0
10	Z	61	0	52	0	0
10	b	61	0	52	0	0
10	g	61	0	52	0	0
10	j	61	0	52	0	0
10	k	61	0	52	0	0
10	l	61	0	52	0	0
10	u	61	0	52	0	0
11	U	61	0	52	2	0
12	2	39	0	34	0	0
12	3	39	0	34	0	0
12	W	39	0	34	1	0
12	e	39	0	34	0	0
12	f	39	0	34	0	0
12	h	39	0	34	0	0
12	i	39	0	34	0	0
12	m	39	0	34	0	0
12	p	39	0	34	0	0
12	r	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	8	28	0	25	0	0
13	c	28	0	25	0	0
13	o	28	0	25	0	0
14	6	61	0	52	1	0
14	w	61	0	52	0	0
15	z	39	0	34	0	0
16	0	39	0	34	0	0
16	7	39	0	34	0	0
17	A	154	0	143	2	0
17	B	154	0	143	0	0
18	A	168	0	144	0	0
18	B	168	0	144	0	0
19	A	44	0	0	0	0
19	B	44	0	0	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
All	All	73258	0	67423	526	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3505:ARG:H	1:B:3505:ARG:HD3	1.38	0.90
1:A:3015:ASP:HB2	1:A:3017:ARG:NH2	1.90	0.87
1:A:2786:GLU:HG2	1:A:2788:THR:H	1.43	0.82
1:A:2708:CYS:SG	1:A:2730:SER:OG	2.40	0.79
1:A:3963:GLY:HA2	1:A:4004:LYS:HE2	1.65	0.79
1:B:4073:SER:HB3	1:B:4075:LYS:HG3	1.64	0.79
1:A:1574:TRP:CE3	5:I:3:LEU:HD23	2.20	0.77
1:A:1173:LYS:HD2	1:A:1178:GLY:HA2	1.69	0.74
1:A:4131:ASN:HD21	1:A:4385:CYS:HB2	1.54	0.73
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.70	0.72
1:B:3983:GLN:NE2	1:B:3988:GLY:O	2.23	0.71
1:A:3431:THR:HG22	1:A:3448:ASN:HB3	1.72	0.71
1:B:4282:PHE:O	1:B:4283:GLU:HG3	1.91	0.70
1:B:4041:MET:SD	1:B:4042:SER:N	2.65	0.70
1:A:4313:VAL:O	1:A:4314:ASN:ND2	2.24	0.69
1:A:3937:CYS:SG	1:A:3938:SER:N	2.65	0.69
1:B:2507:VAL:HG21	1:B:2524:TRP:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3675:THR:HG23	1:A:3677:ALA:H	1.57	0.69
1:B:1003:MET:HG2	1:B:1012:CYS:HB3	1.74	0.69
1:B:2959:ASN:ND2	1:B:2982:ASP:OD2	2.26	0.68
1:A:320:CYS:HA	1:A:329:CYS:HB2	1.75	0.68
1:A:4398:LEU:O	1:A:4400:LYS:NZ	2.23	0.68
1:B:2651:GLN:N	1:B:2651:GLN:OE1	2.27	0.68
14:6:1:NAG:O4	14:6:2:NAG:N2	2.25	0.67
1:B:3943:ILE:HG13	1:B:3955:CYS:HB3	1.75	0.67
2:C:99:LEU:O	2:C:103:GLY:N	2.29	0.66
1:A:1574:TRP:CE3	5:I:3:LEU:CD2	2.79	0.66
1:A:3814:PRO:HG2	1:A:3817:LEU:HD13	1.76	0.66
1:B:4269:ILE:HG22	1:B:4270:ILE:HG12	1.76	0.66
1:B:2939:GLU:HG2	1:B:2941:GLN:H	1.60	0.65
1:B:3372:ILE:HD11	1:B:3381:LEU:HD11	1.80	0.64
2:D:96:TRP:HB2	2:D:110:LYS:HG3	1.79	0.64
1:B:1382:LEU:HD12	1:B:1386:THR:HA	1.79	0.64
1:A:912:MET:HE1	1:A:927:ILE:HG21	1.80	0.64
1:A:2463:LEU:HD11	1:A:2501:ARG:HD2	1.79	0.64
1:A:3876:GLU:OE1	1:A:3876:GLU:N	2.31	0.64
1:A:4100:LEU:HD11	1:A:4384:ARG:HG2	1.79	0.63
1:B:574:ASP:OD1	1:B:577:TYR:N	2.23	0.63
2:D:122:LEU:HD22	2:D:127:LEU:HD22	1.79	0.63
1:B:4204:THR:HG22	1:B:4212:ILE:HG12	1.79	0.63
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.81	0.63
1:A:1574:TRP:CZ3	5:I:3:LEU:HD23	2.34	0.63
1:A:2954:GLN:HA	1:A:2969:PRO:HA	1.79	0.63
1:B:811:ARG:NH2	1:B:814:ASP:OD1	2.31	0.63
2:D:79:LEU:HA	2:D:82:LEU:HD12	1.81	0.63
1:A:882:ARG:HE	1:A:895:HIS:HD2	1.46	0.62
1:A:3295:CYS:SG	1:A:3296:LEU:N	2.72	0.62
1:A:2705:GLN:HB3	1:A:2713:CYS:HB3	1.80	0.62
1:A:1550:LYS:O	1:A:1552:VAL:HG23	2.00	0.61
1:A:1281:ASN:ND2	1:A:1297:CYS:O	2.32	0.61
2:D:282:GLU:HA	2:D:285:LYS:HZ3	1.66	0.61
1:A:1595:GLN:HA	1:A:1598:ILE:HD11	1.82	0.61
1:B:863:ILE:HG22	1:B:864:VAL:HG23	1.82	0.60
1:B:616:THR:HG22	1:B:623:VAL:HG22	1.83	0.60
1:A:2795:ILE:HD11	1:A:2800:VAL:HG12	1.84	0.60
1:A:2546:ILE:HG22	1:A:2547:VAL:HG13	1.82	0.60
1:A:1574:TRP:CD2	5:I:3:LEU:HD23	2.37	0.60
1:A:4068:LYS:HB2	1:A:4077:SER:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3862:ILE:HG13	1:B:3863:CYS:SG	2.41	0.60
2:C:291:ILE:O	2:C:295:ASN:ND2	2.35	0.60
1:B:2933:CYS:HB2	1:B:2938:ASP:HB3	1.83	0.60
1:A:3017:ARG:HD3	1:A:3017:ARG:N	2.17	0.60
1:B:465:VAL:HG12	1:B:465:VAL:O	2.02	0.59
1:B:4295:GLU:N	1:B:4295:GLU:OE1	2.35	0.59
1:A:1551:ASN:OD1	9:X:1:NAG:N2	2.35	0.59
1:A:2809:ASP:OD1	1:A:2811:ASP:N	2.35	0.59
1:A:2648:GLN:HB3	1:A:2651:GLN:HE21	1.68	0.59
1:B:1088:ARG:HB3	1:B:1088:ARG:HH21	1.67	0.59
2:C:56:GLU:OE1	2:C:66:TRP:NE1	2.36	0.59
1:B:451:ASP:OD2	1:B:453:ASN:ND2	2.36	0.59
1:B:36:ASP:HB2	1:B:57:THR:HG21	1.84	0.58
1:B:4100:LEU:HD11	1:B:4384:ARG:HG2	1.83	0.58
2:D:111:GLU:O	2:D:114:LEU:HG	2.01	0.58
1:A:3082:PHE:CD2	1:A:3095:VAL:HG21	2.39	0.58
1:B:431:HIS:HD2	1:B:434:LYS:H	1.50	0.58
1:A:2192:MET:HG3	1:A:2192:MET:O	2.04	0.58
1:B:2210:TYR:HB2	1:B:2236:THR:HA	1.85	0.58
1:A:1367:GLN:NE2	1:A:1371:GLY:O	2.31	0.58
2:C:59:MET:O	2:C:63:ASN:ND2	2.26	0.58
1:B:3016:ARG:HD3	1:B:3045:ARG:HD2	1.85	0.58
2:D:72:LEU:O	2:D:73:HIS:ND1	2.37	0.58
1:A:3982:THR:HB	1:A:3990:ILE:HG23	1.86	0.58
1:A:3984:LEU:HD13	1:A:3987:GLY:HA3	1.85	0.58
1:A:4119:ARG:NH2	1:A:4173:LEU:O	2.36	0.58
1:B:766:LYS:HD3	1:B:777:ILE:HD11	1.86	0.58
1:B:2525:THR:HG22	1:B:2533:ILE:HD12	1.86	0.58
1:A:1497:ASN:OD1	12:W:1:NAG:N2	2.37	0.58
1:A:1574:TRP:CD2	5:I:3:LEU:CD2	2.86	0.58
1:A:738:SER:OG	1:A:739:PRO:HD3	2.03	0.57
1:A:2972:TRP:CZ2	2:D:127:LEU:HD21	2.39	0.57
1:B:268:ARG:HG3	1:B:281:ILE:HG12	1.86	0.57
1:B:2070:MET:HG3	1:B:2072:PRO:HD2	1.86	0.57
1:B:3064:ASP:OD1	1:B:3064:ASP:N	2.33	0.57
1:B:1923:GLU:HB2	1:B:1937:ALA:HB3	1.86	0.57
10:4:1:NAG:H83	10:4:2:NAG:H83	1.85	0.57
1:B:1864:ASN:ND2	1:B:2319:ASP:OD1	2.37	0.57
2:C:281:ARG:O	2:C:285:LYS:HG2	2.05	0.57
1:A:3144:LYS:HB3	1:A:3155:ILE:HD11	1.86	0.57
1:B:2950:CYS:HB3	1:B:2956:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:ARG:HA	2:C:284:LEU:HD12	1.87	0.57
1:A:321:HIS:CD2	1:A:322:GLN:H	2.22	0.56
1:B:1937:ALA:HB1	1:B:1964:PRO:HG2	1.87	0.56
1:A:2484:SER:HB3	1:A:2513:ILE:HD11	1.86	0.56
1:B:3225:LEU:HD13	1:B:3256:MET:HE1	1.87	0.56
1:A:3295:CYS:SG	1:A:3308:MET:HG2	2.45	0.56
1:A:4254:ASP:HB2	1:A:4275:LYS:H	1.71	0.56
1:B:486:LYS:HG2	1:B:736:THR:HG21	1.87	0.56
1:B:616:THR:HB	1:B:644:PRO:HB2	1.88	0.56
1:B:4295:GLU:HG3	1:B:4312:VAL:HG13	1.87	0.56
1:A:295:ASP:OD1	1:A:304:ARG:NH1	2.38	0.56
1:B:3016:ARG:NE	1:B:3044:GLY:O	2.38	0.56
1:B:2959:ASN:O	1:B:2961:ARG:NH1	2.39	0.56
1:B:4098:ILE:O	1:B:4384:ARG:NH1	2.38	0.56
1:A:3066:GLN:HE21	1:A:3069:LEU:H	1.54	0.56
1:B:4398:LEU:HD23	1:B:4399:PRO:HD2	1.88	0.56
1:A:1853:GLY:O	1:A:1856:ARG:NH1	2.30	0.56
1:B:3981:CYS:SG	1:B:3982:THR:N	2.78	0.56
1:A:3693:ARG:HH22	1:A:3708:ARG:HG2	1.70	0.55
1:B:272:CYS:HB2	1:B:295:ASP:HB3	1.88	0.55
1:B:3976:ILE:HG12	1:B:3989:PHE:HE2	1.70	0.55
1:B:3048:PRO:HD2	1:B:3051:PHE:HE1	1.71	0.55
1:A:486:LYS:HG2	1:A:736:THR:HG21	1.87	0.55
1:B:3026:GLU:HA	1:B:3026:GLU:OE1	2.07	0.55
1:A:712:PHE:CE1	1:A:953:ILE:HD11	2.41	0.55
1:A:3617:SER:N	1:A:3627:GLU:OE1	2.39	0.55
1:A:3425:THR:HB	1:A:3453:PRO:HG2	1.88	0.55
1:A:2285:THR:HG21	1:A:2328:THR:HA	1.89	0.54
1:B:1473:ASP:OD1	1:B:1474:PHE:N	2.40	0.54
1:B:4204:THR:HG23	1:B:4236:LEU:HD22	1.88	0.54
1:A:616:THR:HG23	1:A:647:VAL:HG23	1.89	0.54
1:A:2139:VAL:HG22	1:A:2175:LEU:HD13	1.88	0.54
1:B:2081:LEU:H	1:B:2081:LEU:HD22	1.72	0.54
1:B:4256:ILE:HB	1:B:4270:ILE:HB	1.89	0.54
1:B:3146:MET:SD	1:B:3146:MET:N	2.80	0.54
1:B:190:CYS:SG	1:B:191:GLY:N	2.81	0.54
1:B:1088:ARG:HB3	1:B:1088:ARG:NH2	2.22	0.54
1:B:2999:GLU:HA	1:B:3009:ARG:HA	1.89	0.54
2:D:283:GLU:HG2	2:D:348:LEU:HD21	1.88	0.54
1:B:4390:ASN:O	1:B:4401:CYS:HB2	2.08	0.54
1:A:3760:GLU:OE1	1:A:3760:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4130:ASN:HB2	1:A:4389:GLY:O	2.08	0.54
1:A:1636:VAL:HG23	1:A:1637:ILE:HG13	1.90	0.54
1:B:2192:MET:O	1:B:2192:MET:HG3	2.08	0.54
1:A:557:TRP:N	1:A:574:ASP:OD1	2.41	0.53
1:A:3949:CYS:SG	1:A:3990:ILE:HB	2.48	0.53
1:B:3145:LEU:HD22	1:B:3146:MET:H	1.73	0.53
2:D:113:LYS:HA	2:D:116:HIS:CD2	2.42	0.53
1:B:2080:GLU:O	1:B:2080:GLU:HG3	2.08	0.53
1:A:321:HIS:HD2	1:A:322:GLN:H	1.57	0.53
1:A:3090:ILE:HG12	1:A:3094:ARG:HG3	1.91	0.53
2:C:62:LEU:HG	2:C:86:LEU:HD22	1.89	0.53
1:A:2468:VAL:HG12	1:A:2486:PHE:HB3	1.90	0.53
1:B:1598:ILE:HD11	1:B:1601:PRO:HB3	1.88	0.53
1:B:1550:LYS:O	1:B:1590:ARG:NH2	2.38	0.53
1:B:4391:CYS:HA	1:B:4401:CYS:HB2	1.90	0.53
1:A:1497:ASN:OD1	1:A:1499:THR:OG1	2.22	0.53
1:A:2484:SER:HB2	1:A:2510:PRO:HB2	1.90	0.53
1:A:1394:GLU:OE1	1:A:1407:ASN:ND2	2.35	0.53
1:A:4131:ASN:ND2	1:A:4385:CYS:HB2	2.20	0.53
1:A:3504:LEU:HG	1:A:3505:ARG:H	1.74	0.52
1:B:2903:HIS:CD2	1:B:2917:ASN:HD22	2.27	0.52
1:B:4314:ASN:OD1	1:B:4314:ASN:N	2.41	0.52
1:A:2954:GLN:HG2	1:A:2969:PRO:HA	1.91	0.52
1:B:3238:ARG:NH2	1:B:3464:GLN:O	2.43	0.52
1:A:2601:VAL:HB	1:A:2606:ILE:HG22	1.90	0.52
1:A:4024:ARG:N	1:A:4031:GLU:O	2.41	0.52
1:A:4228:GLU:O	1:A:4266:ARG:NH2	2.29	0.52
1:A:1004:LYS:HD2	1:A:1015:ASP:HB2	1.92	0.52
1:B:2697:THR:HG23	1:B:2699:THR:H	1.74	0.52
1:A:3564:ASP:OD2	1:A:3582:ASP:HB2	2.09	0.52
1:A:2194:ARG:HG3	1:A:2210:TYR:CZ	2.45	0.52
1:B:1543:HIS:HB3	1:B:1729:PRO:HG3	1.91	0.52
1:B:3371:ALA:HB3	1:B:3384:ALA:HB3	1.92	0.52
1:A:616:THR:HG23	1:A:647:VAL:CG2	2.39	0.52
1:A:1416:CYS:SG	1:A:1420:TYR:HB2	2.50	0.52
1:B:3978:GLU:OE1	1:B:3978:GLU:N	2.43	0.52
1:B:4299:GLN:NE2	1:B:4307:LYS:HG3	2.25	0.52
1:A:359:GLN:HE21	1:A:566:VAL:HG21	1.73	0.52
1:B:963:ASP:HB3	1:B:966:LEU:HD23	1.92	0.52
1:B:3915:SER:HA	1:B:3918:LYS:HG3	1.92	0.52
1:A:2797:LEU:O	1:A:2798:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:VAL:HG13	1:B:821:ILE:HB	1.93	0.51
1:B:2468:VAL:HG23	1:B:2486:PHE:HB3	1.92	0.51
1:A:3597:GLU:OE1	1:A:3597:GLU:N	2.37	0.51
1:A:3886:GLU:HG3	1:A:3888:PRO:HD2	1.91	0.51
1:A:1980:GLN:O	1:A:1981:TYR:HB2	2.10	0.51
1:B:735:VAL:HG11	1:B:756:TYR:CZ	2.45	0.51
1:B:825:ASN:O	1:B:826:ASN:ND2	2.43	0.51
1:A:1802:ILE:HG23	1:A:1815:PHE:HB3	1.93	0.51
1:A:2955:PHE:HB2	1:A:2970:GLN:HE22	1.75	0.51
1:B:3246:ILE:HG12	1:B:3253:ILE:HG12	1.92	0.51
1:B:3671:ASP:OD1	1:B:3672:GLU:N	2.43	0.51
2:D:64:GLN:HG2	2:D:68:LYS:HD2	1.92	0.51
1:B:1081:PRO:HD2	1:B:1084:TRP:CE3	2.45	0.51
1:B:1574:TRP:CD2	5:P:3:LEU:HD13	2.46	0.51
1:A:2960:SER:O	1:A:2961:ARG:NH2	2.43	0.51
1:A:3966:LEU:O	1:A:3970:ARG:NH1	2.44	0.51
1:B:2210:TYR:CB	1:B:2236:THR:HA	2.41	0.51
1:A:3015:ASP:HB2	1:A:3017:ARG:HH22	1.72	0.50
1:B:2441:ASN:OD1	1:B:2444:ARG:N	2.41	0.50
1:B:3039:PHE:N	1:B:3047:ILE:O	2.44	0.50
1:B:407:ASP:OD1	1:B:407:ASP:N	2.44	0.50
1:B:4299:GLN:HE21	1:B:4307:LYS:HG3	1.75	0.50
1:A:2547:VAL:HG23	1:A:2551:LEU:HD11	1.93	0.50
1:B:3125:ASP:OD1	1:B:3125:ASP:N	2.45	0.50
1:B:3331:HIS:CE1	1:B:3333:GLN:HB3	2.46	0.50
1:A:1000:PRO:HD2	1:A:1003:MET:HE3	1.93	0.50
1:A:2441:ASN:HD21	1:A:2444:ARG:HD3	1.75	0.50
1:B:4234:ASN:HD21	1:B:4251:SER:HB3	1.77	0.50
1:A:471:LEU:HD11	1:A:480:LEU:HD21	1.94	0.50
1:A:1404:HIS:HB2	1:A:1415:ALA:HB3	1.93	0.50
1:B:4078:GLU:OE1	1:B:4078:GLU:HA	2.12	0.50
1:A:447:VAL:O	1:A:460:ILE:N	2.41	0.49
1:B:461:LEU:HB3	1:B:465:VAL:HG21	1.95	0.49
1:B:1363:HIS:ND1	1:B:1389:CYS:SG	2.86	0.49
1:A:436:ARG:NH2	1:A:451:ASP:OD1	2.43	0.49
1:A:460:ILE:HD12	1:A:496:GLU:HA	1.95	0.49
1:A:4079:TYR:HD2	1:A:4080:LEU:H	1.61	0.49
2:C:113:LYS:HG2	2:C:114:LEU:HD23	1.93	0.49
2:D:99:LEU:HB3	2:D:105:ASP:HB2	1.95	0.49
1:A:2519:ARG:NH1	1:A:2564:ASP:OD1	2.46	0.49
1:B:1140:ASP:OD1	1:B:1140:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:CYS:SG	1:A:191:GLY:N	2.86	0.49
1:A:953:ILE:HG23	1:A:956:VAL:HB	1.94	0.49
1:A:3849:PHE:HB3	1:A:3857:ILE:HG23	1.94	0.49
1:A:3863:CYS:O	1:A:3890:ARG:NH1	2.45	0.49
1:A:3128:CYS:SG	1:A:3129:THR:N	2.85	0.49
1:A:3616:ASP:N	1:A:3627:GLU:OE1	2.46	0.49
1:B:2480:ARG:NH2	1:B:2493:SER:OG	2.46	0.49
2:D:78:ARG:HG3	2:D:125:TYR:HD1	1.78	0.49
1:A:1907:ASP:HA	1:A:2035:LEU:HD13	1.94	0.49
1:A:4337:LYS:NZ	1:B:48:ASP:OD2	2.33	0.49
1:B:2268:GLU:HA	1:B:2268:GLU:OE1	2.13	0.49
1:B:4098:ILE:HG23	1:B:4384:ARG:HH11	1.76	0.49
1:B:4314:ASN:ND2	1:B:4316:TRP:HB2	2.28	0.49
1:A:1075:ARG:HD2	1:A:1094:ASP:CB	2.43	0.48
1:A:321:HIS:HD2	1:A:322:GLN:HG2	1.78	0.48
1:B:2194:ARG:HG3	1:B:2210:TYR:CZ	2.48	0.48
1:A:2511:ARG:NH2	1:A:2555:ASN:OD1	2.45	0.48
1:A:484:GLU:OE1	1:A:486:LYS:N	2.46	0.48
1:A:4394:ASP:N	1:A:4400:LYS:HZ1	2.12	0.48
1:B:91:LYS:HD2	1:B:96:GLY:HA3	1.95	0.48
1:B:396:ILE:HG22	1:B:405:VAL:HG22	1.94	0.48
1:B:2969:PRO:HD2	1:B:2972:TRP:CD2	2.48	0.48
1:B:4043:THR:HG22	1:B:4044:HIS:H	1.77	0.48
1:A:494:ASN:OD1	1:A:495:LEU:N	2.47	0.48
1:B:2070:MET:HG2	1:B:2073:ALA:O	2.14	0.48
1:B:2234:ILE:HD11	1:B:2237:PRO:HG3	1.96	0.48
1:B:2921:ILE:HD11	1:B:2938:ASP:HB2	1.96	0.48
2:C:96:TRP:HA	2:C:110:LYS:HZ3	1.79	0.48
1:B:1903:SER:HB3	1:B:1914:LEU:HD11	1.95	0.48
1:B:2957:CYS:HB3	1:B:2984:LEU:HD11	1.96	0.48
1:A:1477:VAL:HG23	1:A:1478:THR:HG23	1.96	0.48
1:A:3135:PHE:CD1	1:A:3135:PHE:C	2.88	0.48
1:B:1514:MET:HG3	1:B:1556:ARG:O	2.14	0.48
1:B:793:ILE:HG21	1:B:971:ASN:OD1	2.14	0.47
1:B:3048:PRO:HD2	1:B:3051:PHE:CE1	2.49	0.47
1:A:197:LEU:H	1:A:197:LEU:HD22	1.79	0.47
1:B:3051:PHE:HB3	1:B:3058:ASP:OD2	2.14	0.47
1:A:98:ASP:OD1	1:A:98:ASP:N	2.42	0.47
1:B:788:LEU:HD13	1:B:799:TRP:HB3	1.95	0.47
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.95	0.47
1:A:1873:PHE:HB3	1:A:1891:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:ARG:HB3	1:B:847:PRO:HD3	1.97	0.47
1:B:2984:LEU:O	1:B:2988:GLN:HG2	2.13	0.47
2:D:110:LYS:O	2:D:114:LEU:HD23	2.14	0.47
1:A:311:CYS:HB2	1:A:327:GLY:HA3	1.96	0.47
1:A:3417:ILE:CD1	1:A:3422:VAL:HG12	2.45	0.47
1:B:699:ASP:OD2	1:B:702:ARG:NH2	2.47	0.47
1:B:1596:GLU:O	1:B:1633:ARG:NH2	2.32	0.47
1:B:299:ASN:OD1	1:B:301:THR:OG1	2.31	0.47
1:B:1381:GLN:HB3	1:B:1392:ILE:HD11	1.96	0.47
1:B:4247:TYR:CD2	1:B:4258:ALA:HB2	2.49	0.47
1:A:2972:TRP:CH2	2:D:127:LEU:HD21	2.50	0.47
1:B:1188:CYS:HB2	1:B:1194:LYS:HE2	1.97	0.47
1:B:1412:PHE:O	1:B:1413:ARG:NH2	2.48	0.47
1:B:1616:MET:CE	1:B:1646:PRO:HB2	2.45	0.47
1:B:3758:PRO:HB2	1:B:3767:ARG:NH1	2.30	0.47
1:B:4068:LYS:HB2	1:B:4077:SER:OG	2.15	0.47
1:B:4070:ASN:HD22	1:B:4073:SER:HB2	1.79	0.47
1:B:2160:LEU:HB2	1:B:2177:ILE:HD11	1.96	0.47
1:A:2519:ARG:HH21	1:A:2519:ARG:HG3	1.80	0.47
1:A:2210:TYR:OH	7:K:2:GLU:OE2	2.28	0.47
1:B:1785:GLU:OE2	1:B:2009:ARG:NH2	2.48	0.47
1:A:460:ILE:HG22	1:A:461:LEU:HG	1.97	0.46
1:A:484:GLU:OE1	1:A:485:THR:N	2.49	0.46
1:A:2602:TYR:HB2	1:A:2643:THR:HG21	1.96	0.46
1:B:34:ARG:NE	1:B:38:GLY:HA2	2.30	0.46
1:B:3553:ARG:NH2	1:B:3555:CYS:HB2	2.30	0.46
1:B:3758:PRO:HB2	1:B:3767:ARG:HH11	1.80	0.46
1:A:3930:CYS:N	1:A:3942:CYS:SG	2.89	0.46
1:A:4080:LEU:HD21	1:A:4083:GLU:HG3	1.96	0.46
1:A:3949:CYS:HA	1:A:3961:GLU:HG3	1.97	0.46
1:A:4022:SER:O	1:A:4032:CYS:HB2	2.15	0.46
1:A:4142:TYR:HB3	1:B:3793:ARG:HB2	1.96	0.46
1:A:4301:LYS:HE3	1:A:4302:PHE:CZ	2.51	0.46
1:B:1907:ASP:HA	1:B:2035:LEU:HD13	1.97	0.46
1:B:3102:CYS:HB3	1:B:3104:ASP:OD1	2.16	0.46
1:B:1734:LEU:HD12	1:B:1734:LEU:HA	1.82	0.46
1:A:2703:GLN:HE21	1:A:2704:LEU:HG	1.80	0.46
1:A:735:VAL:HG11	1:A:756:TYR:CZ	2.51	0.46
1:A:1476:SER:HB3	1:A:1698:GLN:HG3	1.97	0.46
1:A:2573:LEU:HB3	1:A:2575:LYS:HE2	1.98	0.46
1:A:3721:CYS:HB3	1:A:3726:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:ARG:HG3	1:B:1410:GLY:N	2.30	0.46
1:B:2419:ALA:O	1:B:2438:GLN:NE2	2.45	0.46
1:A:465:VAL:O	1:A:468:PRO:HD3	2.15	0.46
1:A:2286:VAL:HG22	1:A:2291:ILE:HG22	1.97	0.46
1:B:33:PHE:CD2	1:B:46:ARG:HG3	2.51	0.46
1:B:3041:CYS:SG	1:B:3045:ARG:HB2	2.56	0.46
1:A:316:CYS:HB3	1:A:343:ARG:HA	1.98	0.45
1:A:3280:ASP:OD2	1:A:3283:SER:N	2.36	0.45
1:A:3449:THR:OG1	1:A:3451:HIS:O	2.34	0.45
1:B:844:TRP:HB2	1:B:870:TRP:HA	1.98	0.45
1:B:1596:GLU:HA	1:B:1596:GLU:OE1	2.16	0.45
1:B:2932:ASP:HB2	1:B:2938:ASP:CG	2.35	0.45
1:B:3417:ILE:CD1	1:B:3422:VAL:HG12	2.46	0.45
1:A:1734:LEU:HD11	1:A:1738:SER:HA	1.98	0.45
1:A:2685:TYR:CE2	1:A:2687:ALA:HB2	2.51	0.45
1:A:3125:ASP:HB2	1:A:3151:SER:HA	1.98	0.45
1:B:4018:ILE:HG22	1:B:4019:CYS:SG	2.56	0.45
1:B:4065:ARG:HD2	1:B:4067:ARG:HD3	1.98	0.45
1:A:422:ARG:HH11	1:A:1091:ASP:CG	2.20	0.45
1:A:3984:LEU:HB3	1:A:3988:GLY:N	2.32	0.45
1:B:1788:ASP:OD2	1:B:2013:ARG:HA	2.16	0.45
1:A:1847:GLU:HB3	1:A:1860:THR:HA	1.99	0.45
1:A:2210:TYR:HB2	1:A:2236:THR:HA	1.98	0.45
1:A:2613:THR:O	1:A:2615:LYS:N	2.50	0.45
1:B:2253:ASP:HB3	1:B:2258:LEU:HD23	1.99	0.45
1:B:3916:ASP:OD1	1:B:3916:ASP:N	2.50	0.45
1:B:757:SER:HB3	1:B:788:LEU:HD21	1.98	0.45
2:D:311:VAL:HA	2:D:314:ILE:HD12	1.97	0.45
1:A:1837:TYR:CZ	1:A:1906:MET:HG2	2.52	0.45
1:B:318:TYR:CD2	1:B:319:GLN:HG2	2.52	0.45
1:B:1564:MET:HE1	1:B:1702:ARG:HE	1.82	0.45
1:B:2797:LEU:O	1:B:2800:VAL:HG22	2.17	0.45
1:B:4384:ARG:HD3	1:B:4411:TYR:CE2	2.52	0.45
1:A:1075:ARG:HD2	1:A:1094:ASP:HB2	1.98	0.45
1:B:266:TYR:HB3	1:B:267:PRO:HD2	1.99	0.45
1:A:321:HIS:CD2	1:A:322:GLN:HG2	2.53	0.45
1:A:1106:THR:HG22	1:A:1107:SER:H	1.81	0.45
1:B:2592:THR:HG22	1:B:2592:THR:O	2.16	0.45
1:B:4295:GLU:HG2	1:B:4309:LYS:HE2	1.99	0.45
2:D:85:ASP:HB3	2:D:121:ILE:HD11	1.99	0.45
1:A:1539:ILE:HD12	1:A:1539:ILE:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:THR:HB	1:B:468:PRO:HG2	1.98	0.44
1:B:1091:ASP:OD1	1:B:1091:ASP:N	2.50	0.44
1:B:2506:ARG:HH21	1:B:2506:ARG:HB3	1.81	0.44
2:C:58:ARG:N	2:C:90:GLU:OE1	2.50	0.44
1:A:89:GLU:N	1:A:99:GLU:OE1	2.50	0.44
1:A:461:LEU:HB3	1:A:465:VAL:HG21	2.00	0.44
1:A:1368:GLY:H	1:A:1372:ALA:HA	1.82	0.44
1:A:3562:CYS:SG	1:A:3566:ASN:HB2	2.57	0.44
1:B:4079:TYR:CG	1:B:4080:LEU:N	2.85	0.44
1:A:1484:SER:HB3	1:A:1515:ILE:HD11	1.99	0.44
1:A:2406:PRO:HG2	1:A:2618:ARG:HH11	1.82	0.44
1:A:2489:GLN:NE2	1:A:2508:SER:O	2.49	0.44
1:A:3146:MET:HG2	1:A:3147:SER:N	2.32	0.44
1:B:474:ASP:HB3	1:B:479:LYS:HB2	1.99	0.44
2:D:118:LEU:O	2:D:122:LEU:HG	2.18	0.44
1:A:687:ARG:HH22	2:C:275:LYS:HE3	1.82	0.44
1:A:3228:LEU:HD13	1:A:3231:VAL:HG21	2.00	0.44
1:B:4100:LEU:HD23	1:B:4123:PRO:HA	1.99	0.44
2:D:273:THR:HG22	2:D:275:LYS:H	1.82	0.44
1:A:3115:GLU:HB2	1:A:3135:PHE:HD2	1.81	0.44
1:A:98:ASP:HA	1:A:102:ASN:ND2	2.33	0.44
1:A:1109:THR:HG23	1:A:1109:THR:O	2.17	0.44
1:B:3223:LEU:HD11	1:B:3226:GLN:HB3	1.99	0.44
1:B:4019:CYS:HB3	1:B:4032:CYS:HB3	1.94	0.44
1:A:3626:ASP:OD1	1:A:3626:ASP:N	2.51	0.44
1:A:3887:SER:N	1:A:3888:PRO:HD2	2.33	0.44
2:D:66:TRP:CZ2	2:D:70:LYS:NZ	2.84	0.44
1:B:308:MET:HG3	1:B:322:GLN:HB3	2.00	0.44
1:B:2962:PRO:N	1:B:2963:PRO:HD2	2.32	0.44
1:B:3626:ASP:OD1	1:B:3626:ASP:N	2.50	0.44
1:B:3962:THR:N	1:B:3990:ILE:HD11	2.32	0.44
1:B:270:TRP:CH2	1:B:272:CYS:HA	2.53	0.43
1:B:1972:SER:HA	1:B:1989:LYS:HD2	2.00	0.43
1:B:2286:VAL:HG22	1:B:2291:ILE:HG22	2.00	0.43
1:A:718:VAL:HB	1:A:735:VAL:HB	2.00	0.43
1:A:2787:PHE:CZ	1:A:2814:ASP:HA	2.53	0.43
1:A:3081:GLN:HB3	1:A:3089:CYS:SG	2.58	0.43
1:B:1616:MET:HE3	1:B:1646:PRO:HB2	1.99	0.43
2:C:76:PRO:HA	2:C:79:LEU:HB3	2.01	0.43
2:C:82:LEU:HD13	2:C:125:TYR:CE2	2.53	0.43
1:A:626:ALA:HB1	1:A:631:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3671:ASP:OD1	1:B:3671:ASP:C	2.57	0.43
2:C:316:ASP:HB3	2:C:319:HIS:HB2	2.00	0.43
1:A:364:ARG:O	1:A:367:ARG:HD3	2.19	0.43
1:A:1616:MET:HG2	1:A:1623:ILE:HG12	2.00	0.43
1:B:1873:PHE:HB3	1:B:1891:HIS:HB2	1.99	0.43
1:B:2507:VAL:HG21	1:B:2524:TRP:NE1	2.30	0.43
1:B:2773:GLU:HA	1:B:2776:CYS:SG	2.59	0.43
1:A:188:PHE:O	1:A:196:ILE:N	2.52	0.43
1:A:780:ASN:OD1	1:A:781:ARG:HG2	2.19	0.43
1:A:1734:LEU:CD1	1:A:1738:SER:HA	2.49	0.43
1:A:3793:ARG:NH1	1:B:4142:TYR:O	2.52	0.43
1:B:2484:SER:HB2	1:B:2510:PRO:HG2	2.01	0.43
1:B:2561:LEU:HD12	1:B:2561:LEU:HA	1.87	0.43
1:B:3037:ASN:O	1:B:3049:ARG:HG2	2.18	0.43
1:B:3225:LEU:HD23	1:B:3228:LEU:HD11	2.01	0.43
1:B:3255:ARG:NE	1:B:3264:GLU:OE2	2.36	0.43
1:B:3857:ILE:HD12	1:B:3857:ILE:O	2.17	0.43
2:D:96:TRP:HE3	2:D:110:LYS:HB3	1.84	0.43
1:A:1186:LEU:HD12	1:A:1186:LEU:O	2.19	0.43
1:A:2636:THR:HG22	1:A:2637:GLN:N	2.33	0.43
1:A:2787:PHE:O	1:A:2788:THR:OG1	2.29	0.43
1:B:1265:THR:HG21	1:B:3177:ILE:HD11	2.00	0.43
1:B:3610:PRO:HG2	1:B:3613:TRP:CD2	2.54	0.43
2:C:97:LYS:O	2:C:100:LYS:N	2.50	0.43
1:A:1623:ILE:HD12	1:A:1637:ILE:HD12	2.00	0.43
1:B:451:ASP:HB3	1:B:454:GLY:O	2.19	0.43
2:C:59:MET:SD	2:C:60:GLU:N	2.91	0.43
1:A:3722:HIS:CG	1:A:3723:PRO:HD2	2.54	0.43
1:B:461:LEU:HD11	1:B:493:VAL:HG11	2.00	0.43
1:A:3980:ASN:OD1	17:A:4710:NAG:N2	2.52	0.43
1:B:2401:SER:HB2	1:B:2413:PHE:CZ	2.54	0.43
1:B:2939:GLU:HG2	1:B:2940:ASP:N	2.33	0.43
1:B:3016:ARG:HB2	1:B:3016:ARG:NH2	2.33	0.43
2:D:80:ALA:O	2:D:83:HIS:ND1	2.48	0.43
2:D:303:ILE:HD13	2:D:303:ILE:HA	1.95	0.43
1:A:865:ASN:N	1:A:865:ASN:OD1	2.50	0.42
1:A:2578:ARG:HD2	1:A:2589:VAL:HG22	2.00	0.42
1:B:2960:SER:HB3	1:B:2964:ASN:HB3	2.01	0.42
1:B:3904:LEU:HD12	1:B:3916:ASP:HA	2.00	0.42
1:A:2428:ASP:HB3	1:A:2433:ARG:HG2	2.01	0.42
1:B:2546:ILE:HD12	1:B:2582:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ASN:HD22	11:U:1:NAG:C7	2.32	0.42
1:A:1838:TYR:CZ	1:A:1847:GLU:HG3	2.54	0.42
1:A:2259:ILE:HB	1:A:2273:ARG:HB2	2.01	0.42
1:A:3052:VAL:HG12	1:A:3053:CYS:SG	2.59	0.42
1:B:1189:THR:OG1	1:B:1190:SER:N	2.52	0.42
1:B:4065:ARG:HD3	1:B:4081:GLU:OE2	2.19	0.42
1:A:2810:ASN:HB2	17:A:4707:NAG:O5	2.19	0.42
1:B:740:SER:HB2	1:B:742:PHE:CE2	2.55	0.42
2:D:96:TRP:CH2	2:D:111:GLU:HB2	2.54	0.42
1:B:1906:MET:SD	1:B:2036:PRO:HG2	2.59	0.42
1:B:4284:ASP:HA	1:B:4301:LYS:HE2	2.01	0.42
1:A:521:GLY:C	1:A:542:MET:HG3	2.40	0.42
1:B:1886:LEU:N	1:B:1904:ALA:O	2.45	0.42
1:B:2235:VAL:HG12	1:B:2236:THR:HG23	2.02	0.42
1:B:2699:THR:O	1:B:2700:ARG:HD3	2.20	0.42
1:B:2914:GLN:HA	1:B:2920:CYS:HB3	2.02	0.42
2:C:97:LYS:O	2:C:97:LYS:HD2	2.20	0.42
2:D:262:ASP:OD1	2:D:263:LEU:N	2.53	0.42
1:A:376:TYR:HB3	1:A:384:CYS:HB3	2.02	0.42
1:A:3015:ASP:HB2	1:A:3017:ARG:CZ	2.46	0.42
1:B:2668:ALA:HB2	1:B:2677:GLN:HE22	1.84	0.42
1:A:3275:GLU:OE1	1:A:3326:ARG:NE	2.45	0.42
1:A:3997:PHE:HB3	1:A:4007:CYS:HB3	2.02	0.42
1:B:431:HIS:CD2	1:B:434:LYS:H	2.33	0.42
1:B:2517:PRO:HA	1:B:2538:LEU:HD11	2.01	0.42
1:B:4061:PRO:HD2	1:B:4319:GLN:O	2.20	0.42
2:D:324:LYS:O	2:D:328:VAL:HG13	2.20	0.42
1:B:445:GLU:OE2	1:B:738:SER:OG	2.28	0.42
1:B:4213:GLU:HG2	1:B:4224:VAL:HG12	2.02	0.42
1:B:4234:ASN:HD21	1:B:4251:SER:CB	2.32	0.42
1:A:361:CYS:SG	1:A:362:GLU:N	2.93	0.41
1:A:4076:PHE:HZ	1:A:4311:LEU:HD13	1.85	0.41
1:B:2538:LEU:HD12	1:B:2669:PRO:O	2.20	0.41
1:B:2701:CYS:SG	1:B:2705:GLN:HB2	2.60	0.41
1:B:3245:TRP:CE2	1:B:3254:GLU:HB2	2.55	0.41
1:B:3981:CYS:HA	1:B:3991:CYS:HA	2.00	0.41
2:C:82:LEU:HD22	2:C:125:TYR:CD1	2.55	0.41
1:A:896:SER:OG	1:A:901:LEU:O	2.23	0.41
1:A:1081:PRO:HD2	1:A:1084:TRP:CE3	2.55	0.41
1:A:4121:TYR:CD2	1:A:4382:PRO:HB3	2.55	0.41
1:B:3998:LYS:O	1:B:4008:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:CYS:HB3	1:A:1414:CYS:HB3	1.98	0.41
1:A:3609:ILE:HD12	1:A:3609:ILE:O	2.18	0.41
1:B:3205:PHE:HA	1:B:3455:ASP:O	2.21	0.41
1:A:882:ARG:HE	1:A:895:HIS:CD2	2.32	0.41
1:A:2350:SER:O	1:A:2350:SER:OG	2.34	0.41
1:A:3736:PRO:HD2	1:A:3739:TRP:CE3	2.55	0.41
1:B:3601:TRP:CD2	1:B:3614:GLN:NE2	2.89	0.41
1:A:357:CYS:HB3	1:A:370:CYS:HB3	1.89	0.41
1:A:398:SER:HB3	1:A:645:HIS:O	2.20	0.41
1:A:1642:VAL:HA	1:B:2592:THR:HG21	2.02	0.41
1:B:4314:ASN:HD22	1:B:4316:TRP:HB2	1.84	0.41
1:A:88:ASP:N	1:A:99:GLU:OE1	2.50	0.41
1:A:631:GLU:OE1	1:A:633:ASN:N	2.49	0.41
1:A:933:GLY:O	1:A:953:ILE:HG22	2.20	0.41
1:B:2155:TRP:CH2	1:B:2200:PRO:HD2	2.55	0.41
1:B:2428:ASP:HB2	1:B:2435:PHE:HE2	1.85	0.41
1:A:2696:ASP:HA	1:A:2700:ARG:HH12	1.86	0.41
1:B:1975:TYR:CE2	1:B:1986:ARG:HD3	2.56	0.41
2:C:97:LYS:HD2	2:C:100:LYS:HB2	2.03	0.41
1:A:3672:GLU:O	1:A:3675:THR:HG22	2.21	0.41
1:A:3860:PHE:CE1	1:A:3861:TRP:CD1	3.09	0.41
1:B:476:ILE:HG22	1:B:660:ASN:HB3	2.02	0.41
1:B:1134:ASP:OD1	1:B:1134:ASP:N	2.54	0.41
1:B:2552:VAL:HB	1:B:2572:SER:HB3	2.03	0.41
1:B:4413:GLU:OE1	1:B:4413:GLU:N	2.54	0.41
2:C:100:LYS:NZ	2:C:105:ASP:HB3	2.36	0.41
1:A:3417:ILE:HD13	1:A:3422:VAL:HG12	2.03	0.41
1:A:4019:CYS:SG	1:A:4020:PRO:HD2	2.60	0.41
1:B:54:LEU:HD13	1:B:54:LEU:HA	1.95	0.41
1:B:4232:TRP:N	1:B:4232:TRP:CD1	2.88	0.41
1:A:2618:ARG:O	1:A:2627:LEU:HA	2.21	0.40
1:A:2709:LEU:HD12	1:A:2730:SER:HB2	2.03	0.40
1:A:2970:GLN:NE2	1:A:2973:VAL:HG21	2.35	0.40
1:A:3759:ARG:HH22	1:A:3765:GLU:CD	2.24	0.40
1:A:3984:LEU:HD13	1:A:3987:GLY:CA	2.52	0.40
1:B:2066:MET:HG2	1:B:2077:PHE:O	2.20	0.40
1:B:2142:GLY:O	1:B:2164:ASN:ND2	2.54	0.40
1:B:3970:ARG:CZ	1:B:3976:ILE:HD13	2.51	0.40
2:C:96:TRP:HA	2:C:110:LYS:NZ	2.35	0.40
2:D:283:GLU:OE2	2:D:344:HIS:NE2	2.40	0.40
11:U:1:NAG:H61	11:U:2:NAG:H82	3.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1401:CYS:HB3	1:B:1405:CYS:HB2	2.04	0.40
1:B:3246:ILE:HD11	1:B:3277:LEU:HB3	2.04	0.40
1:B:3934:GLU:HA	1:B:3944:SER:HA	2.02	0.40
1:B:4413:GLU:HG2	1:B:4414:VAL:HG13	2.03	0.40
2:C:97:LYS:HA	2:C:100:LYS:HG2	2.04	0.40
1:A:359:GLN:OE1	1:A:384:CYS:HB2	2.20	0.40
1:A:624:MET:HE3	1:A:636:VAL:HA	2.03	0.40
1:A:3479:SER:HG	1:A:3480:HIS:CE1	2.34	0.40
1:A:4401:CYS:HB2	1:A:4411:TYR:HA	2.03	0.40
1:B:2071:LEU:HB2	1:B:2072:PRO:HD3	2.02	0.40
1:B:4057:LEU:HD12	1:B:4323:PHE:HD2	1.87	0.40
1:A:3553:ARG:NH1	1:A:3559:GLN:O	2.53	0.40
1:B:447:VAL:HG23	1:B:465:VAL:HG11	2.03	0.40
1:B:4273:ALA:O	1:B:4274:MET:HG2	2.21	0.40
1:A:1173:LYS:CD	1:A:1178:GLY:HA2	2.47	0.40
1:B:4057:LEU:HB2	1:B:4323:PHE:HB3	2.03	0.40
1:B:4119:ARG:HH11	1:B:4173:LEU:C	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4304/4660 (92%)	3983 (92%)	319 (7%)	2 (0%)	100	100
1	B	4304/4660 (92%)	3994 (93%)	308 (7%)	2 (0%)	100	100
2	C	173/360 (48%)	170 (98%)	3 (2%)	0	100	100
2	D	173/360 (48%)	171 (99%)	2 (1%)	0	100	100
4	H	1/5 (20%)	1 (100%)	0	0	100	100
4	O	1/5 (20%)	1 (100%)	0	0	100	100
5	I	1/6 (17%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	1/6 (17%)	1 (100%)	0	0	100	100
6	J	1/3 (33%)	0	1 (100%)	0	100	100
6	Q	1/3 (33%)	1 (100%)	0	0	100	100
7	K	2/5 (40%)	0	2 (100%)	0	100	100
7	R	2/5 (40%)	2 (100%)	0	0	100	100
8	L	1/5 (20%)	0	1 (100%)	0	100	100
8	M	1/5 (20%)	1 (100%)	0	0	100	100
8	S	1/5 (20%)	0	1 (100%)	0	100	100
8	T	1/5 (20%)	1 (100%)	0	0	100	100
All	All	8968/10098 (89%)	8327 (93%)	637 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2874	SER
1	A	2874	SER
1	B	2858	ILE
1	A	410	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3791/4089 (93%)	3672 (97%)	119 (3%)	35	56
1	B	3790/4089 (93%)	3688 (97%)	102 (3%)	40	60
2	C	163/326 (50%)	156 (96%)	7 (4%)	25	48
2	D	163/326 (50%)	159 (98%)	4 (2%)	42	62
4	H	1/1 (100%)	1 (100%)	0	100	100
4	O	1/1 (100%)	1 (100%)	0	100	100
5	I	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	1/1 (100%)	0	1 (100%)	0	0
6	J	1/1 (100%)	1 (100%)	0	100	100
6	Q	1/1 (100%)	1 (100%)	0	100	100
7	K	2/2 (100%)	2 (100%)	0	100	100
7	R	2/2 (100%)	1 (50%)	1 (50%)	0	0
8	L	1/1 (100%)	1 (100%)	0	100	100
8	M	1/1 (100%)	1 (100%)	0	100	100
8	S	1/1 (100%)	1 (100%)	0	100	100
8	T	1/1 (100%)	1 (100%)	0	100	100
All	All	7921/8844 (90%)	7687 (97%)	234 (3%)	37	57

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	74	CYS
1	A	98	ASP
1	A	198	ARG
1	A	215	ARG
1	A	221	THR
1	A	248	GLN
1	A	259	ASN
1	A	268	ARG
1	A	283	LYS
1	A	311	CYS
1	A	329	CYS
1	A	470	ASN
1	A	516	LEU
1	A	549	ASP
1	A	579	TYR
1	A	631	GLU
1	A	681	ASN
1	A	711	LEU
1	A	725	LEU
1	A	759	LEU
1	A	772	THR
1	A	841	LEU
1	A	856	ASP
1	A	887	ASP

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Mol	Chain	Res	Type
1	A	992	ASN
1	A	995	ARG
1	A	1018	ARG
1	A	1093	LEU
1	A	1173	LYS
1	A	1366	MET
1	A	1408	MET
1	A	1436	ASN
1	A	1465	ASP
1	A	1468	PHE
1	A	1472	LEU
1	A	1636	VAL
1	A	1656	VAL
1	A	1728	CYS
1	A	1745	ASP
1	A	2070	MET
1	A	2126	ARG
1	A	2170	THR
1	A	2210	TYR
1	A	2242	MET
1	A	2338	SER
1	A	2363	GLU
1	A	2394	SER
1	A	2439	LYS
1	A	2441	ASN
1	A	2494	MET
1	A	2507	VAL
1	A	2532	LYS
1	A	2570	ASP
1	A	2578	ARG
1	A	2626	ASP
1	A	2633	ARG
1	A	2701	CYS
1	A	2722	ASN
1	A	2781	CYS
1	A	2823	CYS
1	A	2835	ILE
1	A	2849	CYS
1	A	2856	ASN
1	A	2868	ASN
1	A	2914	GLN
1	A	2919	ARG

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Mol	Chain	Res	Type
1	A	2924	ASN
1	A	2927	CYS
1	A	2938	ASP
1	A	2971	TYR
1	A	3012	PHE
1	A	3017	ARG
1	A	3027	ARG
1	A	3086	ASN
1	A	3092	MET
1	A	3096	CYS
1	A	3106	SER
1	A	3135	PHE
1	A	3146	MET
1	A	3150	ARG
1	A	3206	SER
1	A	3212	ARG
1	A	3220	SER
1	A	3262	ASN
1	A	3277	LEU
1	A	3375	ASP
1	A	3378	ASN
1	A	3415	LEU
1	A	3449	THR
1	A	3450	THR
1	A	3509	LEU
1	A	3549	LEU
1	A	3578	GLN
1	A	3782	GLN
1	A	3784	ASN
1	A	3793	ARG
1	A	3797	MET
1	A	3812	CYS
1	A	3826	LEU
1	A	3874	ASP
1	A	3922	CYS
1	A	3924	LYS
1	A	3979	GLN
1	A	4004	LYS
1	A	4032	CYS
1	A	4075	LYS
1	A	4157	HIS
1	A	4174	ASP

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Mol	Chain	Res	Type
1	A	4201	MET
1	A	4217	MET
1	A	4243	ASP
1	A	4280	ASP
1	A	4284	ASP
1	A	4321	ARG
1	A	4366	THR
1	A	4379	MET
1	A	4386	MET
1	A	4401	CYS
1	B	33	PHE
1	B	39	TYR
1	B	46	ARG
1	B	58	ASP
1	B	65	ARG
1	B	72	PHE
1	B	187	GLU
1	B	219	TYR
1	B	247	CYS
1	B	272	CYS
1	B	278	CYS
1	B	335	HIS
1	B	350	ASP
1	B	359	GLN
1	B	362	GLU
1	B	365	GLN
1	B	516	LEU
1	B	530	SER
1	B	534	GLN
1	B	563	LEU
1	B	613	VAL
1	B	741	PHE
1	B	746	ASP
1	B	849	LYS
1	B	895	HIS
1	B	899	ASP
1	B	995	ARG
1	B	1028	LEU
1	B	1088	ARG
1	B	1091	ASP
1	B	1134	ASP
1	B	1194	LYS

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Mol	Chain	Res	Type
1	B	1201	CYS
1	B	1250	GLU
1	B	1300	MET
1	B	1349	CYS
1	B	1352	ASP
1	B	1409	ARG
1	B	1517	VAL
1	B	1550	LYS
1	B	1636	VAL
1	B	1666	VAL
1	B	1673	HIS
1	B	1728	CYS
1	B	1745	ASP
1	B	1783	ASP
1	B	1791	GLN
1	B	1851	LEU
1	B	1936	TRP
1	B	1967	LEU
1	B	2013	ARG
1	B	2080	GLU
1	B	2153	LEU
1	B	2174	VAL
1	B	2225	ASN
1	B	2297	ASN
1	B	2378	ASN
1	B	2407	ARG
1	B	2430	ARG
1	B	2444	ARG
1	B	2519	ARG
1	B	2677	GLN
1	B	2680	HIS
1	B	2753	ARG
1	B	2786	GLU
1	B	2807	CYS
1	B	2839	ARG
1	B	2876	GLN
1	B	2961	ARG
1	B	2966	ARG
1	B	2984	LEU
1	B	2992	MET
1	B	2993	ARG
1	B	3000	PHE

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Mol	Chain	Res	Type
1	B	3092	MET
1	B	3146	MET
1	B	3148	ASP
1	B	3150	ARG
1	B	3401	ARG
1	B	3426	ASP
1	B	3467	MET
1	B	3500	GLN
1	B	3505	ARG
1	B	3545	ASP
1	B	3571	GLN
1	B	3588	ARG
1	B	3635	ARG
1	B	3689	LYS
1	B	3737	LEU
1	B	3755	ASN
1	B	3793	ARG
1	B	3822	ARG
1	B	3878	HIS
1	B	3942	CYS
1	B	3965	ASN
1	B	3971	THR
1	B	4045	TYR
1	B	4048	ARG
1	B	4065	ARG
1	B	4261	TYR
1	B	4274	MET
1	B	4321	ARG
2	C	259	ARG
2	C	268	GLN
2	C	277	LEU
2	C	305	HIS
2	C	307	LYS
2	C	342	LYS
2	C	346	GLN
2	D	64	GLN
2	D	79	LEU
2	D	93	GLU
2	D	336	GLU
5	P	3	LEU
7	R	3	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	321	HIS
1	A	382	GLN
1	A	412	ASN
1	A	444	GLN
1	A	456	ASN
1	A	639	GLN
1	A	681	ASN
1	A	895	HIS
1	A	985	HIS
1	A	992	ASN
1	A	1058	GLN
1	A	1254	HIS
1	A	1393	ASN
1	A	1891	HIS
1	A	1920	GLN
1	A	1921	HIS
1	A	1963	HIS
1	A	2001	ASN
1	A	2489	GLN
1	A	2595	HIS
1	A	2651	GLN
1	A	2703	GLN
1	A	2808	HIS
1	A	3066	GLN
1	A	3262	ASN
1	A	3523	ASN
1	A	3878	HIS
1	A	3941	ASN
1	A	4221	HIS
1	A	4314	ASN
1	B	315	ASN
1	B	412	ASN
1	B	431	HIS
1	B	826	ASN
1	B	1033	ASN
1	B	1192	GLN
1	B	1283	ASN
1	B	1891	HIS
1	B	1980	GLN
1	B	2212	GLN
1	B	2297	ASN

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Mol	Chain	Res	Type
1	B	2378	ASN
1	B	2414	GLN
1	B	2500	ASN
1	B	2710	ASN
1	B	2903	HIS
1	B	3336	HIS
1	B	3378	ASN
1	B	4008	GLN
1	B	4131	ASN
1	B	4234	ASN
2	C	295	ASN
2	D	268	GLN
2	D	294	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

146 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	$\# Z > 2$
16	NAG	0	1	16,1	14,14,15	0.49	0	17,19,21	1.42	1 (5%)
16	NAG	0	2	16	14,14,15	0.38	0	17,19,21	1.41	3 (17%)
16	BMA	0	3	16	11,11,12	0.32	0	15,15,17	0.54	0
10	NAG	1	1	10,1	14,14,15	0.49	0	17,19,21	0.86	0
10	NAG	1	2	10	14,14,15	0.43	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	1	3	10	11,11,12	0.27	0	15,15,17	0.90	1 (6%)
10	MAN	1	4	10	11,11,12	0.30	0	15,15,17	0.69	0
10	MAN	1	5	10	11,11,12	0.29	0	15,15,17	0.60	0
12	NAG	2	1	12,1	14,14,15	0.89	0	17,19,21	1.52	5 (29%)
12	NAG	2	2	12	14,14,15	1.18	2 (14%)	17,19,21	1.04	1 (5%)
12	BMA	2	3	12	11,11,12	1.07	2 (18%)	15,15,17	1.00	1 (6%)
12	NAG	3	1	12,1	14,14,15	0.44	0	17,19,21	0.53	0
12	NAG	3	2	12	14,14,15	0.47	0	17,19,21	0.59	0
12	BMA	3	3	12	11,11,12	0.79	0	15,15,17	0.85	1 (6%)
10	NAG	4	1	10,1	14,14,15	0.41	0	17,19,21	0.99	1 (5%)
10	NAG	4	2	10	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
10	BMA	4	3	10	11,11,12	0.31	0	15,15,17	1.04	2 (13%)
10	MAN	4	4	10	11,11,12	0.30	0	15,15,17	0.54	0
10	MAN	4	5	10	11,11,12	0.34	0	15,15,17	0.55	0
10	NAG	5	1	10,1	14,14,15	0.49	0	17,19,21	0.89	1 (5%)
10	NAG	5	2	10	14,14,15	0.46	0	17,19,21	0.38	0
10	BMA	5	3	10	11,11,12	0.34	0	15,15,17	0.69	0
10	MAN	5	4	10	11,11,12	0.27	0	15,15,17	0.62	0
10	MAN	5	5	10	11,11,12	0.22	0	15,15,17	0.66	1 (6%)
14	NAG	6	1	14,1	14,14,15	0.44	0	17,19,21	0.77	0
14	NAG	6	2	14	14,14,15	0.44	0	17,19,21	0.86	0
14	BMA	6	3	14	11,11,12	0.39	0	15,15,17	1.04	0
14	MAN	6	4	14	11,11,12	0.27	0	15,15,17	0.88	2 (13%)
14	MAN	6	5	14	11,11,12	0.31	0	15,15,17	0.62	0
16	NAG	7	1	16,1	14,14,15	0.43	0	17,19,21	0.50	0
16	NAG	7	2	16	14,14,15	0.44	0	17,19,21	0.41	0
16	BMA	7	3	16	11,11,12	0.23	0	15,15,17	0.66	0
13	NAG	8	1	13,1	14,14,15	0.68	0	17,19,21	1.36	2 (11%)
13	NAG	8	2	13	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
10	NAG	9	1	10,1	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
10	NAG	9	2	10	14,14,15	0.40	0	17,19,21	0.47	0
10	BMA	9	3	10	11,11,12	0.27	0	15,15,17	0.71	0
10	MAN	9	4	10	11,11,12	0.27	0	15,15,17	0.65	0
10	MAN	9	5	10	11,11,12	0.26	0	15,15,17	0.54	0
9	NAG	E	1	9,1	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
9	NAG	E	2	9	14,14,15	0.38	0	17,19,21	0.53	0
10	NAG	F	1	10,1	14,14,15	0.40	0	17,19,21	0.53	0
10	NAG	F	2	10	14,14,15	0.40	0	17,19,21	0.36	0
10	BMA	F	3	10	11,11,12	0.27	0	15,15,17	0.70	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	F	4	10	11,11,12	0.34	0	15,15,17	0.58	0
10	MAN	F	5	10	11,11,12	0.22	0	15,15,17	0.62	0
11	NAG	U	1	11,1	14,14,15	0.41	0	17,19,21	0.56	0
11	NAG	U	2	11	14,14,15	0.49	0	17,19,21	1.77	4 (23%)
11	BMA	U	3	11	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
11	MAN	U	4	11	11,11,12	0.30	0	15,15,17	0.69	0
11	MAN	U	5	11	11,11,12	0.36	0	15,15,17	0.79	2 (13%)
9	NAG	V	1	9,1	14,14,15	0.51	0	17,19,21	1.29	2 (11%)
9	NAG	V	2	9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
12	NAG	W	1	12,1	14,14,15	0.42	0	17,19,21	0.72	1 (5%)
12	NAG	W	2	12	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
12	BMA	W	3	12	11,11,12	0.35	0	15,15,17	0.70	0
9	NAG	X	1	9,1	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.60	0
9	NAG	Y	1	9,1	14,14,15	0.39	0	17,19,21	0.41	0
9	NAG	Y	2	9	14,14,15	0.40	0	17,19,21	0.69	0
10	NAG	Z	1	10,1	14,14,15	0.46	0	17,19,21	1.32	1 (5%)
10	NAG	Z	2	10	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
10	BMA	Z	3	10	11,11,12	0.33	0	15,15,17	0.66	0
10	MAN	Z	4	10	11,11,12	0.28	0	15,15,17	0.50	0
10	MAN	Z	5	10	11,11,12	0.24	0	15,15,17	0.56	0
9	NAG	a	1	9,1	14,14,15	0.40	0	17,19,21	0.71	0
9	NAG	a	2	9	14,14,15	0.40	0	17,19,21	0.35	0
10	NAG	b	1	10,1	14,14,15	0.41	0	17,19,21	0.41	0
10	NAG	b	2	10	14,14,15	0.40	0	17,19,21	0.42	0
10	BMA	b	3	10	11,11,12	0.34	0	15,15,17	0.83	1 (6%)
10	MAN	b	4	10	11,11,12	0.28	0	15,15,17	0.67	0
10	MAN	b	5	10	11,11,12	0.23	0	15,15,17	0.54	0
13	NAG	c	1	13,1	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
13	NAG	c	2	13	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
9	NAG	d	1	9,1	14,14,15	0.40	0	17,19,21	0.62	0
9	NAG	d	2	9	14,14,15	0.39	0	17,19,21	0.50	0
12	NAG	e	1	12,1	14,14,15	0.41	0	17,19,21	0.39	0
12	NAG	e	2	12	14,14,15	0.42	0	17,19,21	0.58	0
12	BMA	e	3	12	11,11,12	0.32	0	15,15,17	0.79	1 (6%)
12	NAG	f	1	12,1	14,14,15	0.42	0	17,19,21	0.45	0
12	NAG	f	2	12	14,14,15	0.42	0	17,19,21	0.54	0
12	BMA	f	3	12	11,11,12	0.22	0	15,15,17	0.63	1 (6%)
10	NAG	g	1	10,1	14,14,15	0.46	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	g	2	10	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	BMA	g	3	10	11,11,12	0.40	0	15,15,17	0.79	1 (6%)
10	MAN	g	4	10	11,11,12	0.30	0	15,15,17	0.58	0
10	MAN	g	5	10	11,11,12	0.27	0	15,15,17	0.64	0
12	NAG	h	1	12,1	14,14,15	0.41	0	17,19,21	0.70	0
12	NAG	h	2	12	14,14,15	0.43	0	17,19,21	0.49	0
12	BMA	h	3	12	11,11,12	0.29	0	15,15,17	0.57	0
12	NAG	i	1	12,1	14,14,15	0.47	0	17,19,21	0.80	0
12	NAG	i	2	12	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
12	BMA	i	3	12	11,11,12	0.62	0	15,15,17	0.84	1 (6%)
10	NAG	j	1	10,1	14,14,15	0.40	0	17,19,21	1.30	3 (17%)
10	NAG	j	2	10	14,14,15	0.41	0	17,19,21	0.38	0
10	BMA	j	3	10	11,11,12	0.55	0	15,15,17	0.79	0
10	MAN	j	4	10	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
10	MAN	j	5	10	11,11,12	0.38	0	15,15,17	0.65	0
10	NAG	k	1	10,1	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
10	NAG	k	2	10	14,14,15	0.49	0	17,19,21	1.11	2 (11%)
10	BMA	k	3	10	11,11,12	0.26	0	15,15,17	0.64	0
10	MAN	k	4	10	11,11,12	0.31	0	15,15,17	0.93	2 (13%)
10	MAN	k	5	10	11,11,12	0.33	0	15,15,17	0.56	0
10	NAG	l	1	10,1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	NAG	l	2	10	14,14,15	0.43	0	17,19,21	0.37	0
10	BMA	l	3	10	11,11,12	0.34	0	15,15,17	1.21	2 (13%)
10	MAN	l	4	10	11,11,12	0.29	0	15,15,17	0.70	0
10	MAN	l	5	10	11,11,12	0.33	0	15,15,17	0.53	0
12	NAG	m	1	12,1	14,14,15	1.07	1 (7%)	17,19,21	1.19	1 (5%)
12	NAG	m	2	12	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
12	BMA	m	3	12	11,11,12	0.28	0	15,15,17	0.61	0
9	NAG	n	1	9,1	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
9	NAG	n	2	9	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
13	NAG	o	1	13,1	14,14,15	0.40	0	17,19,21	0.82	0
13	NAG	o	2	13	14,14,15	0.41	0	17,19,21	0.41	0
12	NAG	p	1	12,1	14,14,15	0.42	0	17,19,21	0.71	0
12	NAG	p	2	12	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
12	BMA	p	3	12	11,11,12	0.26	0	15,15,17	0.67	0
9	NAG	q	1	9,1	14,14,15	1.13	1 (7%)	17,19,21	1.14	1 (5%)
9	NAG	q	2	9	14,14,15	0.92	1 (7%)	17,19,21	1.07	1 (5%)
12	NAG	r	1	12,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	r	2	12	14,14,15	0.41	0	17,19,21	0.57	0
12	BMA	r	3	12	11,11,12	0.30	0	15,15,17	0.66	0
9	NAG	s	1	9,1	14,14,15	0.44	0	17,19,21	1.02	2 (11%)
9	NAG	s	2	9	14,14,15	0.40	0	17,19,21	0.61	0
9	NAG	t	1	9,1	14,14,15	0.98	0	17,19,21	1.55	3 (17%)
9	NAG	t	2	9	14,14,15	1.08	1 (7%)	17,19,21	1.53	1 (5%)
10	NAG	u	1	10,1	14,14,15	0.48	0	17,19,21	0.56	0
10	NAG	u	2	10	14,14,15	0.45	0	17,19,21	0.70	0
10	BMA	u	3	10	11,11,12	0.40	0	15,15,17	0.72	1 (6%)
10	MAN	u	4	10	11,11,12	0.24	0	15,15,17	0.60	0
10	MAN	u	5	10	11,11,12	0.27	0	15,15,17	0.64	0
9	NAG	v	1	9,1	14,14,15	0.45	0	17,19,21	0.49	0
9	NAG	v	2	9	14,14,15	0.39	0	17,19,21	0.39	0
14	NAG	w	1	14,1	14,14,15	0.52	0	17,19,21	1.20	2 (11%)
14	NAG	w	2	14	14,14,15	0.46	0	17,19,21	1.34	3 (17%)
14	BMA	w	3	14	11,11,12	0.42	0	15,15,17	0.66	0
14	MAN	w	4	14	11,11,12	0.29	0	15,15,17	0.62	0
14	MAN	w	5	14	11,11,12	0.27	0	15,15,17	0.57	0
9	NAG	x	1	9,1	14,14,15	0.51	0	17,19,21	0.85	0
9	NAG	x	2	9	14,14,15	0.40	0	17,19,21	0.69	0
9	NAG	y	1	9,1	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
9	NAG	y	2	9	14,14,15	0.41	0	17,19,21	0.43	0
15	NAG	z	1	1,15	14,14,15	0.54	0	17,19,21	0.82	1 (5%)
15	NAG	z	2	15	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
15	BMA	z	3	15	11,11,12	0.37	0	15,15,17	0.69	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
16	NAG	0	1	16,1	-	2/6/23/26	0/1/1/1
16	NAG	0	2	16	-	0/6/23/26	0/1/1/1
16	BMA	0	3	16	-	0/2/19/22	0/1/1/1
10	NAG	1	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1
10	BMA	1	3	10	-	2/2/19/22	0/1/1/1
10	MAN	1	4	10	-	0/2/19/22	0/1/1/1
10	MAN	1	5	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	2	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	2	2	12	-	1/6/23/26	0/1/1/1
12	BMA	2	3	12	-	0/2/19/22	0/1/1/1
12	NAG	3	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	3	2	12	-	0/6/23/26	0/1/1/1
12	BMA	3	3	12	-	0/2/19/22	0/1/1/1
10	NAG	4	1	10,1	-	6/6/23/26	0/1/1/1
10	NAG	4	2	10	-	5/6/23/26	0/1/1/1
10	BMA	4	3	10	-	2/2/19/22	0/1/1/1
10	MAN	4	4	10	-	0/2/19/22	0/1/1/1
10	MAN	4	5	10	-	0/2/19/22	0/1/1/1
10	NAG	5	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	5	2	10	-	0/6/23/26	0/1/1/1
10	BMA	5	3	10	-	2/2/19/22	0/1/1/1
10	MAN	5	4	10	-	0/2/19/22	0/1/1/1
10	MAN	5	5	10	-	0/2/19/22	0/1/1/1
14	NAG	6	1	14,1	-	2/6/23/26	0/1/1/1
14	NAG	6	2	14	-	4/6/23/26	0/1/1/1
14	BMA	6	3	14	-	0/2/19/22	0/1/1/1
14	MAN	6	4	14	-	1/2/19/22	0/1/1/1
14	MAN	6	5	14	-	1/2/19/22	0/1/1/1
16	NAG	7	1	16,1	-	0/6/23/26	0/1/1/1
16	NAG	7	2	16	-	3/6/23/26	0/1/1/1
16	BMA	7	3	16	-	0/2/19/22	0/1/1/1
13	NAG	8	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	8	2	13	-	2/6/23/26	0/1/1/1
10	NAG	9	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	9	2	10	-	0/6/23/26	0/1/1/1
10	BMA	9	3	10	-	2/2/19/22	0/1/1/1
10	MAN	9	4	10	-	0/2/19/22	0/1/1/1
10	MAN	9	5	10	-	0/2/19/22	0/1/1/1
9	NAG	E	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	E	2	9	-	0/6/23/26	0/1/1/1
10	NAG	F	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
10	MAN	F	5	10	-	0/2/19/22	0/1/1/1
11	NAG	U	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	U	3	11	-	1/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	1/2/19/22	0/1/1/1
9	NAG	V	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
12	NAG	W	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	W	2	12	-	2/6/23/26	0/1/1/1
12	BMA	W	3	12	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	NAG	Y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	3/6/23/26	0/1/1/1
10	NAG	Z	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
9	NAG	a	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
10	NAG	b	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	1/6/23/26	0/1/1/1
10	BMA	b	3	10	-	0/2/19/22	0/1/1/1
10	MAN	b	4	10	-	0/2/19/22	0/1/1/1
10	MAN	b	5	10	-	0/2/19/22	0/1/1/1
13	NAG	c	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	c	2	13	-	1/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
12	NAG	e	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
12	NAG	f	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	f	2	12	-	0/6/23/26	0/1/1/1
12	BMA	f	3	12	-	0/2/19/22	0/1/1/1
10	NAG	g	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	g	2	10	-	0/6/23/26	0/1/1/1
10	BMA	g	3	10	-	0/2/19/22	0/1/1/1
10	MAN	g	4	10	-	0/2/19/22	0/1/1/1
10	MAN	g	5	10	-	1/2/19/22	0/1/1/1
12	NAG	h	1	12,1	-	3/6/23/26	0/1/1/1
12	NAG	h	2	12	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	NAG	i	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
10	NAG	j	1	10,1	-	3/6/23/26	0/1/1/1
10	NAG	j	2	10	-	4/6/23/26	0/1/1/1
10	BMA	j	3	10	-	2/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
10	MAN	j	5	10	-	1/2/19/22	0/1/1/1
10	NAG	k	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	k	2	10	-	0/6/23/26	0/1/1/1
10	BMA	k	3	10	-	0/2/19/22	0/1/1/1
10	MAN	k	4	10	-	0/2/19/22	0/1/1/1
10	MAN	k	5	10	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1
10	MAN	l	4	10	-	1/2/19/22	0/1/1/1
10	MAN	l	5	10	-	1/2/19/22	0/1/1/1
12	NAG	m	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	m	2	12	-	2/6/23/26	0/1/1/1
12	BMA	m	3	12	-	0/2/19/22	0/1/1/1
9	NAG	n	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1
13	NAG	o	1	13,1	-	0/6/23/26	0/1/1/1
13	NAG	o	2	13	-	2/6/23/26	0/1/1/1
12	NAG	p	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
12	BMA	p	3	12	-	0/2/19/22	0/1/1/1
9	NAG	q	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	q	2	9	-	0/6/23/26	0/1/1/1
12	NAG	r	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	r	2	12	-	3/6/23/26	0/1/1/1
12	BMA	r	3	12	-	1/2/19/22	0/1/1/1
9	NAG	s	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	s	2	9	-	0/6/23/26	0/1/1/1
9	NAG	t	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
10	NAG	u	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	u	3	10	-	2/2/19/22	0/1/1/1
10	MAN	u	4	10	-	0/2/19/22	0/1/1/1
10	MAN	u	5	10	-	0/2/19/22	0/1/1/1
9	NAG	v	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	v	2	9	-	0/6/23/26	0/1/1/1
14	NAG	w	1	14,1	-	4/6/23/26	0/1/1/1
14	NAG	w	2	14	-	3/6/23/26	0/1/1/1
14	BMA	w	3	14	-	0/2/19/22	0/1/1/1
14	MAN	w	4	14	-	1/2/19/22	0/1/1/1
14	MAN	w	5	14	-	1/2/19/22	0/1/1/1
9	NAG	x	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	3/6/23/26	0/1/1/1
9	NAG	y	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	y	2	9	-	1/6/23/26	0/1/1/1
15	NAG	z	1	1,15	-	2/6/23/26	0/1/1/1
15	NAG	z	2	15	-	1/6/23/26	0/1/1/1
15	BMA	z	3	15	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	NAG	O5-C5	2.57	1.48	1.43
9	q	1	NAG	O5-C5	2.45	1.48	1.43
9	t	2	NAG	C1-C2	2.36	1.55	1.52
12	2	2	NAG	O5-C5	2.31	1.48	1.43
9	q	2	NAG	O5-C5	2.23	1.48	1.43
12	2	3	BMA	O5-C5	2.18	1.47	1.43
12	2	3	BMA	O5-C1	2.06	1.47	1.43
12	2	2	NAG	C1-C2	2.05	1.55	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	0	1	NAG	C1-O5-C5	5.01	118.98	112.19
9	t	2	NAG	C1-O5-C5	4.88	118.80	112.19
11	U	2	NAG	C4-C3-C2	4.72	117.93	111.02
9	t	1	NAG	C4-C3-C2	4.47	117.57	111.02
15	z	2	NAG	O5-C1-C2	-4.16	104.72	111.29
13	8	1	NAG	O5-C1-C2	4.00	117.60	111.29
10	Z	1	NAG	O5-C1-C2	-3.76	105.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	w	2	NAG	O5-C1-C2	-3.67	105.49	111.29
10	Z	2	NAG	C1-O5-C5	3.51	116.95	112.19
16	0	2	NAG	O5-C1-C2	3.43	116.70	111.29
9	V	1	NAG	C1-O5-C5	3.38	116.77	112.19
14	w	1	NAG	C4-C3-C2	3.33	115.89	111.02
9	E	1	NAG	O5-C1-C2	-3.32	106.04	111.29
9	n	1	NAG	C1-C2-N2	3.32	116.16	110.49
10	j	1	NAG	O5-C1-C2	-3.16	106.30	111.29
11	U	2	NAG	C3-C4-C5	3.15	115.86	110.24
10	l	3	BMA	C1-C2-C3	3.08	113.46	109.67
13	c	2	NAG	C1-O5-C5	3.08	116.37	112.19
9	q	2	NAG	O5-C1-C2	-3.03	106.51	111.29
12	m	1	NAG	C1-O5-C5	2.94	116.18	112.19
12	2	1	NAG	C3-C4-C5	2.93	115.47	110.24
10	1	3	BMA	C1-C2-C3	2.91	113.24	109.67
10	j	4	MAN	C1-O5-C5	2.90	116.12	112.19
9	V	2	NAG	C1-O5-C5	2.89	116.11	112.19
11	U	2	NAG	O5-C1-C2	-2.88	106.74	111.29
9	q	1	NAG	C1-O5-C5	2.85	116.05	112.19
9	V	1	NAG	O5-C1-C2	2.82	115.75	111.29
10	4	1	NAG	C1-O5-C5	2.78	115.96	112.19
12	i	2	NAG	C1-O5-C5	2.75	115.92	112.19
10	k	1	NAG	C1-O5-C5	2.74	115.91	112.19
12	2	3	BMA	C1-O5-C5	2.70	115.85	112.19
9	t	1	NAG	C1-C2-N2	2.70	115.10	110.49
16	0	2	NAG	O3-C3-C2	-2.69	103.89	109.47
10	k	4	MAN	C1-C2-C3	2.62	112.89	109.67
11	U	3	BMA	O5-C1-C2	-2.61	106.75	110.77
10	4	3	BMA	C1-C2-C3	2.60	112.86	109.67
10	4	2	NAG	C1-O5-C5	2.59	115.71	112.19
12	i	3	BMA	C1-O5-C5	2.56	115.66	112.19
13	8	2	NAG	C1-C2-N2	2.52	114.79	110.49
12	2	1	NAG	C4-C3-C2	2.51	114.69	111.02
13	8	1	NAG	C1-O5-C5	2.46	115.52	112.19
10	4	3	BMA	C1-O5-C5	2.45	115.52	112.19
9	s	1	NAG	O5-C1-C2	2.44	115.14	111.29
12	e	3	BMA	C1-C2-C3	2.44	112.66	109.67
10	l	1	NAG	C1-O5-C5	2.43	115.49	112.19
12	2	1	NAG	C1-C2-N2	2.42	114.62	110.49
11	U	2	NAG	O3-C3-C2	-2.38	104.55	109.47
10	j	1	NAG	C3-C4-C5	2.36	114.45	110.24
14	w	1	NAG	C3-C4-C5	2.35	114.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	3	BMA	C1-O5-C5	2.32	115.34	112.19
12	2	1	NAG	C2-N2-C7	2.31	126.19	122.90
10	k	2	NAG	C1-O5-C5	2.31	115.32	112.19
12	2	2	NAG	C1-O5-C5	2.29	115.30	112.19
9	t	1	NAG	O5-C1-C2	-2.29	107.67	111.29
13	c	1	NAG	C4-C3-C2	2.29	114.37	111.02
10	F	3	BMA	C1-C2-C3	2.27	112.46	109.67
10	b	3	BMA	C1-C2-C3	2.25	112.44	109.67
10	k	2	NAG	O3-C3-C2	2.24	114.11	109.47
14	6	4	MAN	C1-O5-C5	2.24	115.23	112.19
10	5	1	NAG	C1-C2-N2	2.24	114.32	110.49
10	9	1	NAG	C1-C2-N2	2.23	114.30	110.49
14	w	2	NAG	C1-O5-C5	-2.22	109.19	112.19
12	r	1	NAG	O5-C1-C2	-2.20	107.82	111.29
12	2	1	NAG	O4-C4-C3	-2.19	105.28	110.35
12	p	2	NAG	C1-C2-N2	2.19	114.23	110.49
10	l	3	BMA	O3-C3-C2	-2.18	105.81	109.99
12	W	1	NAG	C1-O5-C5	2.18	115.15	112.19
10	k	4	MAN	C1-O5-C5	2.17	115.13	112.19
14	6	4	MAN	C1-C2-C3	2.16	112.31	109.67
10	g	3	BMA	C1-C2-C3	2.13	112.29	109.67
15	z	2	NAG	C1-C2-N2	2.12	114.12	110.49
12	m	2	NAG	O5-C1-C2	-2.12	107.94	111.29
10	Z	2	NAG	C4-C3-C2	-2.11	107.93	111.02
11	U	5	MAN	C1-O5-C5	2.10	115.04	112.19
12	W	2	NAG	O5-C1-C2	-2.10	107.98	111.29
15	z	1	NAG	O4-C4-C5	-2.09	104.10	109.30
10	j	1	NAG	C4-C3-C2	2.08	114.07	111.02
9	n	2	NAG	C1-C2-N2	2.08	114.04	110.49
14	w	2	NAG	C3-C4-C5	2.08	113.95	110.24
10	u	3	BMA	C1-C2-C3	2.05	112.19	109.67
10	g	2	NAG	C1-O5-C5	2.05	114.97	112.19
16	0	2	NAG	C2-N2-C7	-2.05	119.99	122.90
10	5	5	MAN	C1-C2-C3	2.04	112.17	109.67
12	f	3	BMA	C1-C2-C3	2.04	112.17	109.67
11	U	5	MAN	C1-C2-C3	2.03	112.17	109.67
9	y	1	NAG	C1-C2-N2	2.03	113.96	110.49
10	l	2	NAG	O5-C1-C2	-2.03	108.08	111.29
9	s	1	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	4	1	NAG	C1-C2-N2-C7
12	h	1	NAG	C3-C2-N2-C7
12	h	1	NAG	C8-C7-N2-C2
12	h	1	NAG	O7-C7-N2-C2
14	w	1	NAG	C1-C2-N2-C7
14	w	1	NAG	C8-C7-N2-C2
14	w	1	NAG	O7-C7-N2-C2
14	6	2	NAG	C8-C7-N2-C2
14	6	2	NAG	O7-C7-N2-C2
16	7	2	NAG	C8-C7-N2-C2
16	7	2	NAG	O7-C7-N2-C2
10	4	1	NAG	C8-C7-N2-C2
14	6	1	NAG	C8-C7-N2-C2
14	6	1	NAG	O7-C7-N2-C2
10	u	3	BMA	O5-C5-C6-O6
9	x	2	NAG	C8-C7-N2-C2
9	y	1	NAG	C8-C7-N2-C2
9	y	1	NAG	O7-C7-N2-C2
10	4	1	NAG	O7-C7-N2-C2
10	9	1	NAG	C8-C7-N2-C2
13	o	2	NAG	C8-C7-N2-C2
15	z	1	NAG	C8-C7-N2-C2
10	j	2	NAG	O5-C5-C6-O6
11	U	2	NAG	C8-C7-N2-C2
15	z	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O5-C5-C6-O6
10	j	1	NAG	C1-C2-N2-C7
12	h	2	NAG	C1-C2-N2-C7
16	7	2	NAG	C1-C2-N2-C7
10	u	3	BMA	C4-C5-C6-O6
9	x	2	NAG	O7-C7-N2-C2
10	l	1	NAG	C8-C7-N2-C2
10	9	1	NAG	O7-C7-N2-C2
11	U	2	NAG	O7-C7-N2-C2
12	W	2	NAG	C8-C7-N2-C2
12	h	2	NAG	C8-C7-N2-C2
13	o	2	NAG	O7-C7-N2-C2
11	U	2	NAG	C4-C5-C6-O6
9	x	2	NAG	C1-C2-N2-C7
9	y	1	NAG	C1-C2-N2-C7
12	h	2	NAG	O7-C7-N2-C2
14	6	2	NAG	C1-C2-N2-C7
10	4	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	j	2	NAG	C4-C5-C6-O6
10	l	1	NAG	O7-C7-N2-C2
12	p	1	NAG	C8-C7-N2-C2
16	0	1	NAG	C8-C7-N2-C2
10	j	1	NAG	O5-C5-C6-O6
14	w	1	NAG	O5-C5-C6-O6
10	4	2	NAG	C4-C5-C6-O6
12	m	1	NAG	O5-C5-C6-O6
12	2	1	NAG	C1-C2-N2-C7
10	4	3	BMA	C4-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6
11	U	3	BMA	O5-C5-C6-O6
10	9	3	BMA	O5-C5-C6-O6
14	6	4	MAN	O5-C5-C6-O6
14	w	2	NAG	C1-C2-N2-C7
12	m	2	NAG	C8-C7-N2-C2
12	W	2	NAG	O7-C7-N2-C2
12	p	1	NAG	O7-C7-N2-C2
9	Y	2	NAG	C1-C2-N2-C7
14	w	4	MAN	O5-C5-C6-O6
12	r	3	BMA	O5-C5-C6-O6
9	Y	2	NAG	C8-C7-N2-C2
16	0	1	NAG	O7-C7-N2-C2
9	y	2	NAG	O5-C5-C6-O6
10	l	4	MAN	O5-C5-C6-O6
10	j	5	MAN	O5-C5-C6-O6
10	l	5	MAN	O5-C5-C6-O6
10	g	5	MAN	O5-C5-C6-O6
9	s	1	NAG	C8-C7-N2-C2
14	6	5	MAN	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
14	w	5	MAN	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
10	j	2	NAG	C1-C2-N2-C7
12	r	2	NAG	O5-C5-C6-O6
14	w	2	NAG	O5-C5-C6-O6
10	j	1	NAG	C3-C2-N2-C7
14	6	2	NAG	C3-C2-N2-C7
10	1	3	BMA	C4-C5-C6-O6
12	2	2	NAG	C1-C2-N2-C7
9	v	1	NAG	C8-C7-N2-C2
12	e	1	NAG	C4-C5-C6-O6

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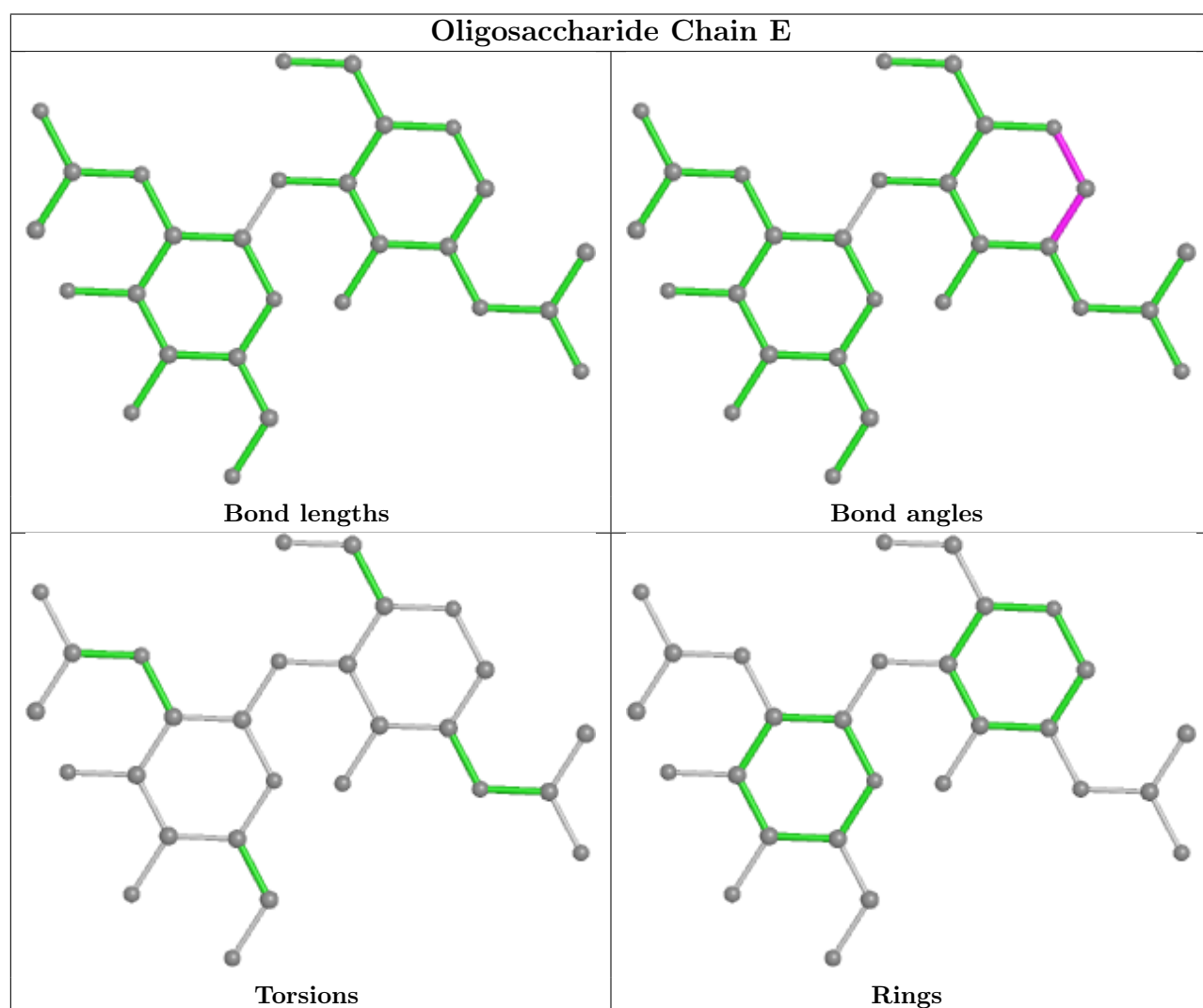
Mol	Chain	Res	Type	Atoms
10	1	3	BMA	O5-C5-C6-O6
10	4	2	NAG	O5-C5-C6-O6
10	5	3	BMA	C4-C5-C6-O6
9	Y	2	NAG	O7-C7-N2-C2
12	m	2	NAG	O7-C7-N2-C2
12	r	2	NAG	C8-C7-N2-C2
12	e	2	NAG	C8-C7-N2-C2
15	z	3	BMA	O5-C5-C6-O6
10	u	2	NAG	C8-C7-N2-C2
9	v	1	NAG	O7-C7-N2-C2
10	5	3	BMA	O5-C5-C6-O6
12	e	1	NAG	O5-C5-C6-O6
10	j	3	BMA	C4-C5-C6-O6
9	t	1	NAG	C3-C2-N2-C7
10	4	1	NAG	C3-C2-N2-C7
10	4	2	NAG	C3-C2-N2-C7
12	h	2	NAG	C3-C2-N2-C7
10	u	2	NAG	O7-C7-N2-C2
12	e	2	NAG	O7-C7-N2-C2
9	n	2	NAG	C1-C2-N2-C7
9	X	1	NAG	C8-C7-N2-C2
12	r	2	NAG	O7-C7-N2-C2
10	u	1	NAG	C8-C7-N2-C2
10	9	3	BMA	C4-C5-C6-O6
10	j	3	BMA	O5-C5-C6-O6
10	4	2	NAG	O7-C7-N2-C2
10	4	2	NAG	C8-C7-N2-C2
12	m	1	NAG	C4-C5-C6-O6
10	4	1	NAG	O5-C5-C6-O6
13	8	2	NAG	C1-C2-N2-C7
9	X	1	NAG	O7-C7-N2-C2
10	4	1	NAG	C4-C5-C6-O6
10	j	2	NAG	C3-C2-N2-C7
10	5	1	NAG	C3-C2-N2-C7
13	8	1	NAG	C3-C2-N2-C7
13	8	2	NAG	C3-C2-N2-C7
14	w	2	NAG	C3-C2-N2-C7
15	z	2	NAG	C3-C2-N2-C7
13	c	2	NAG	C4-C5-C6-O6

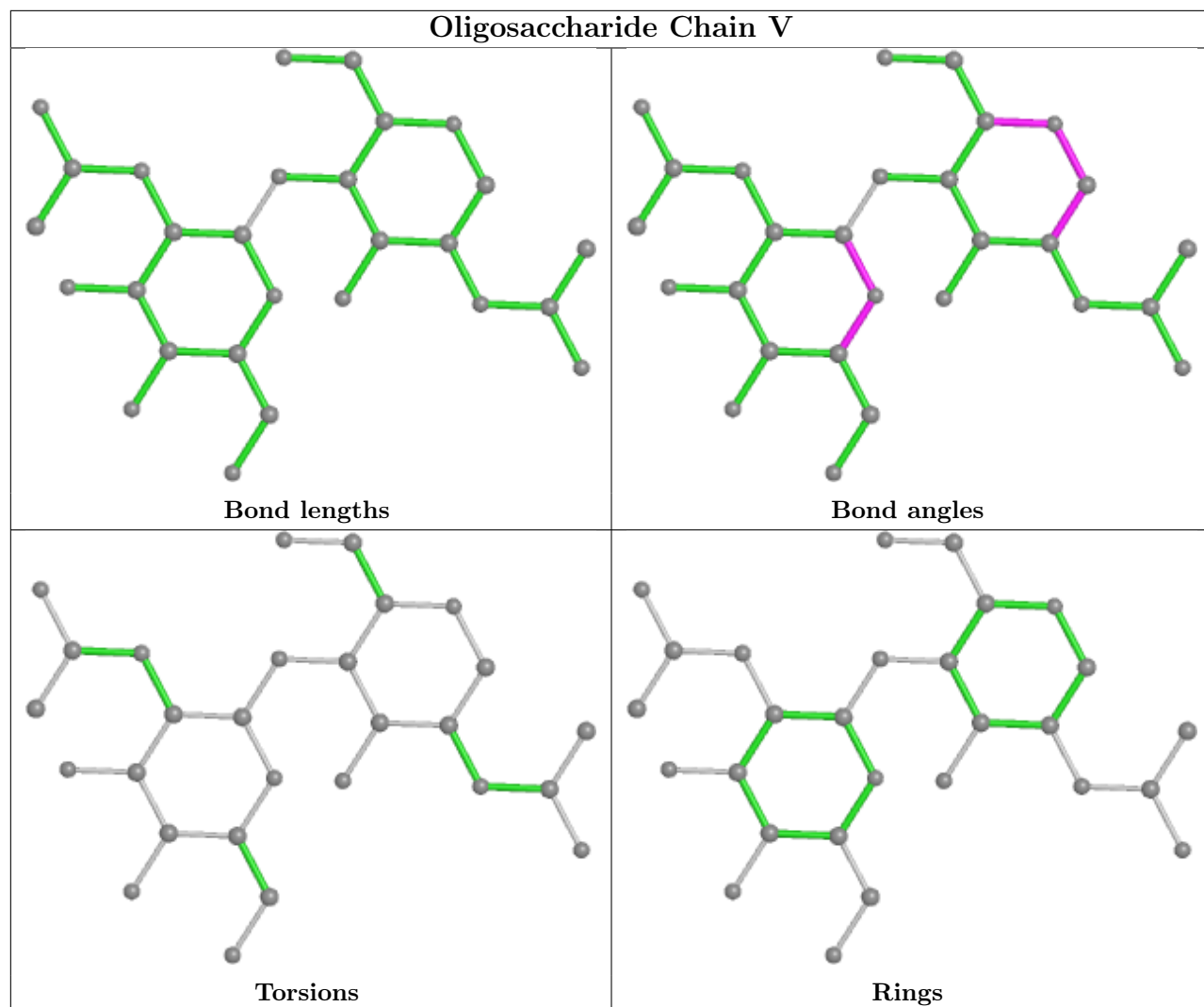
There are no ring outliers.

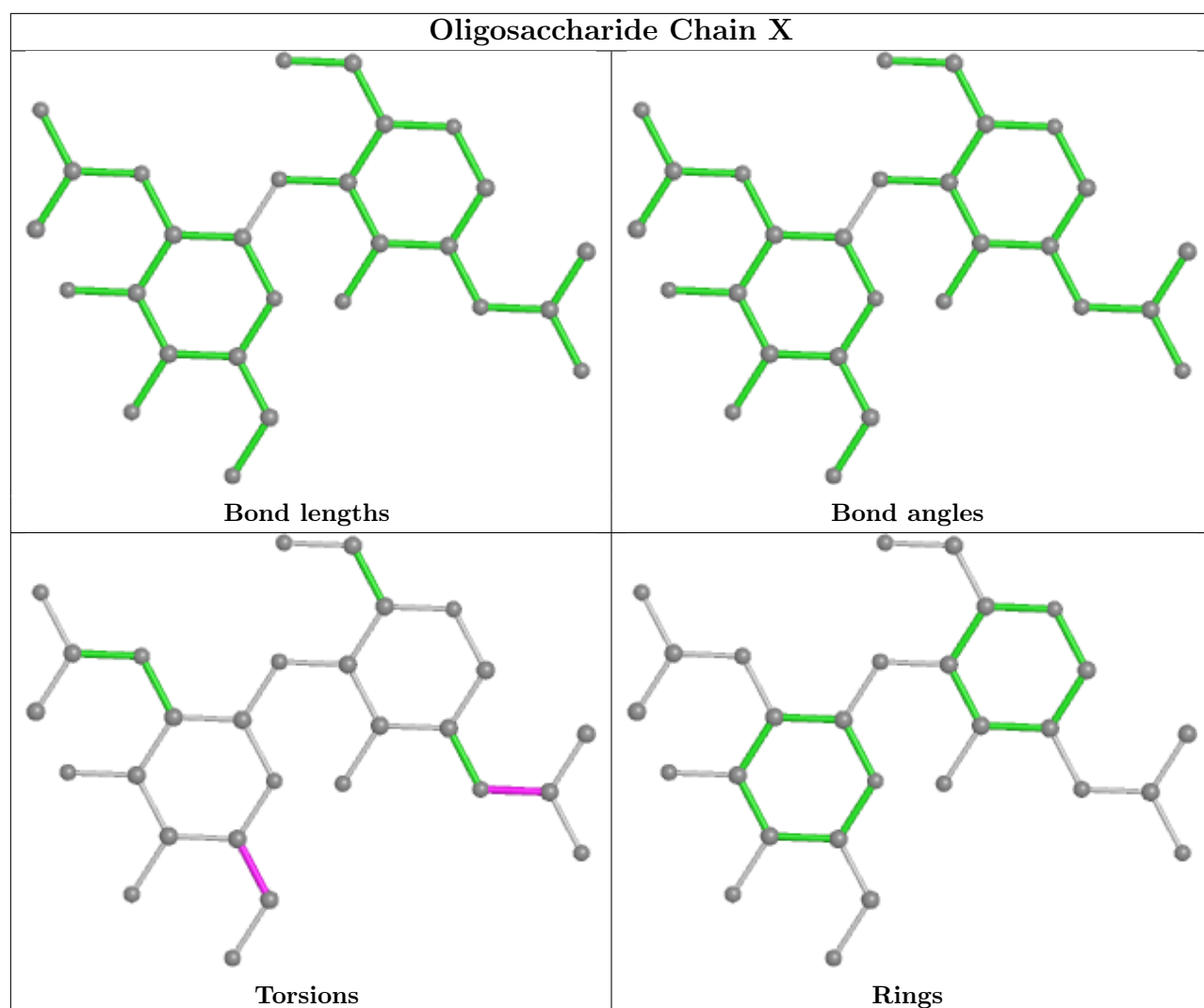
8 monomers are involved in 6 short contacts:

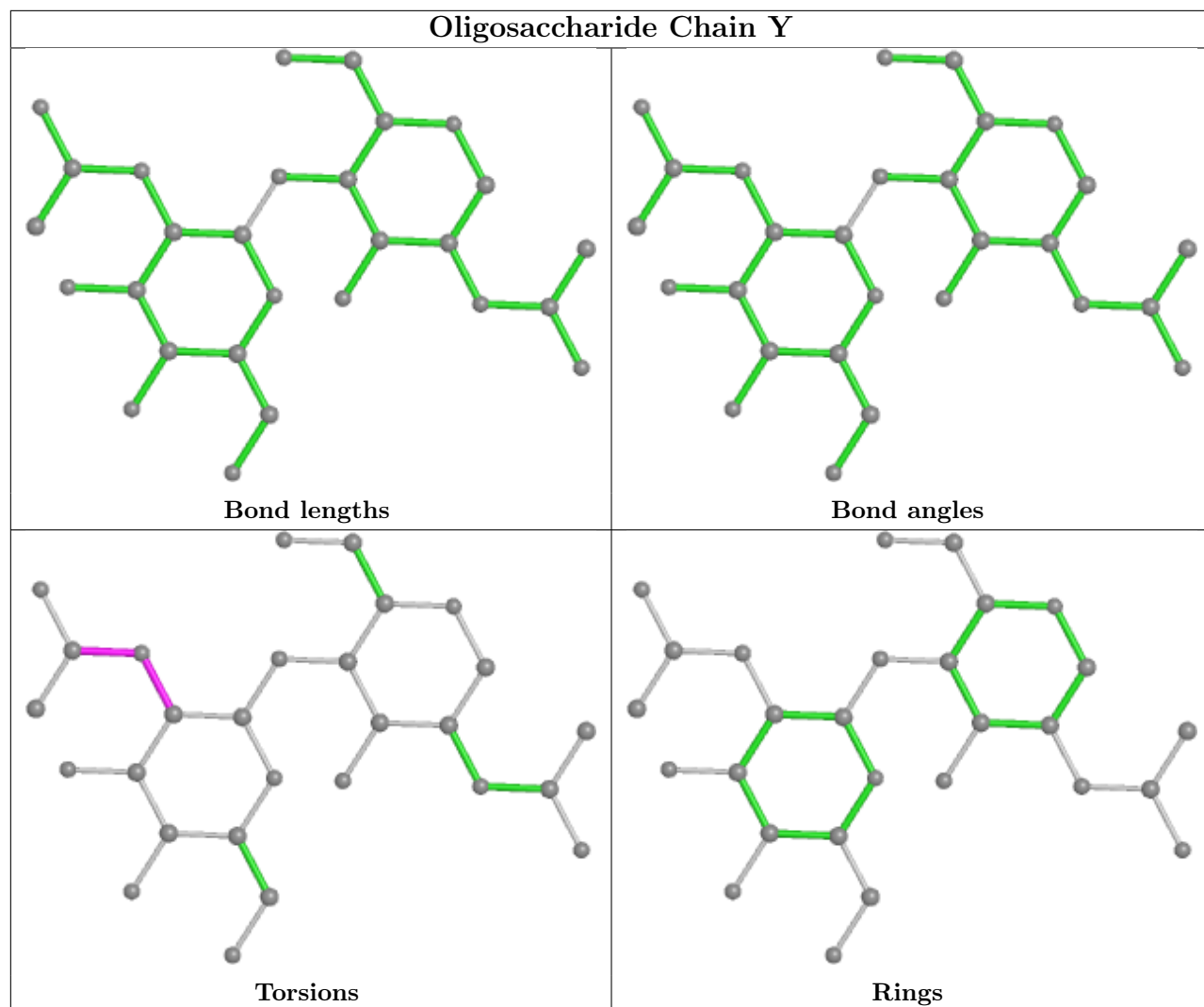
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	1	NAG	1	0
14	6	1	NAG	1	0
12	W	1	NAG	1	0
10	4	1	NAG	1	0
14	6	2	NAG	1	0
11	U	1	NAG	2	0
11	U	2	NAG	1	0
10	4	2	NAG	1	0

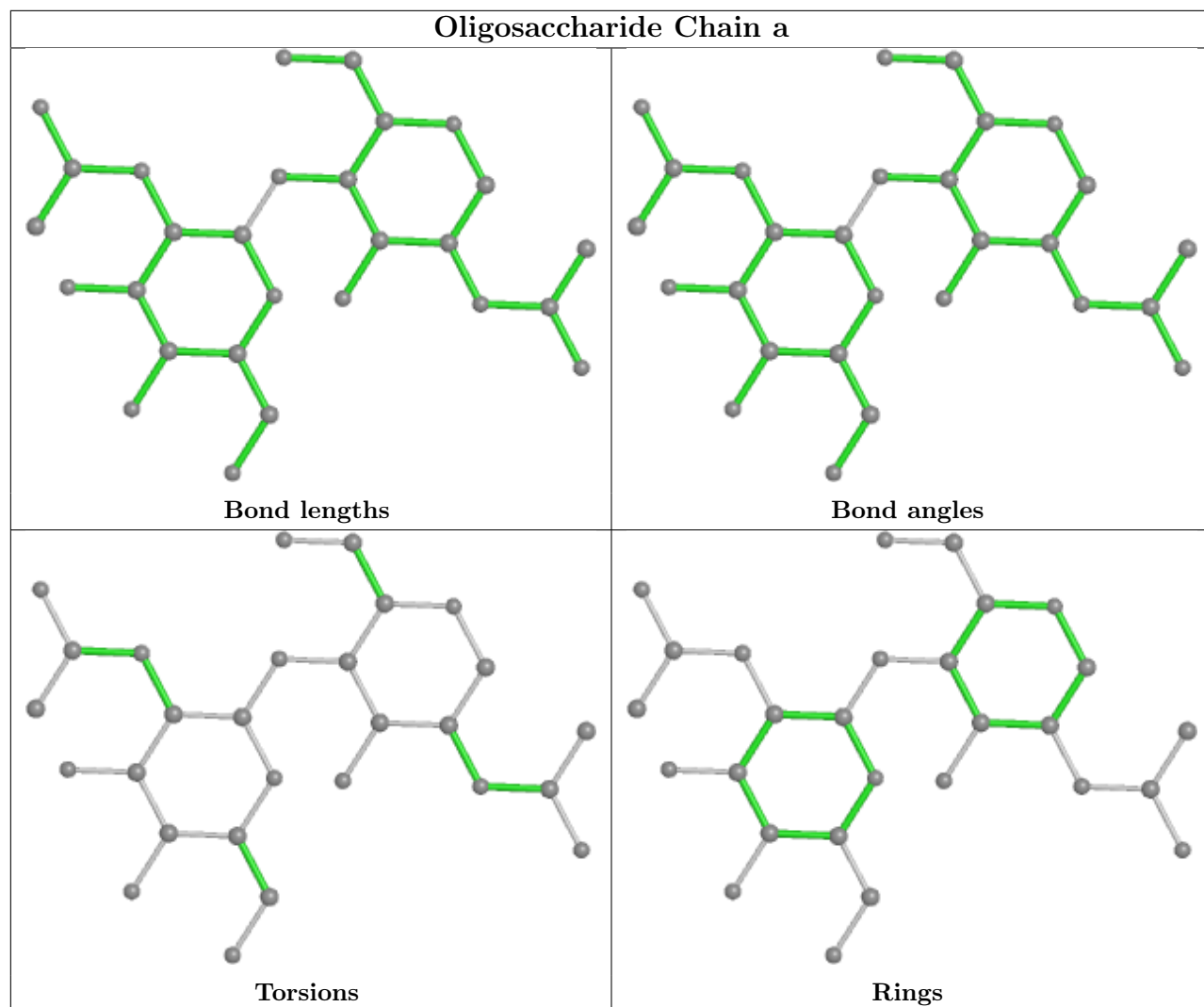
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

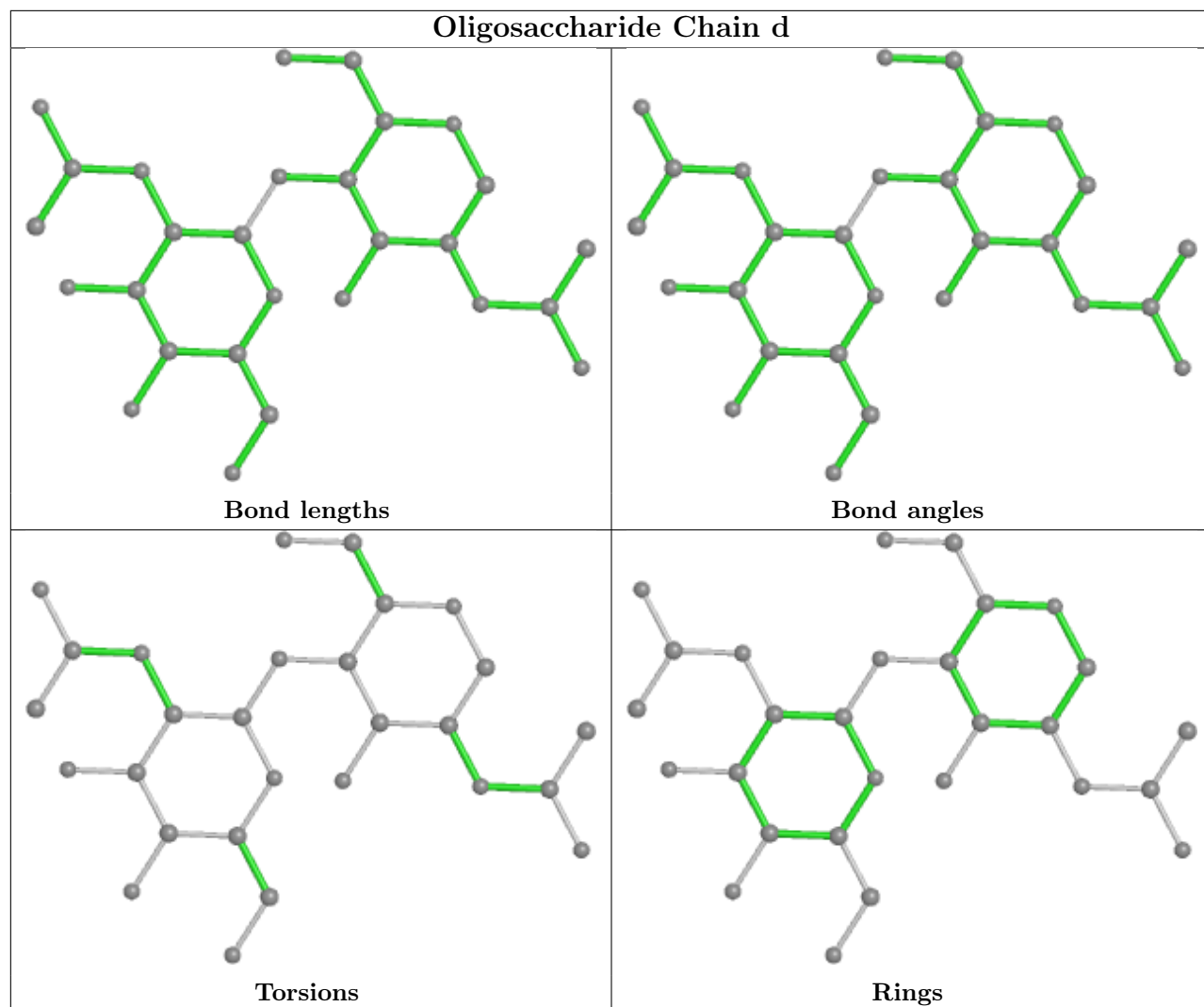


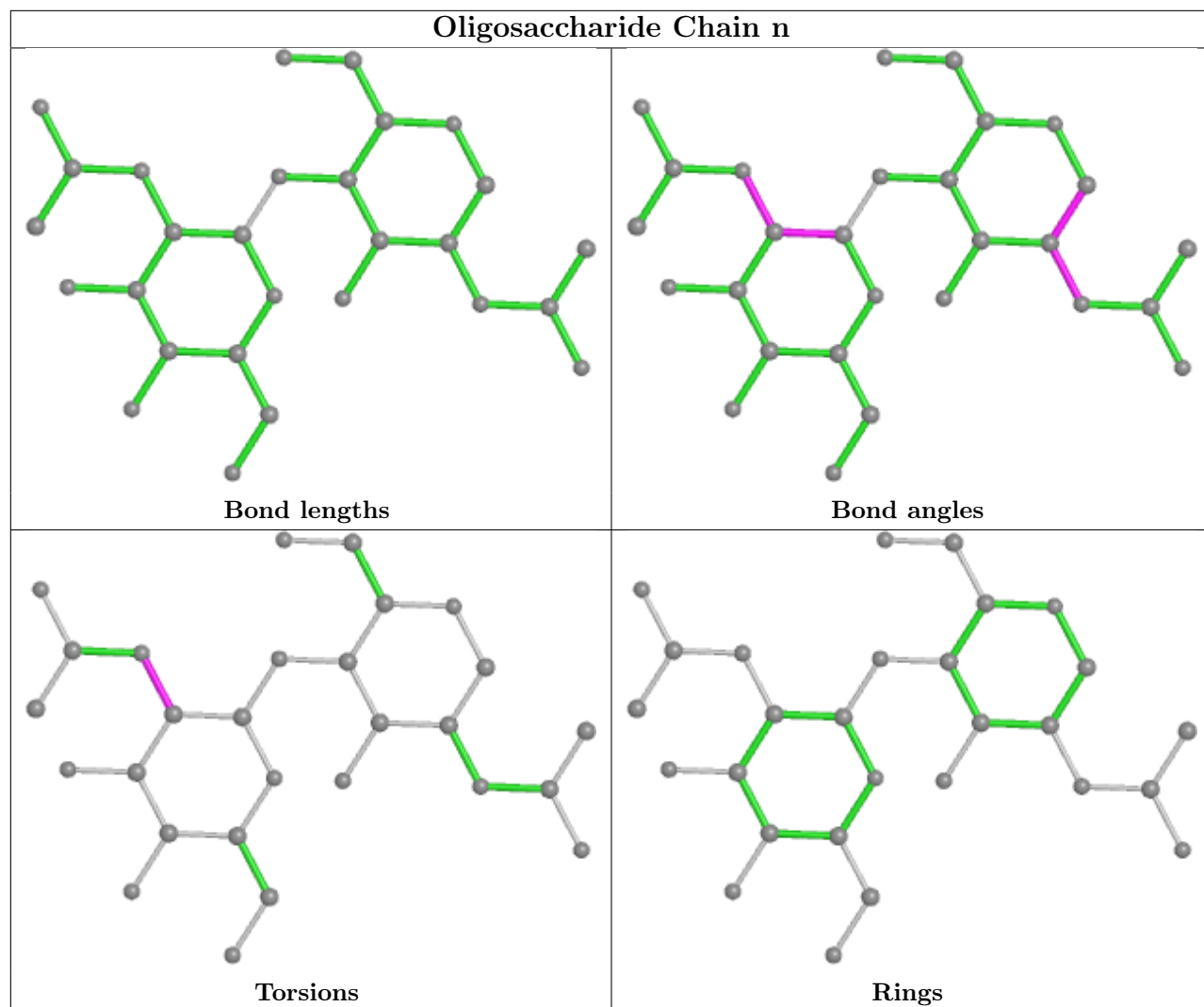


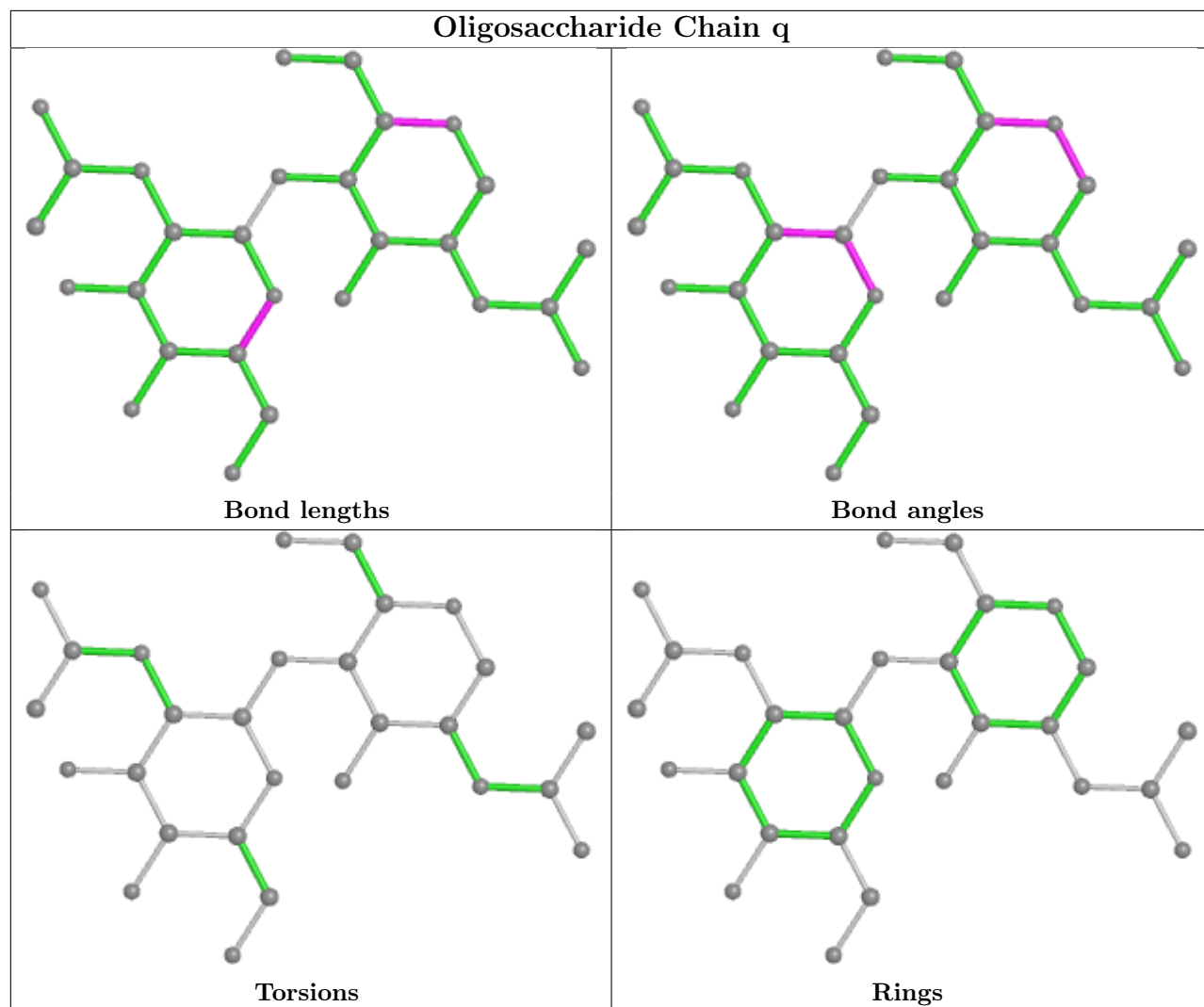


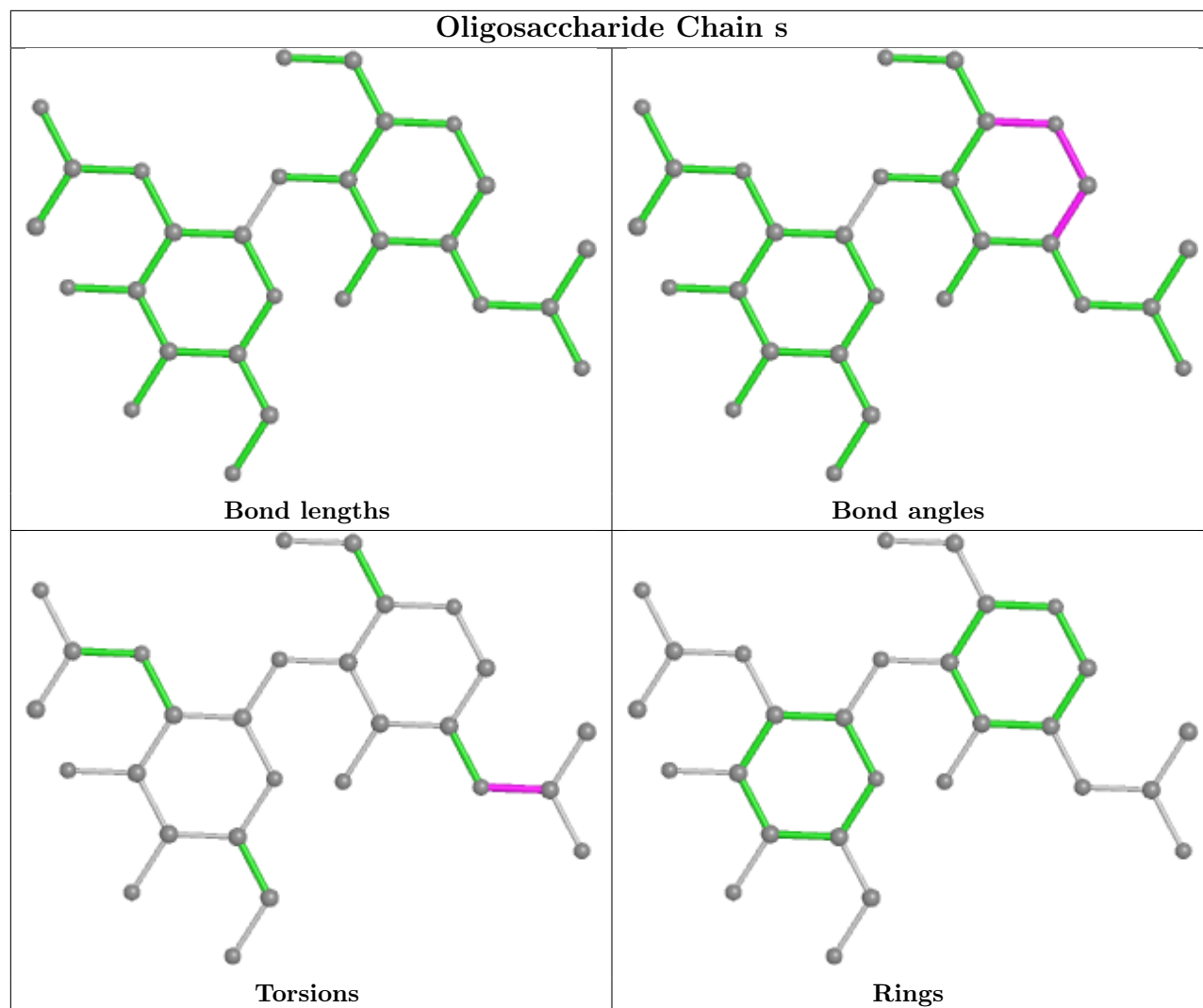


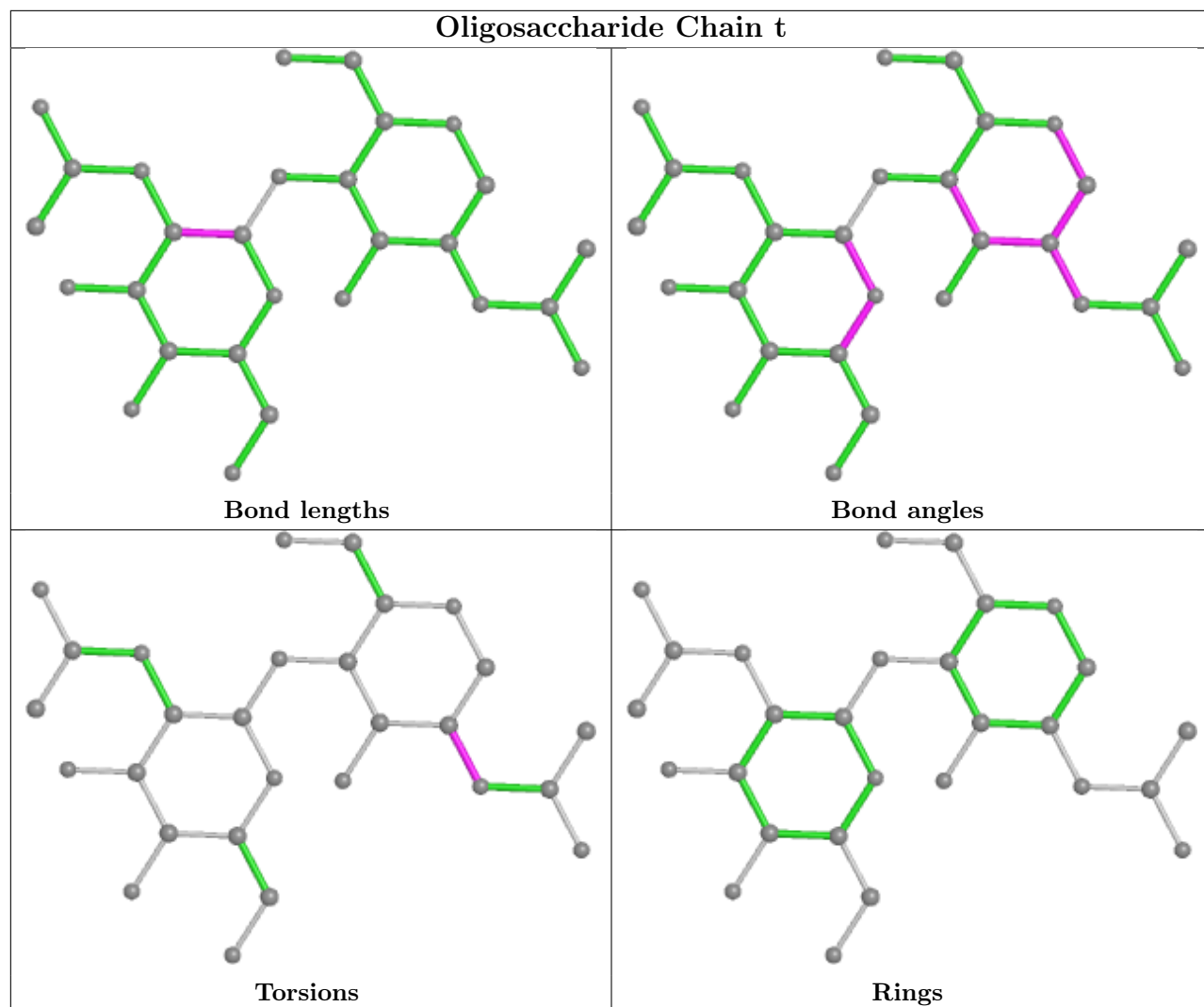


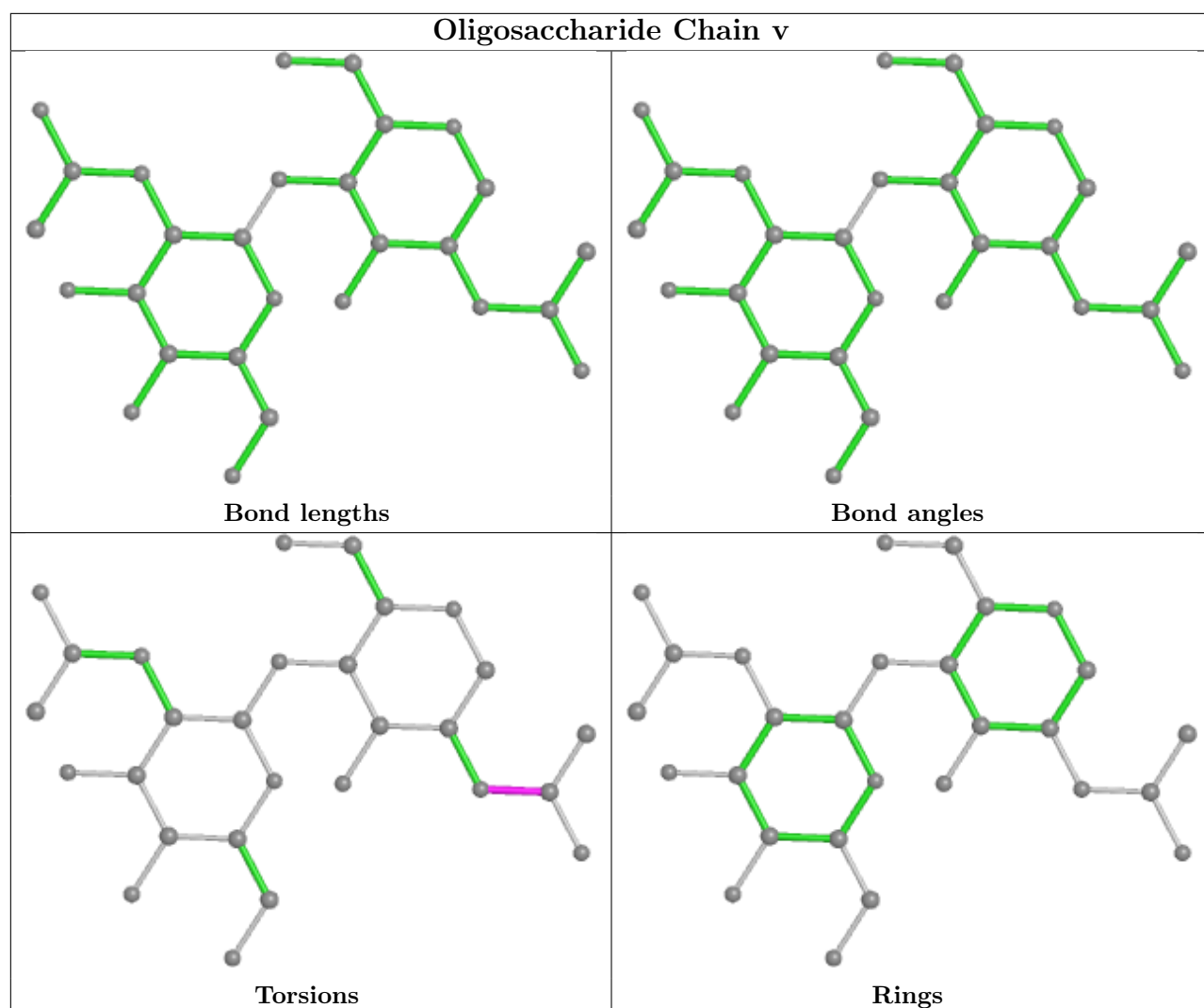


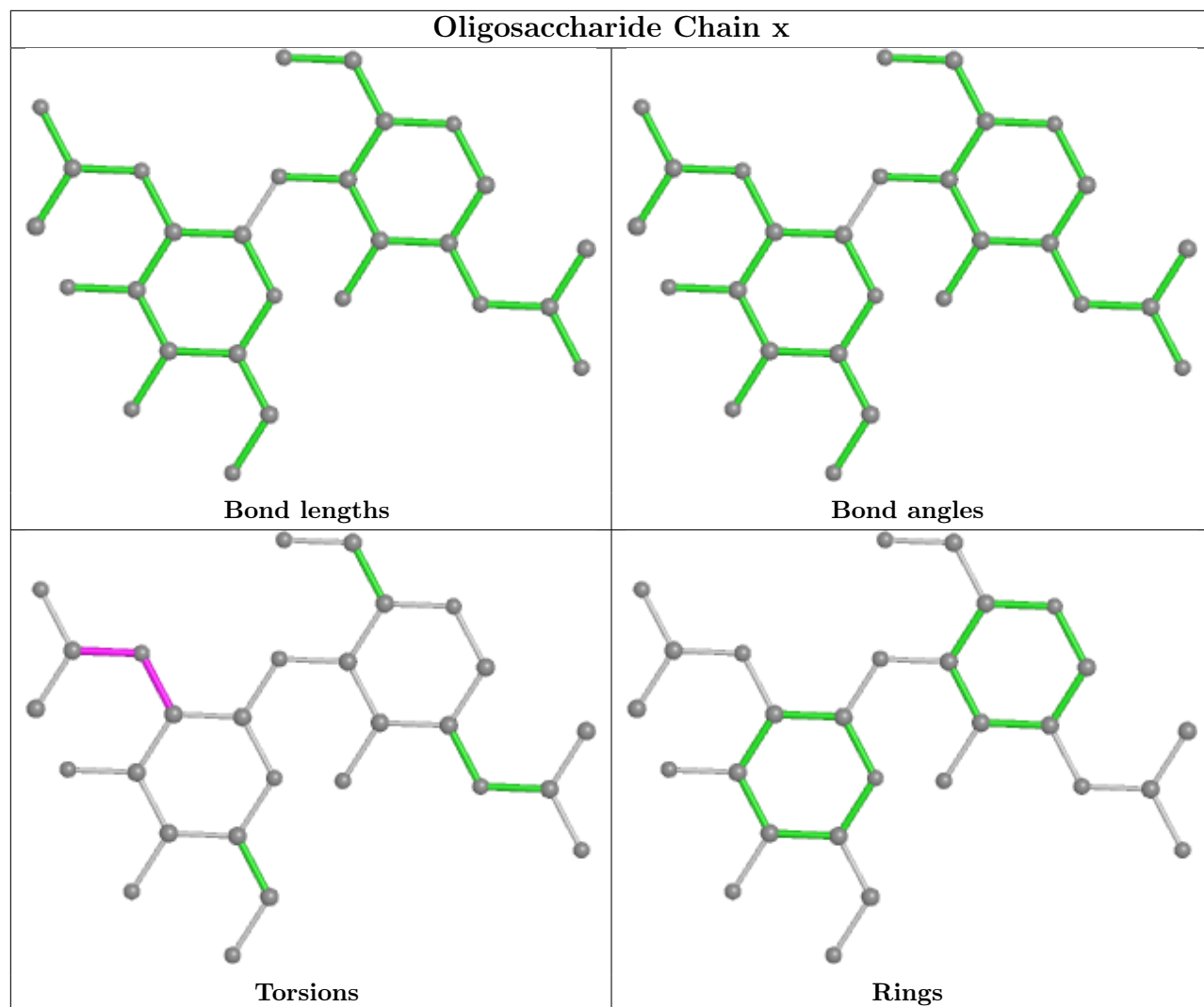


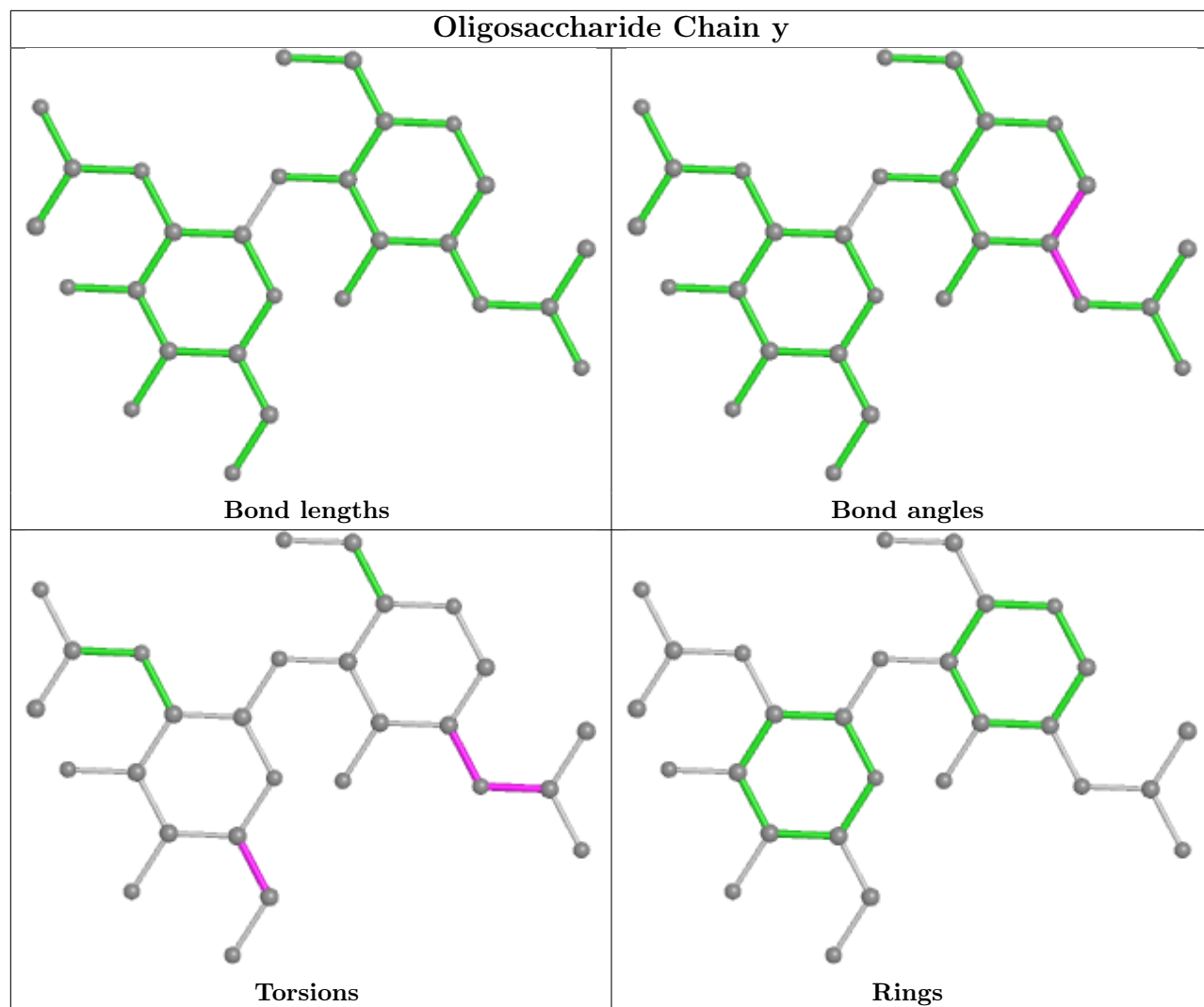


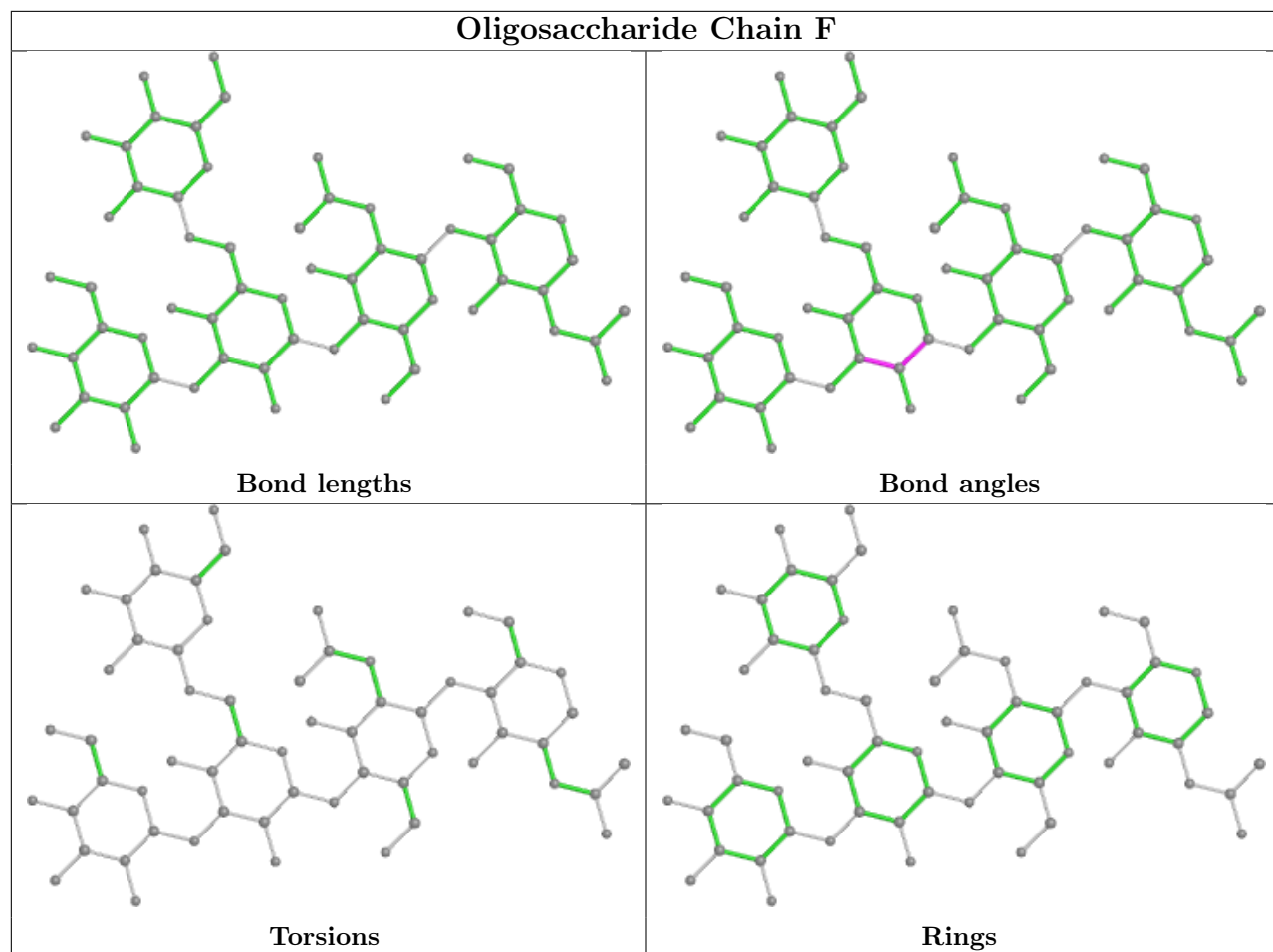


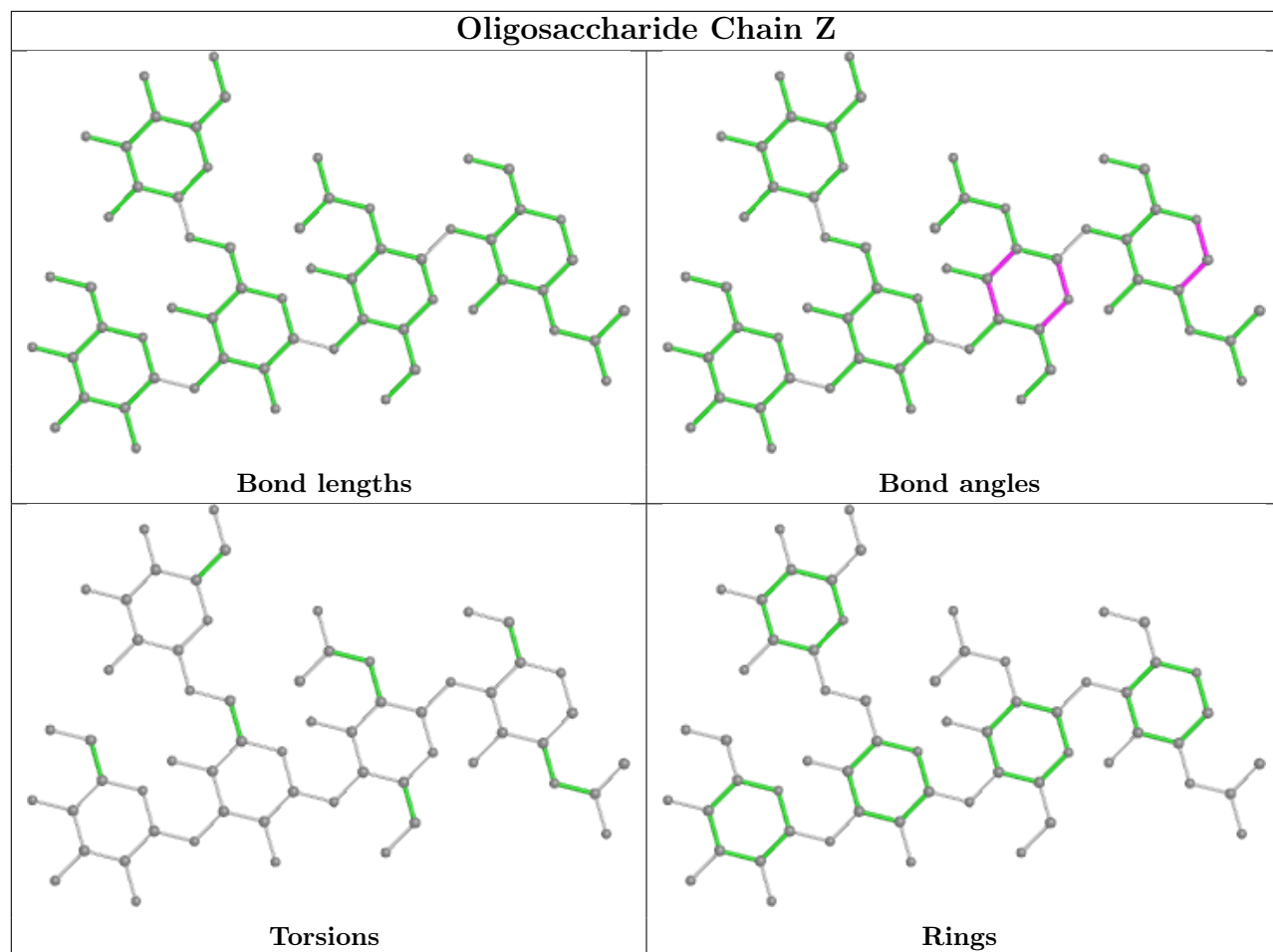


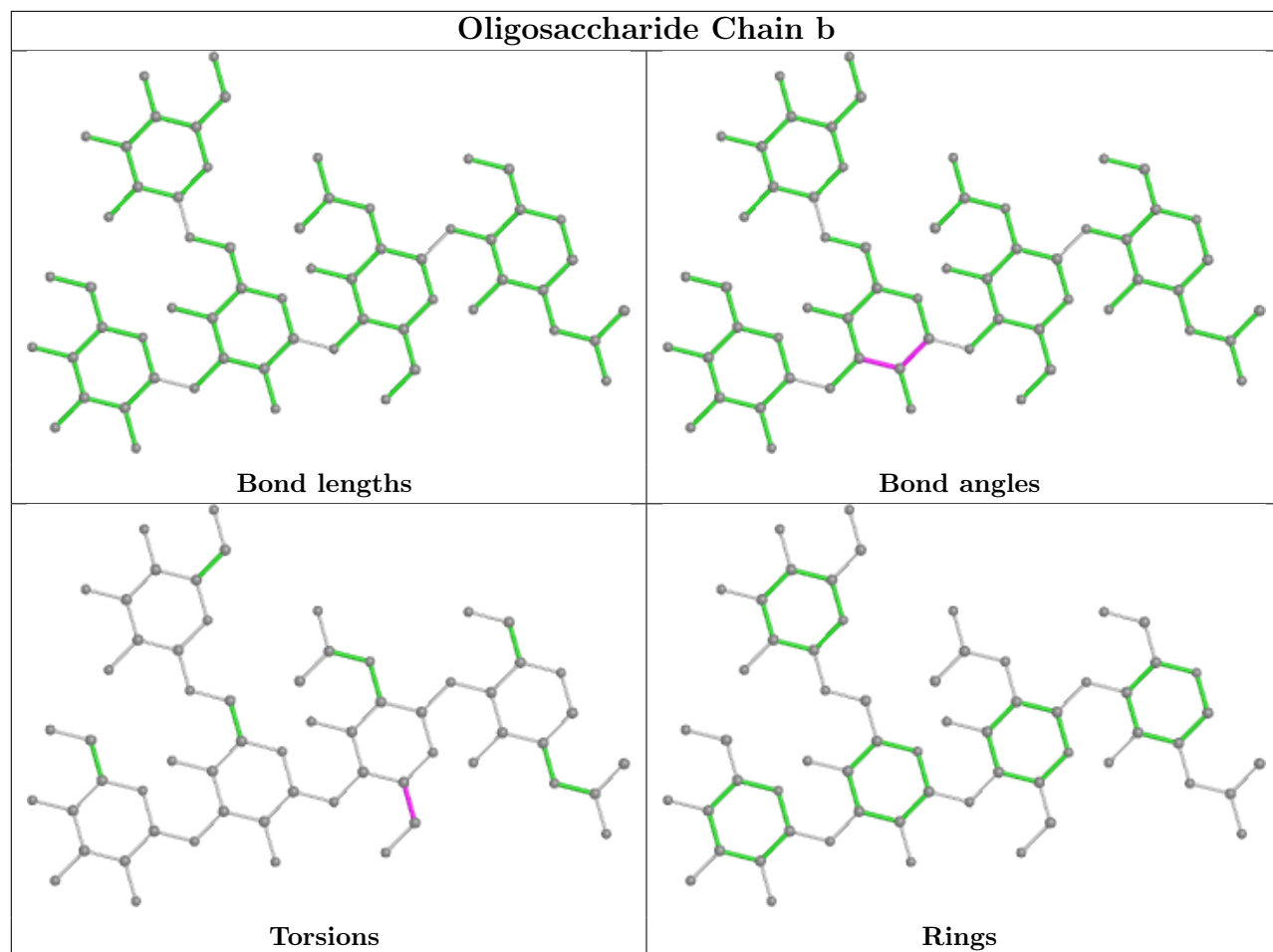


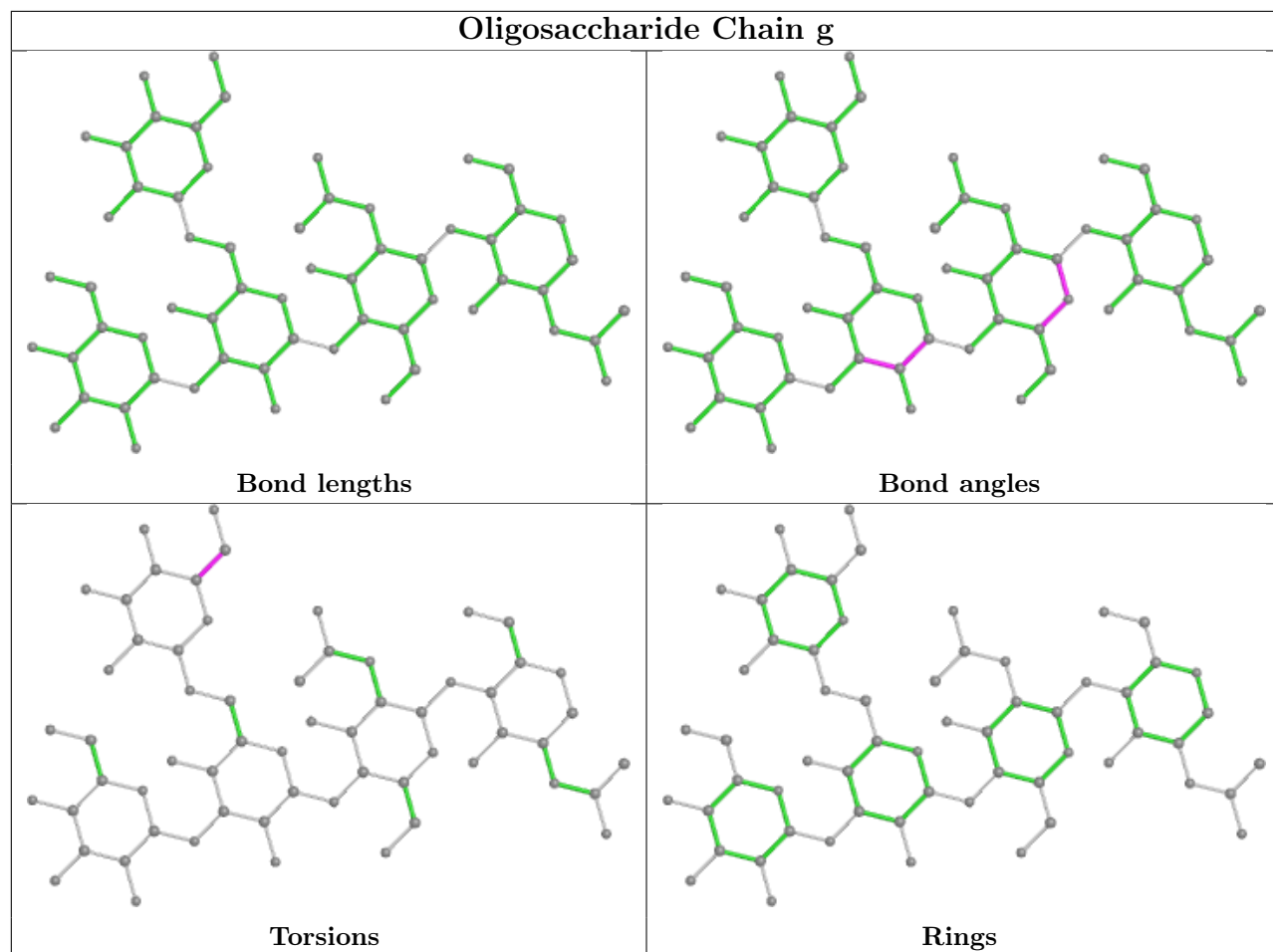


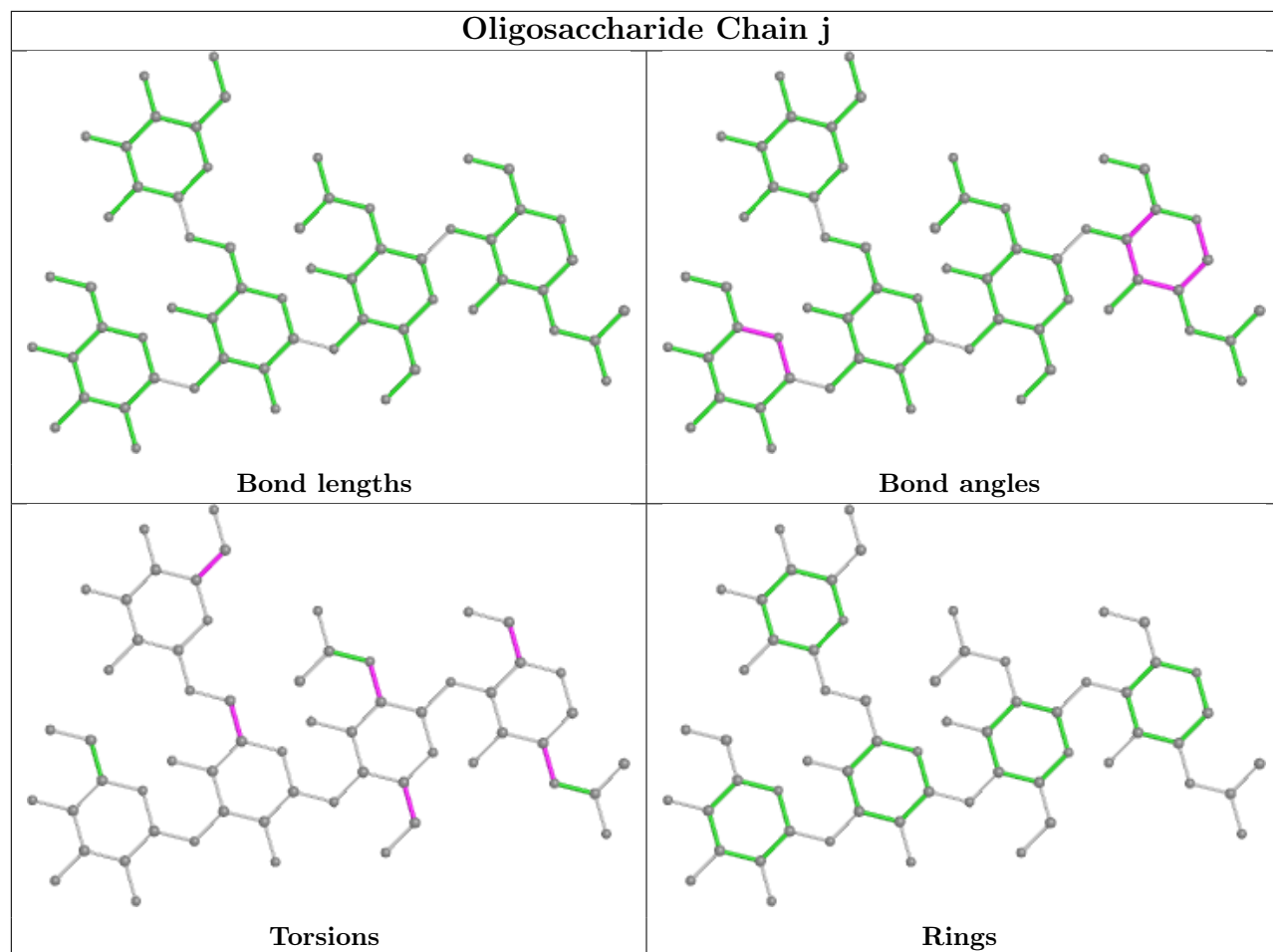


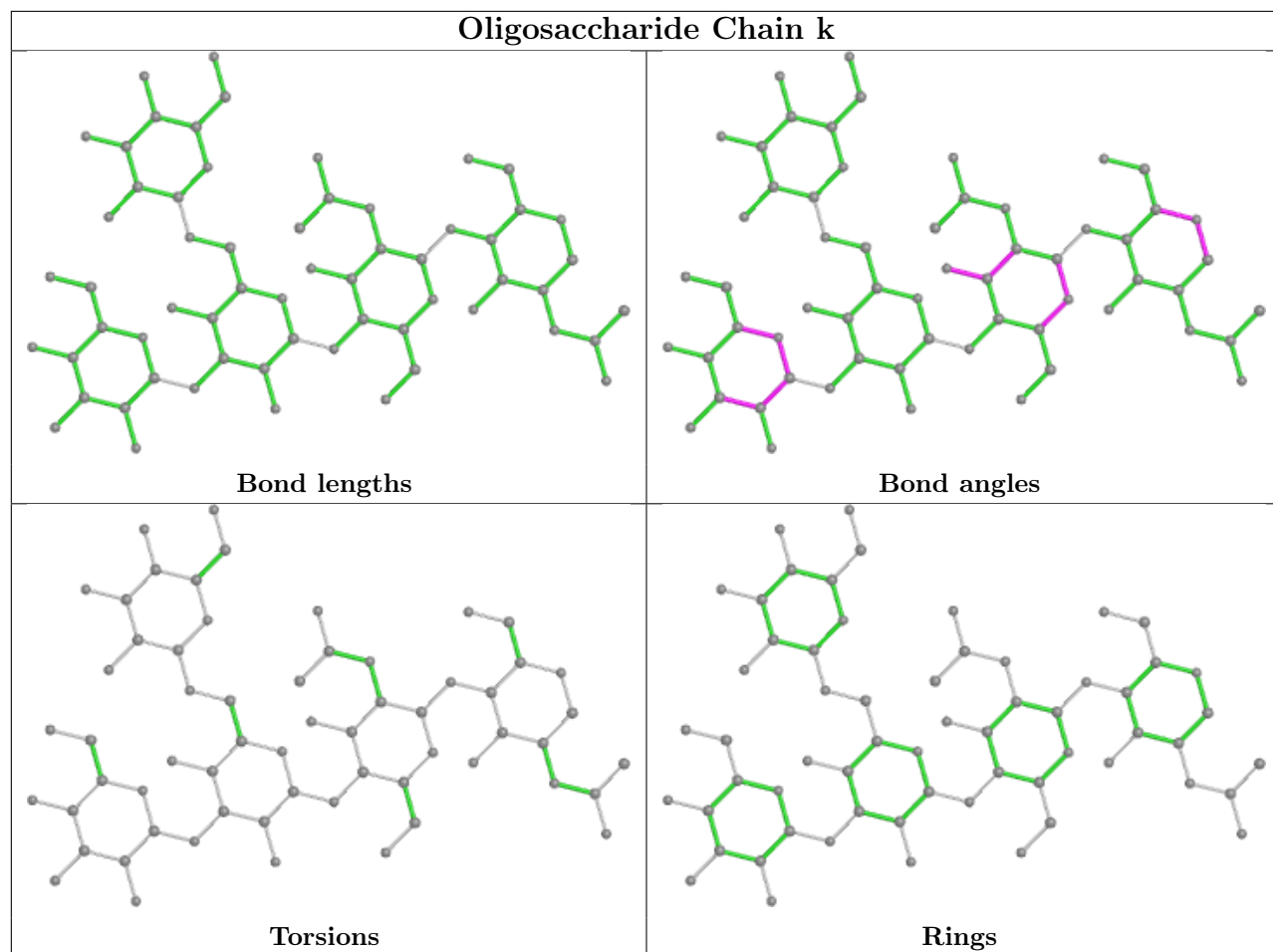


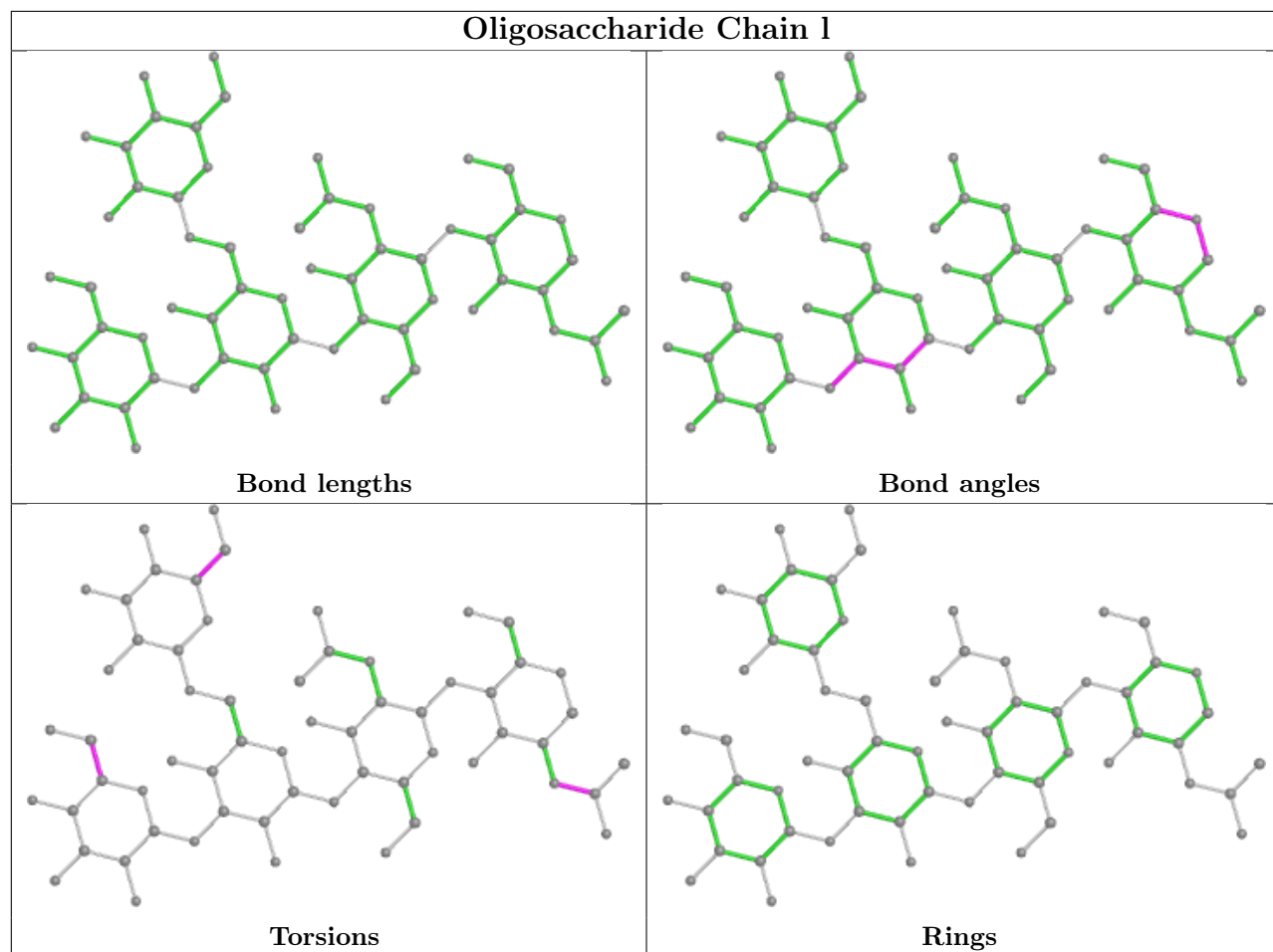


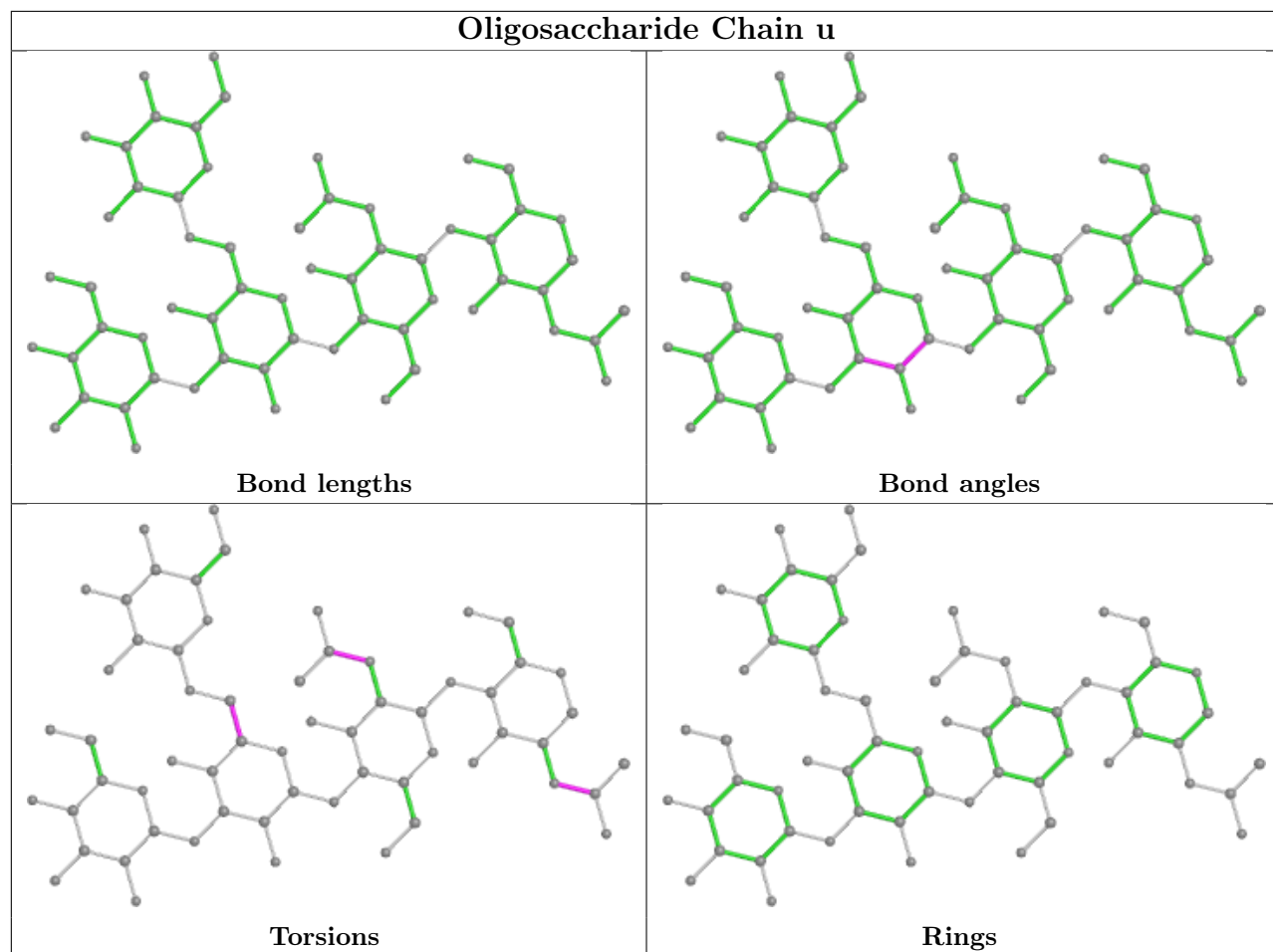


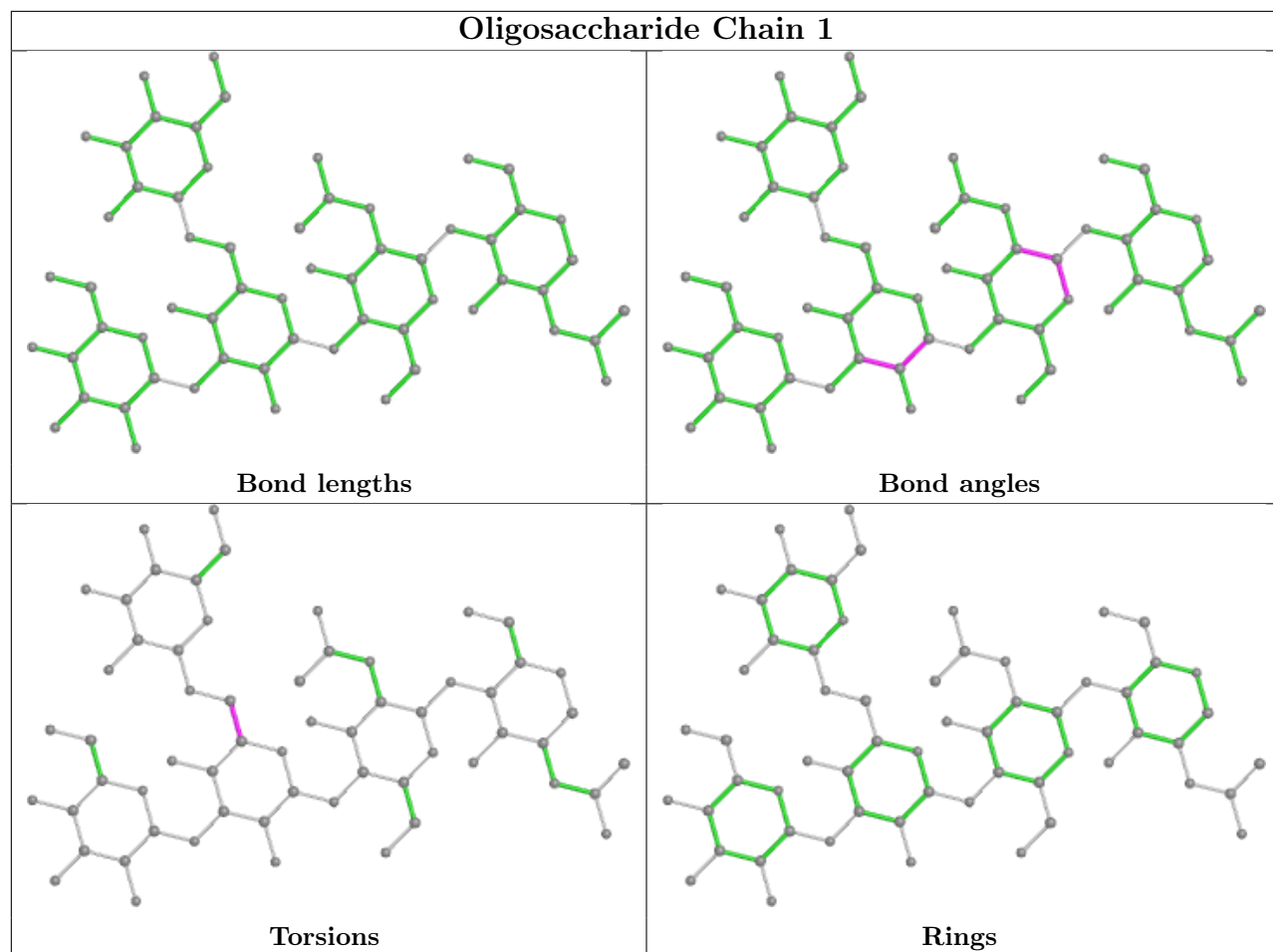


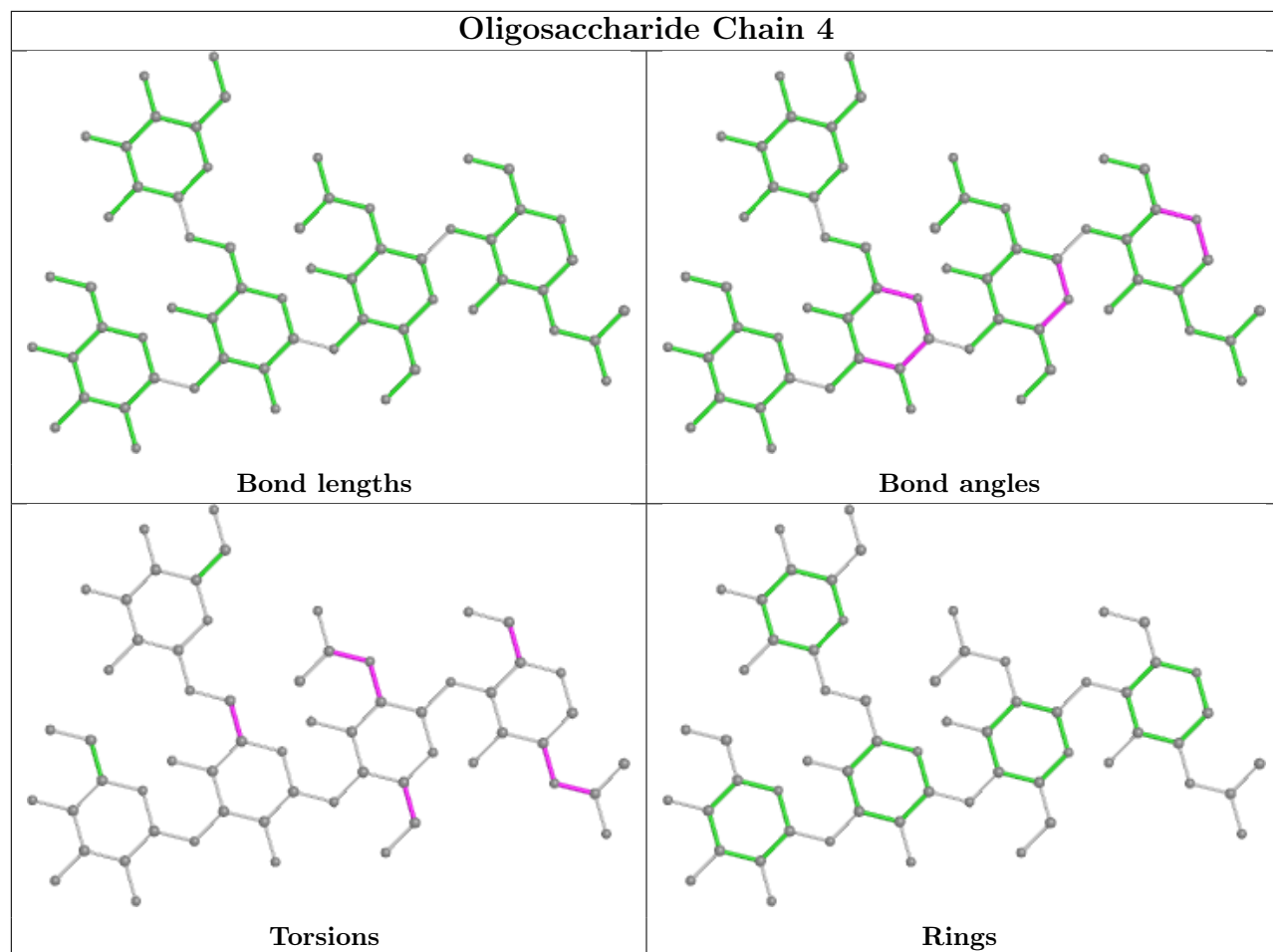


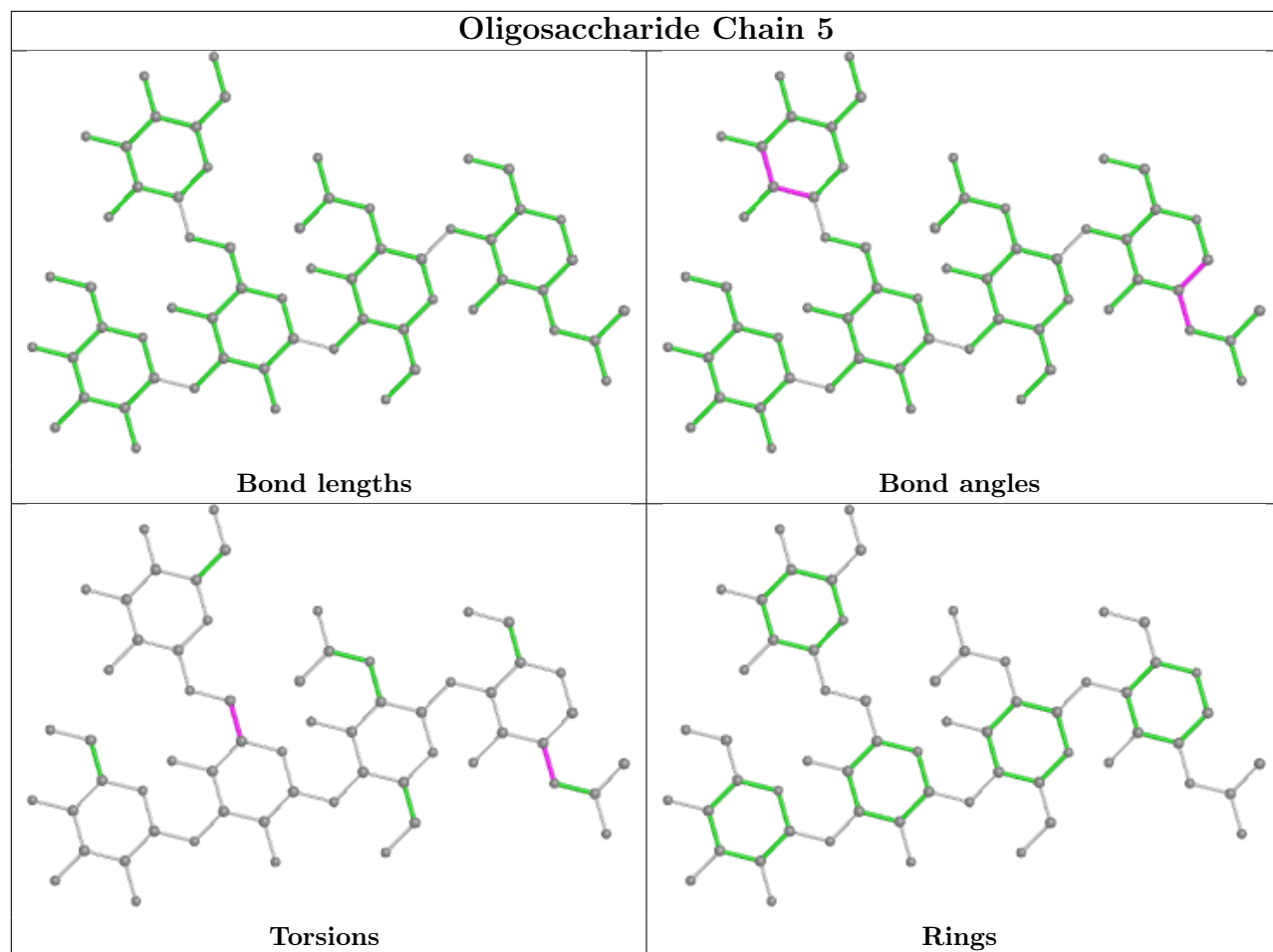


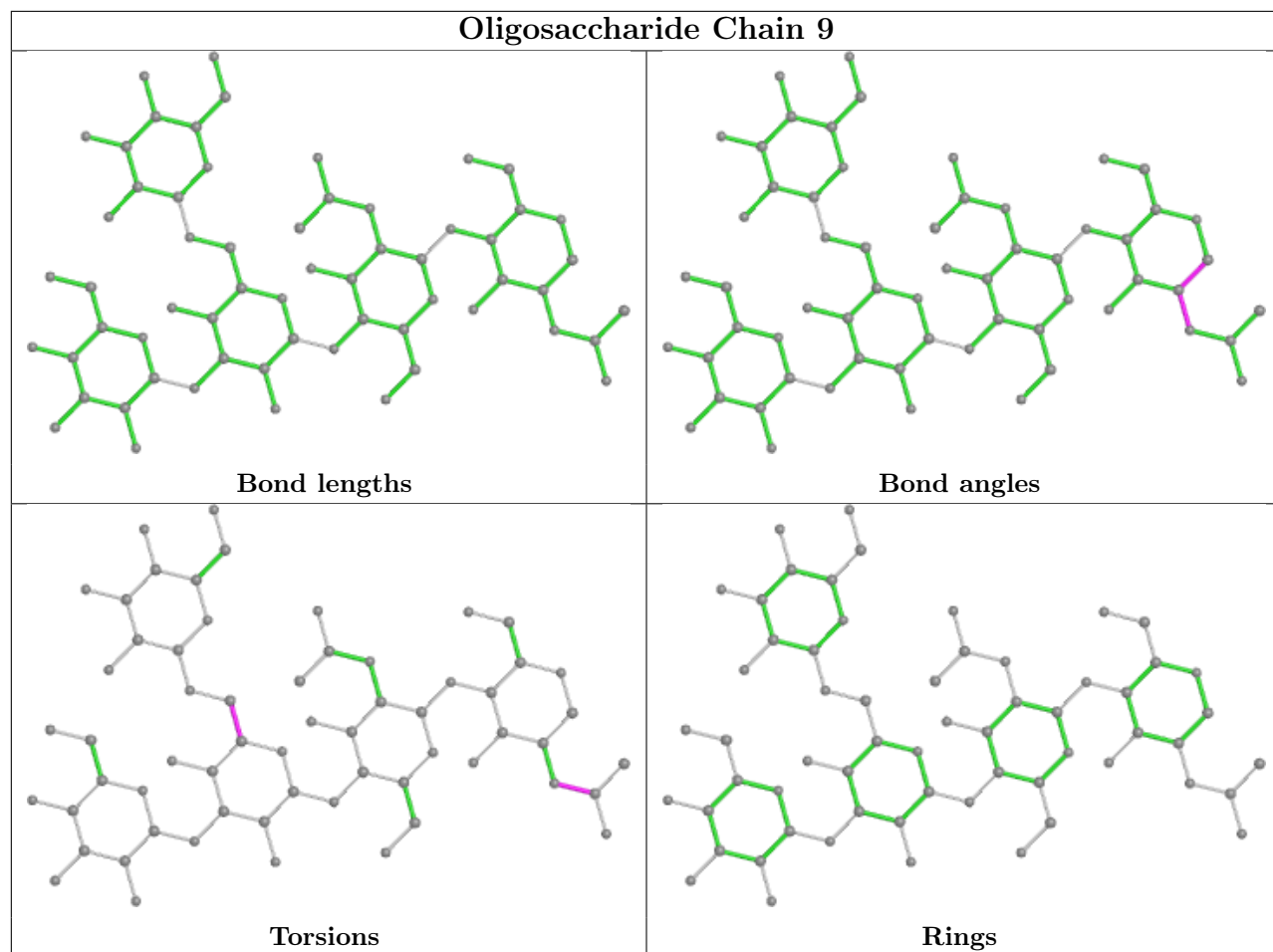


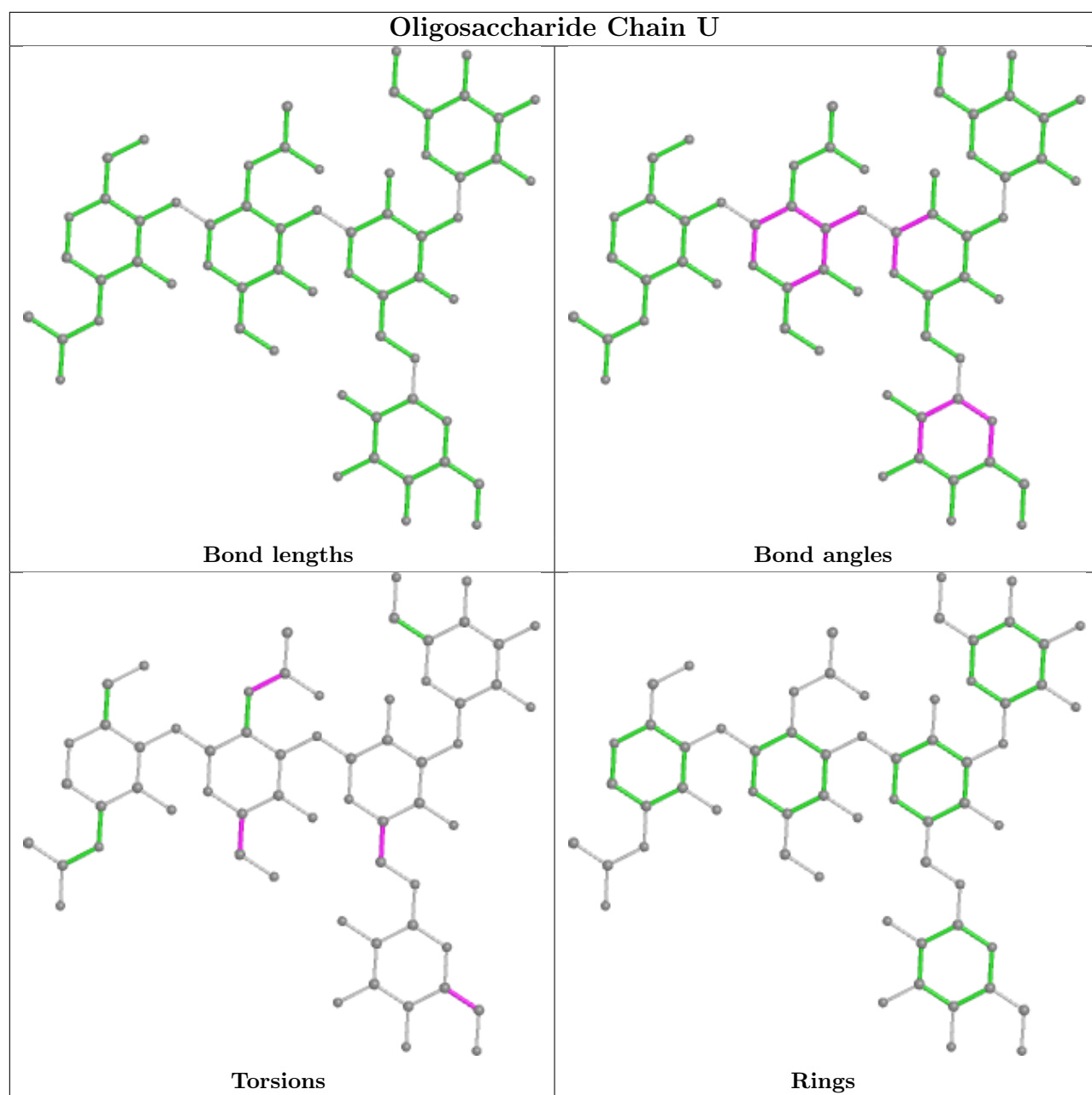


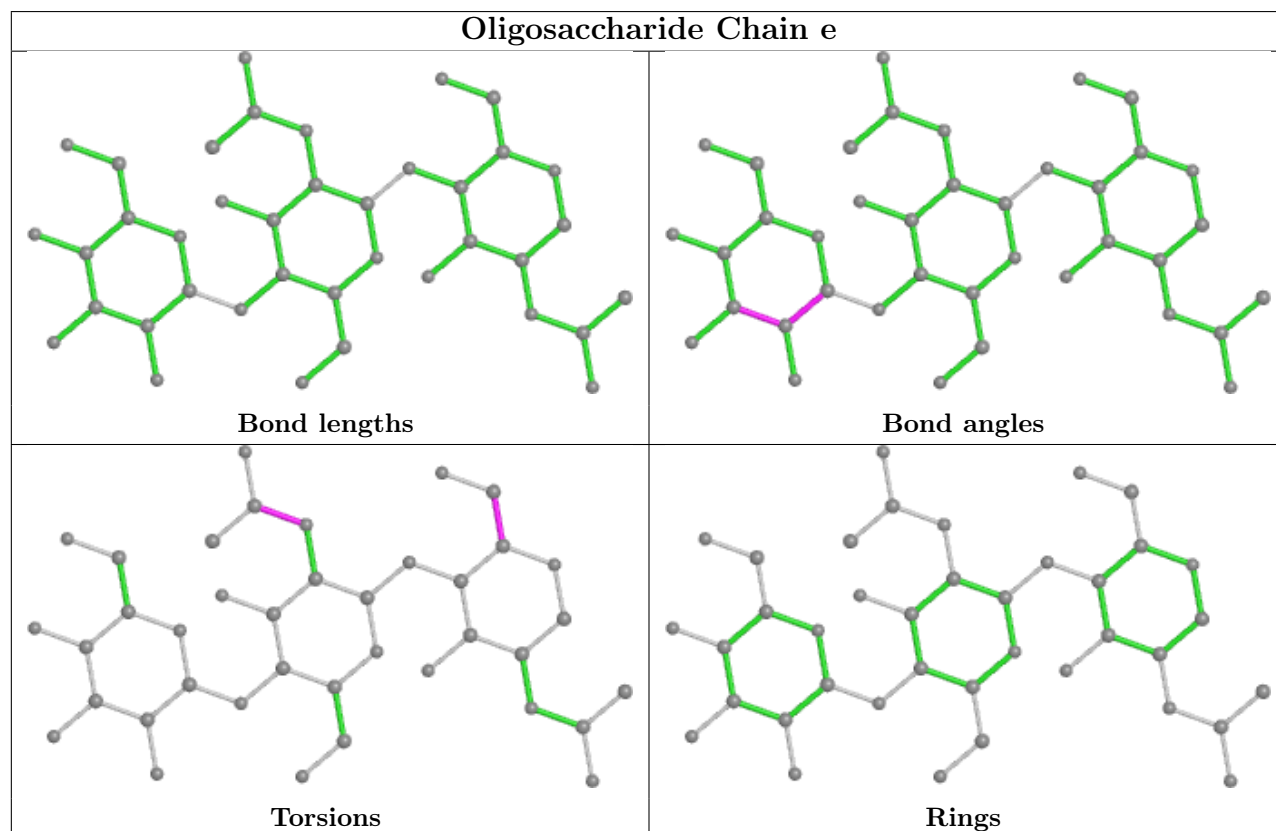
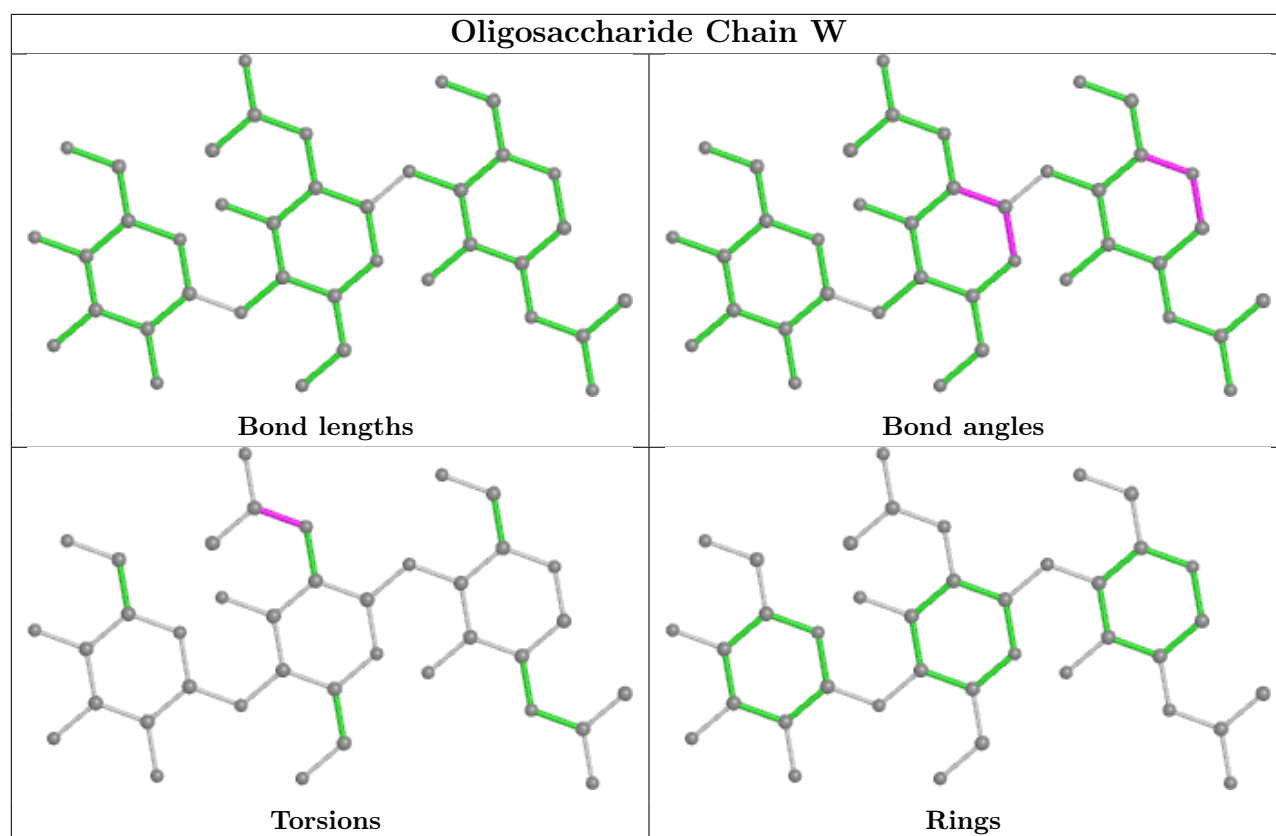


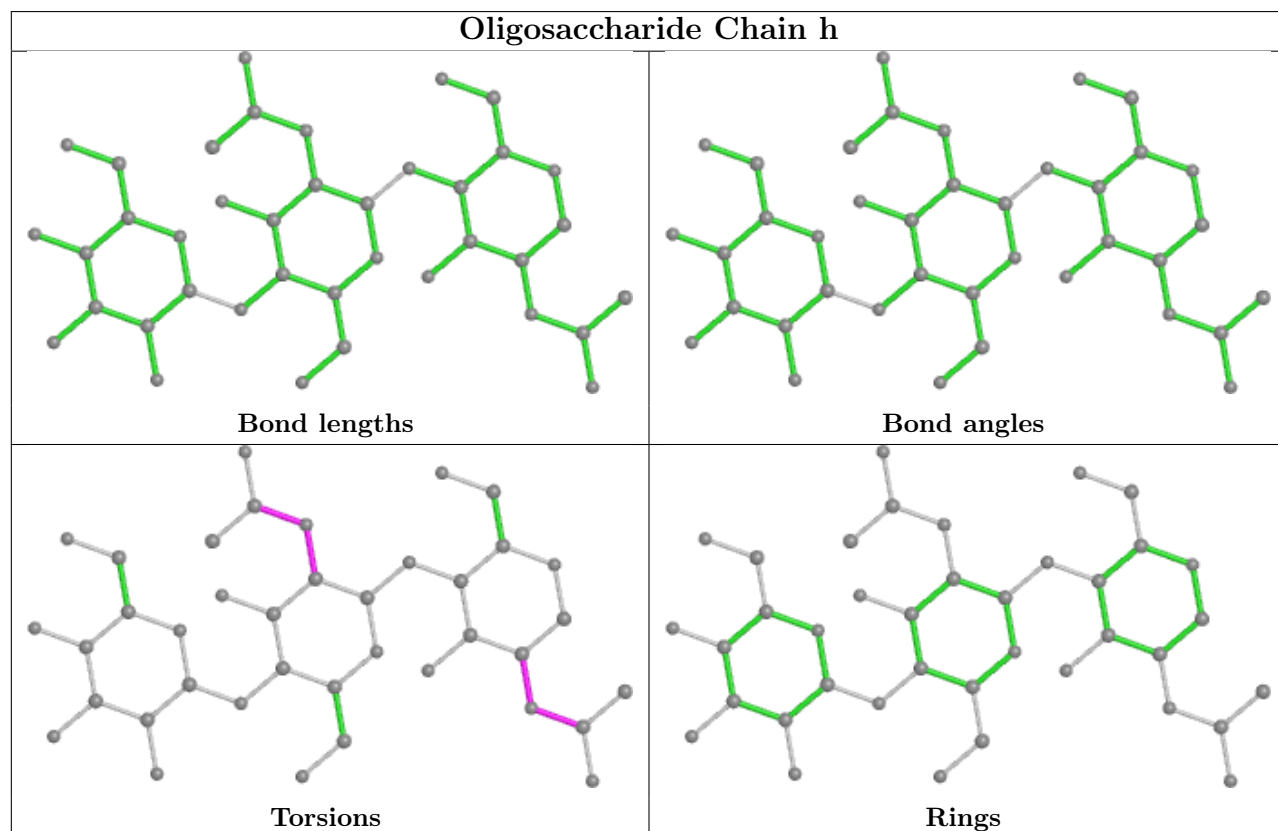
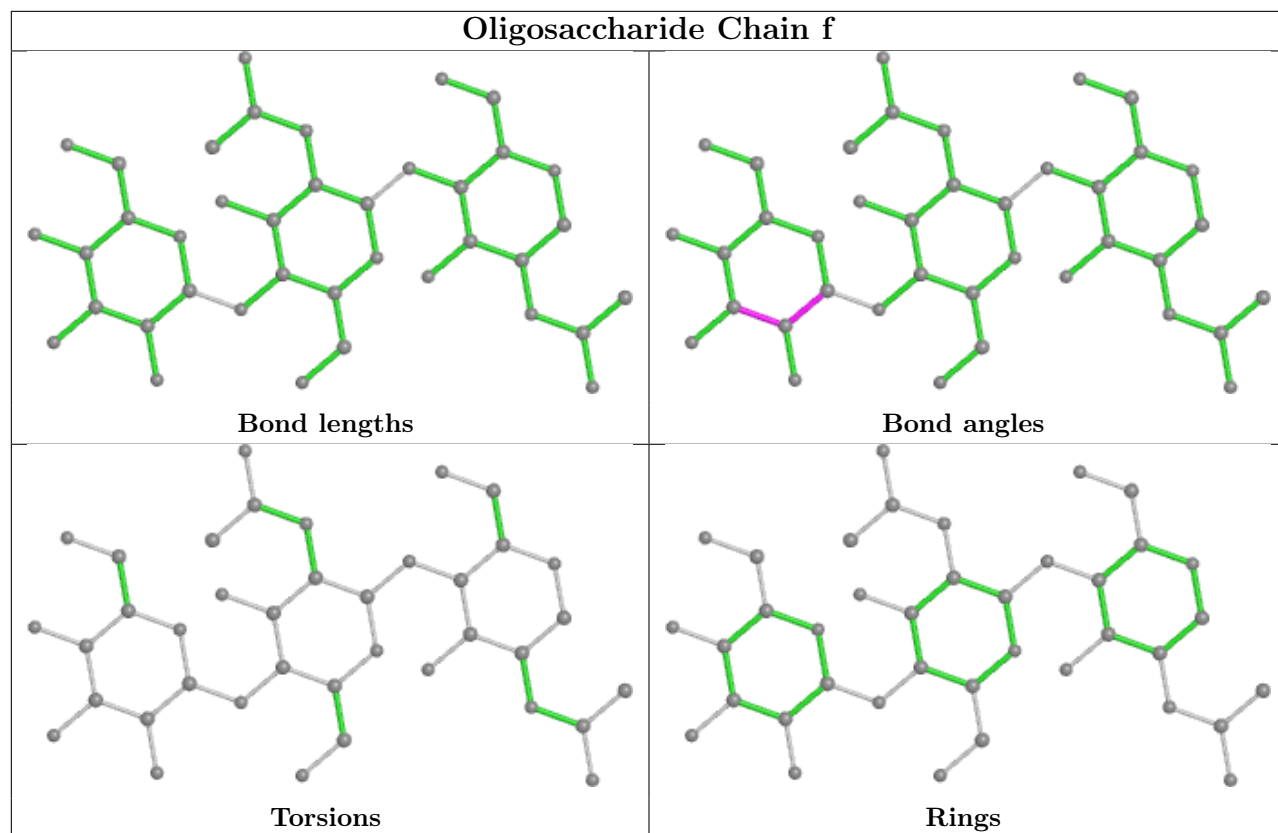


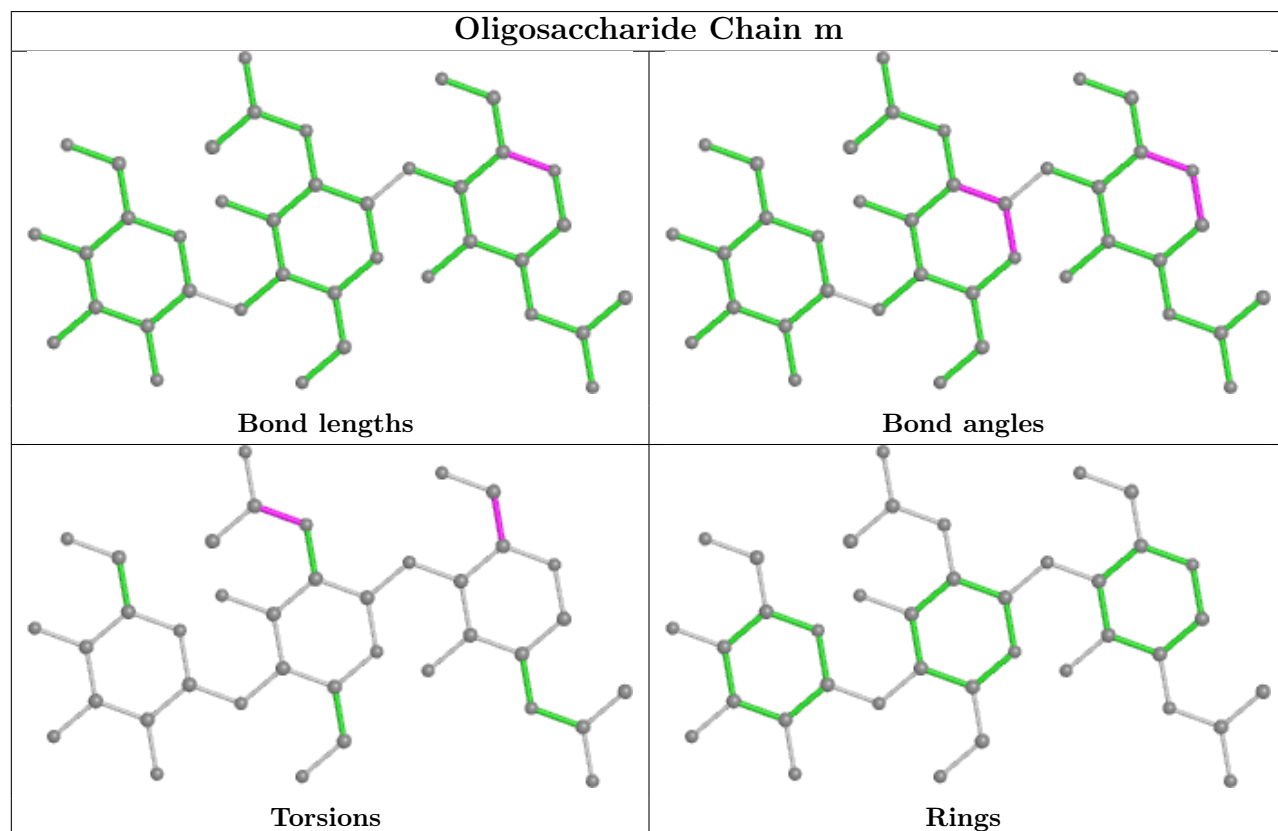
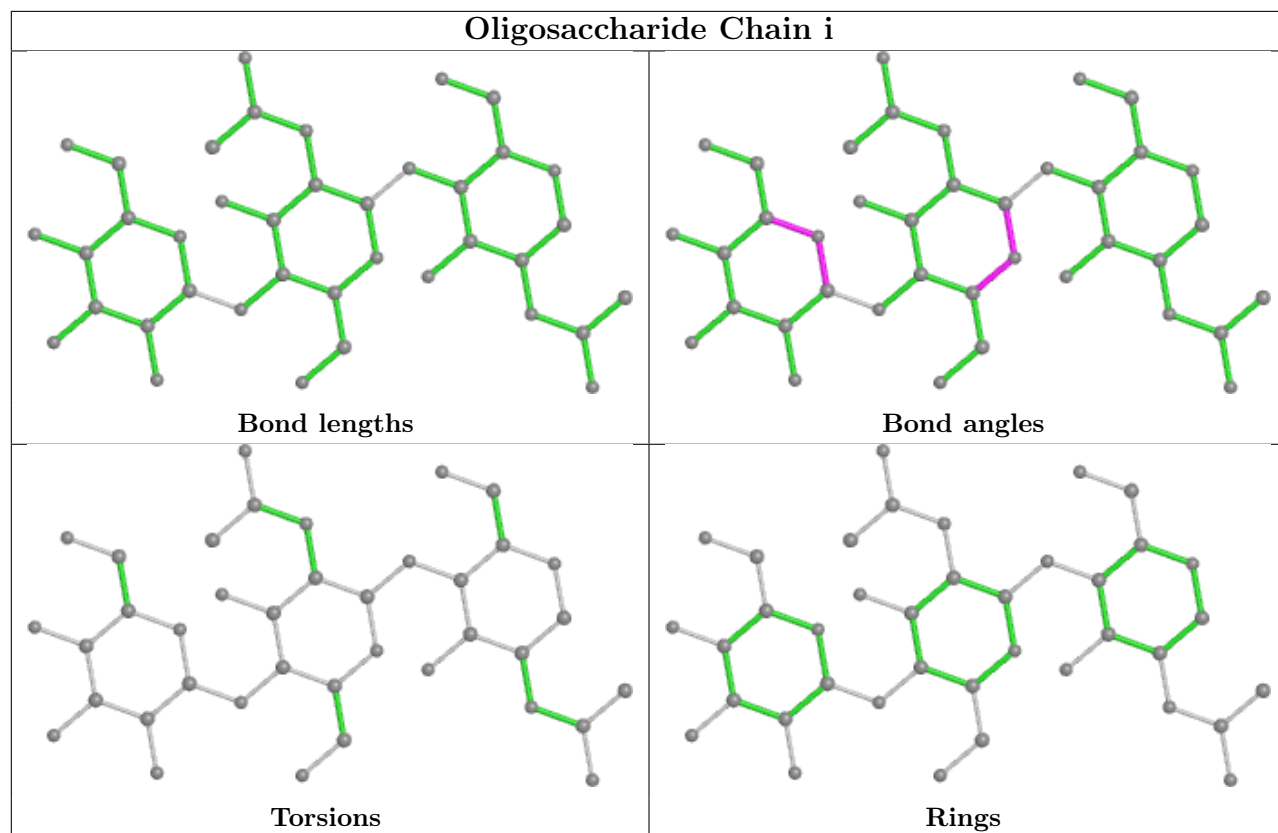


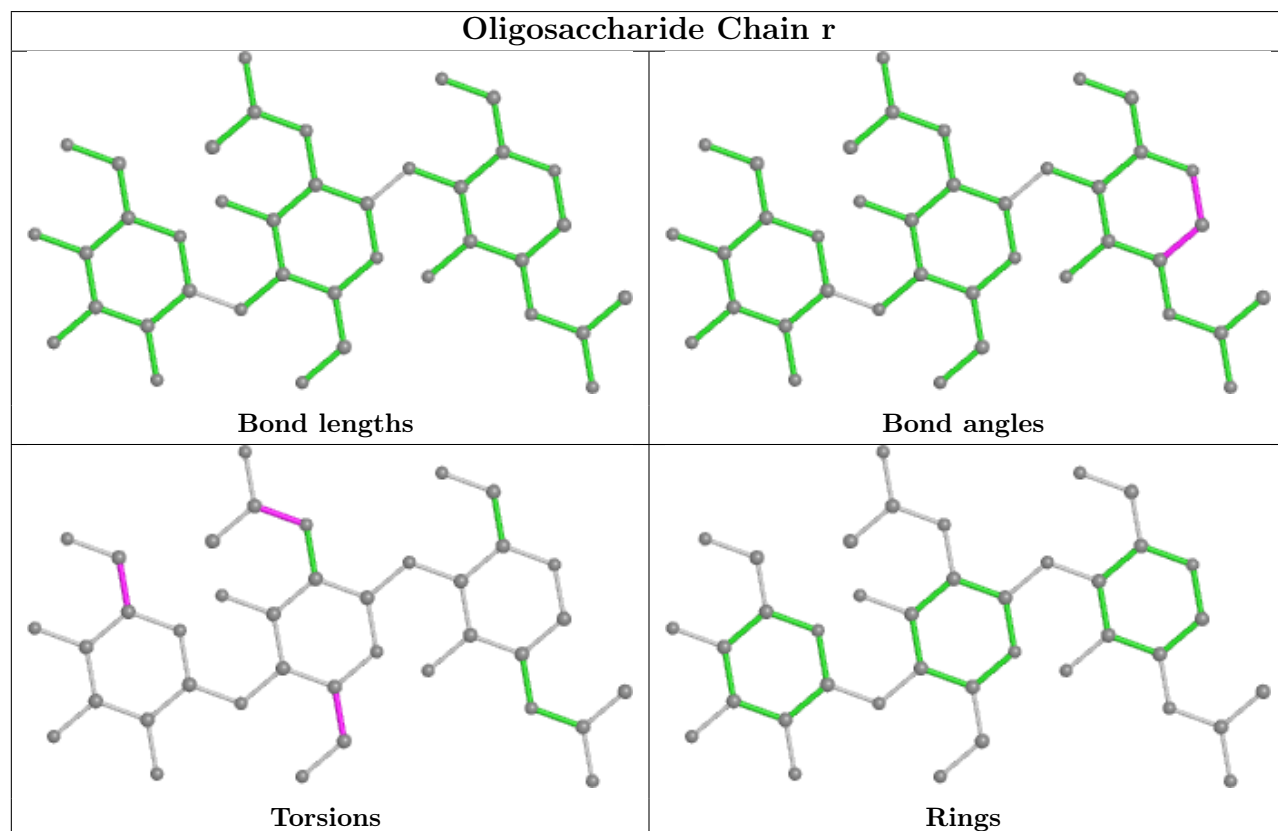
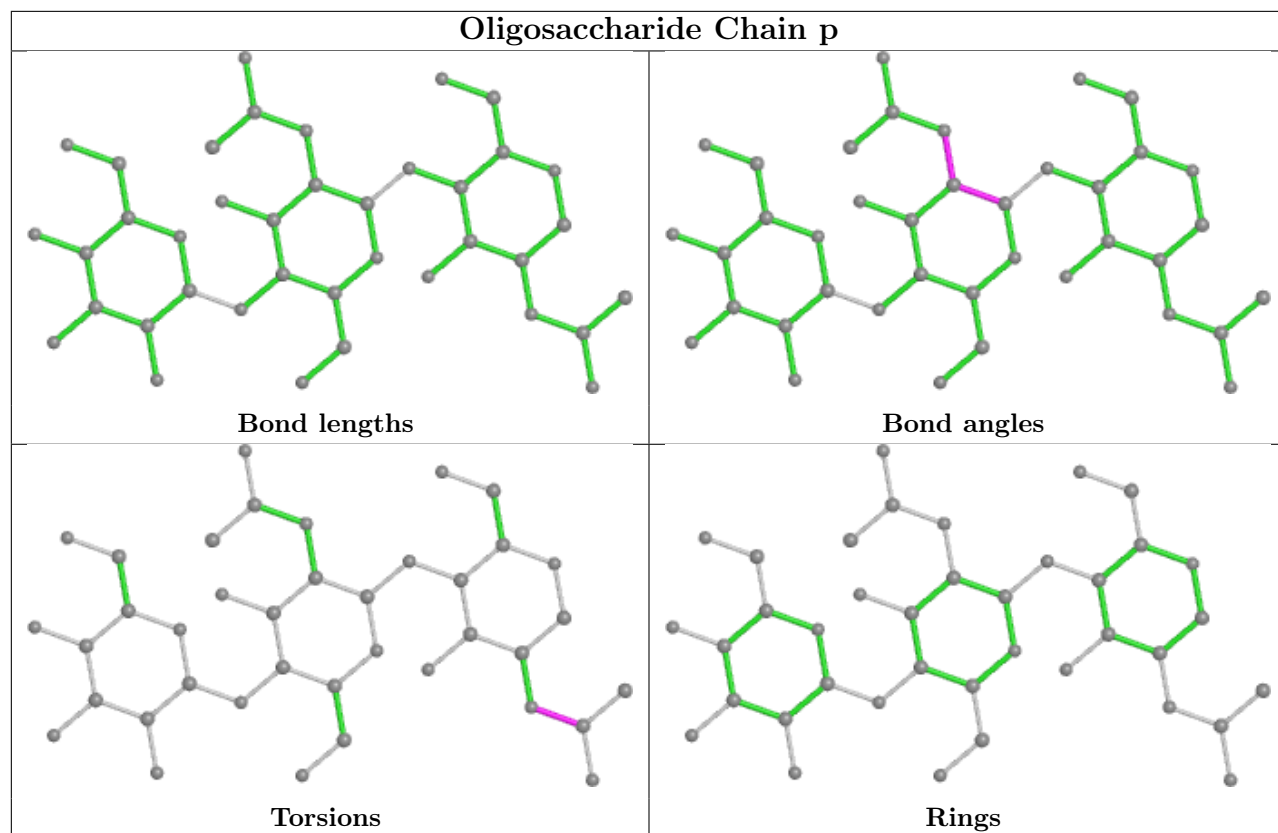


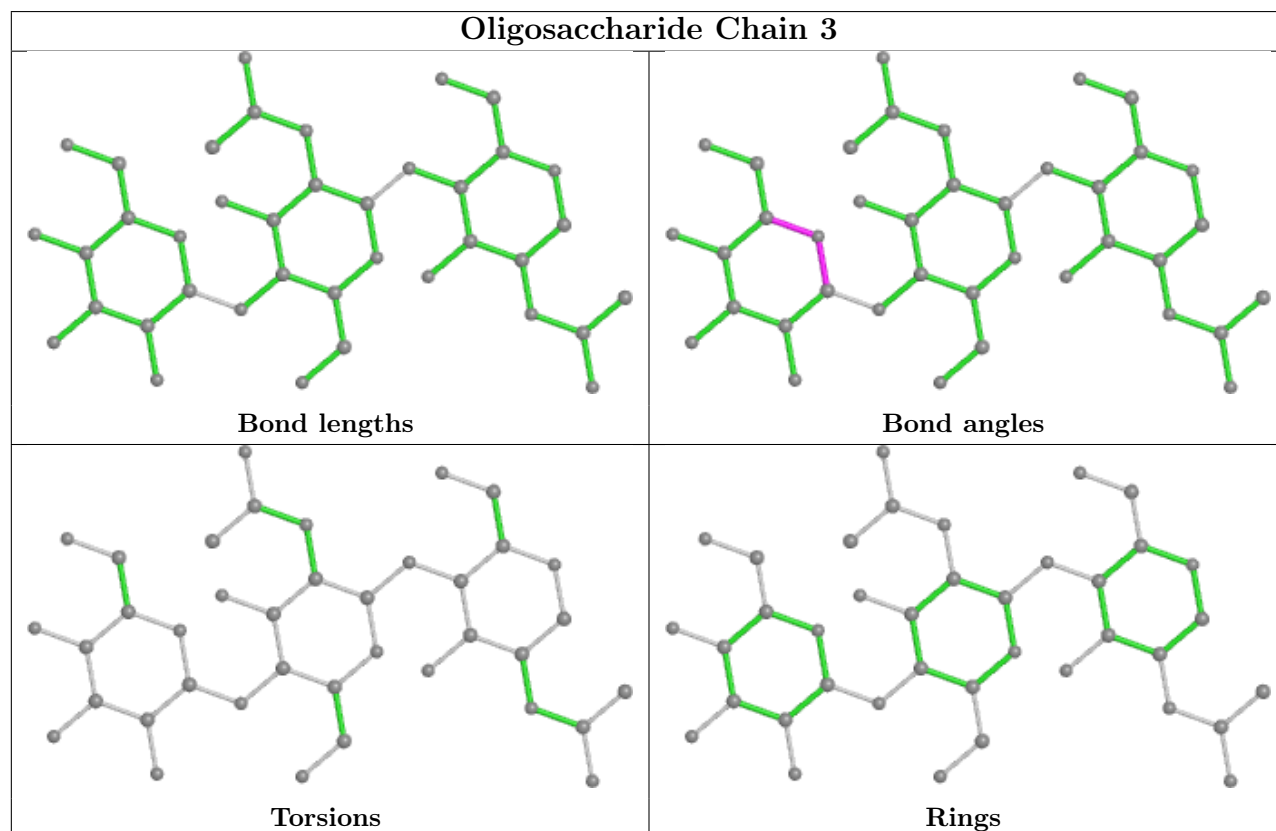
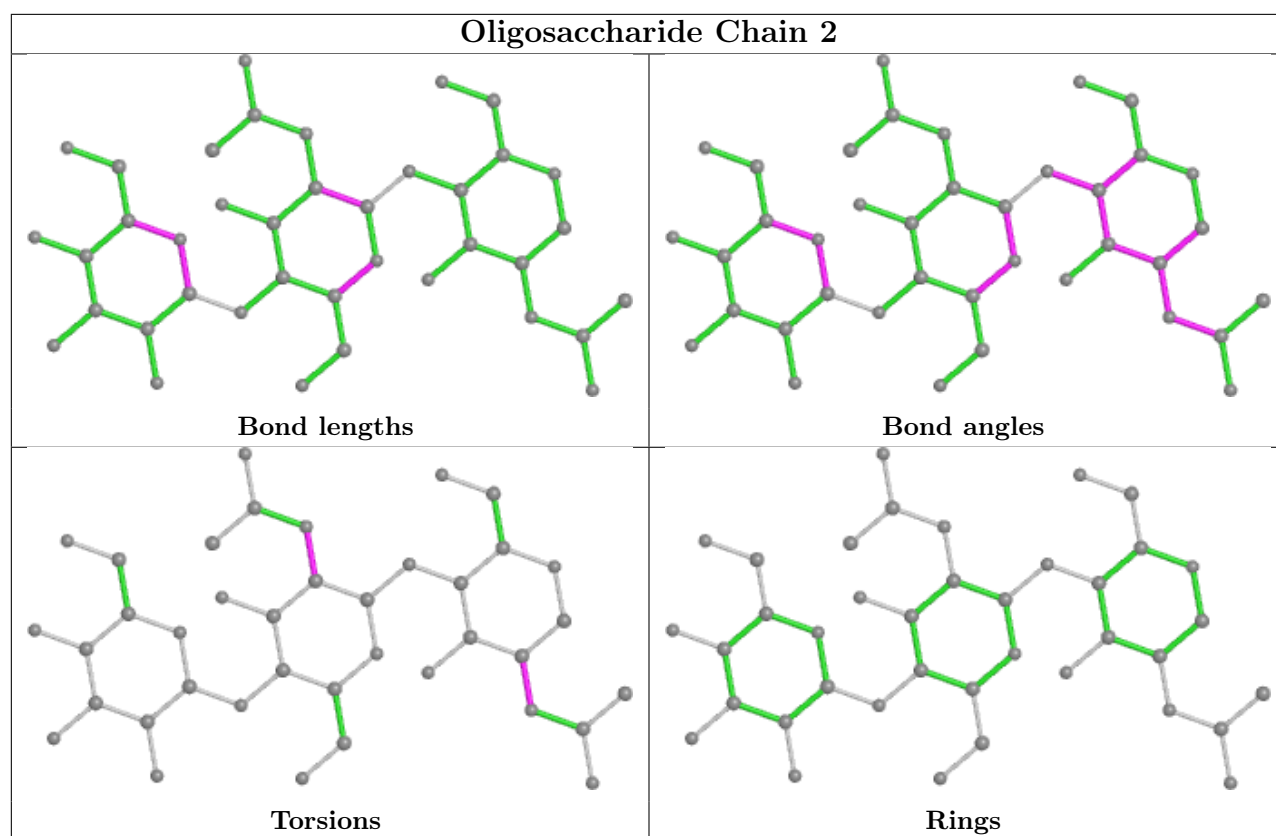


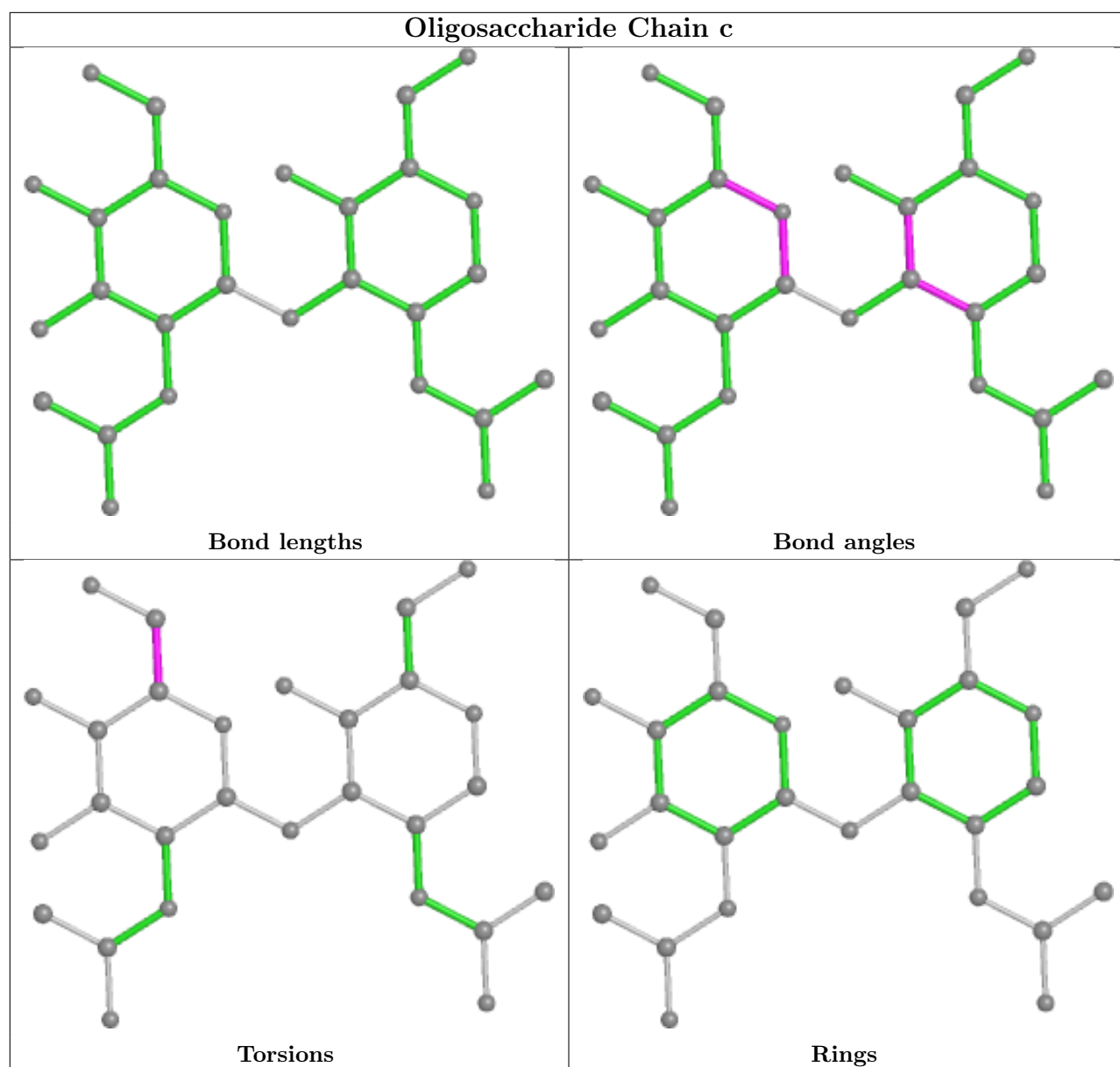


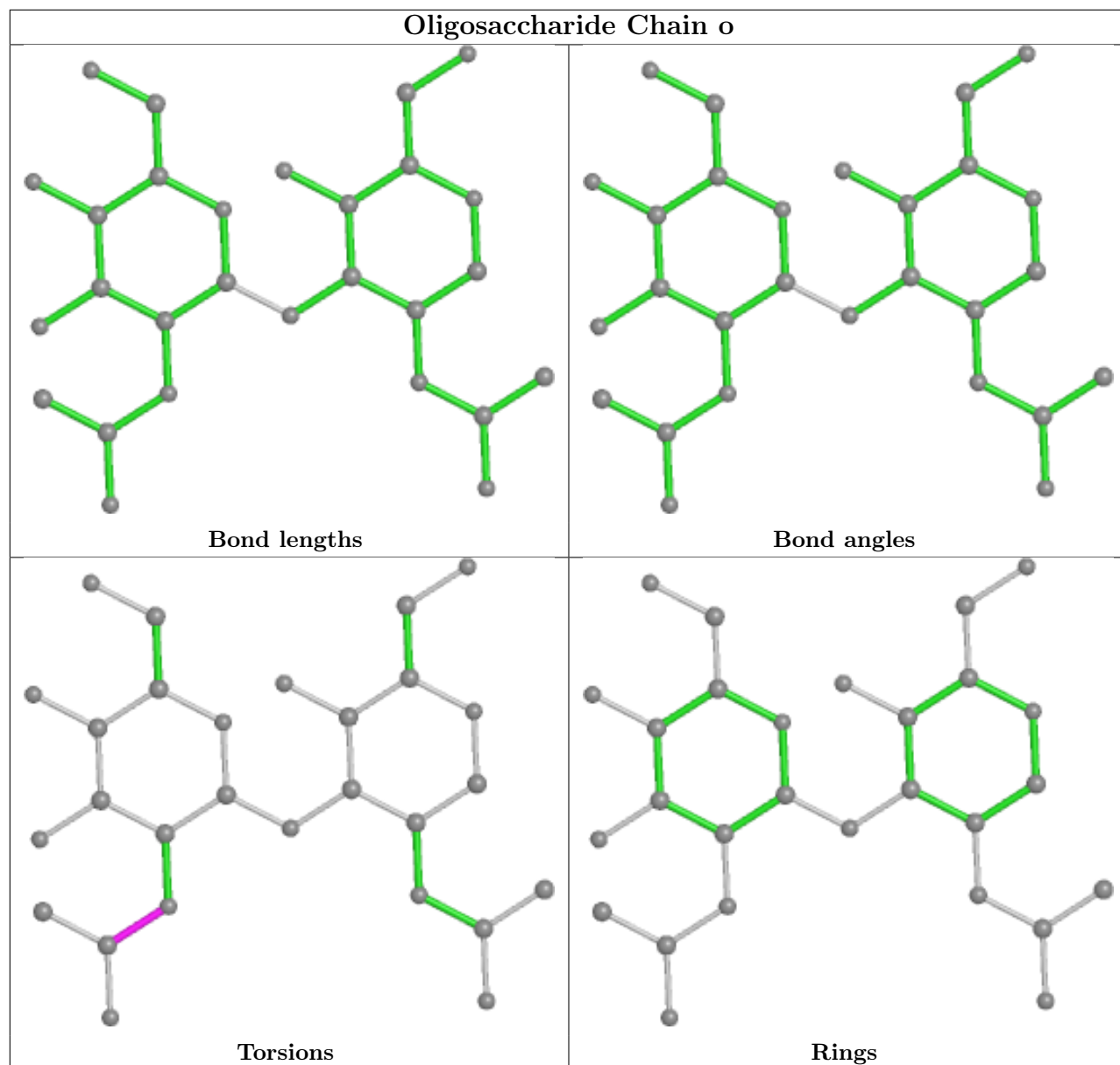


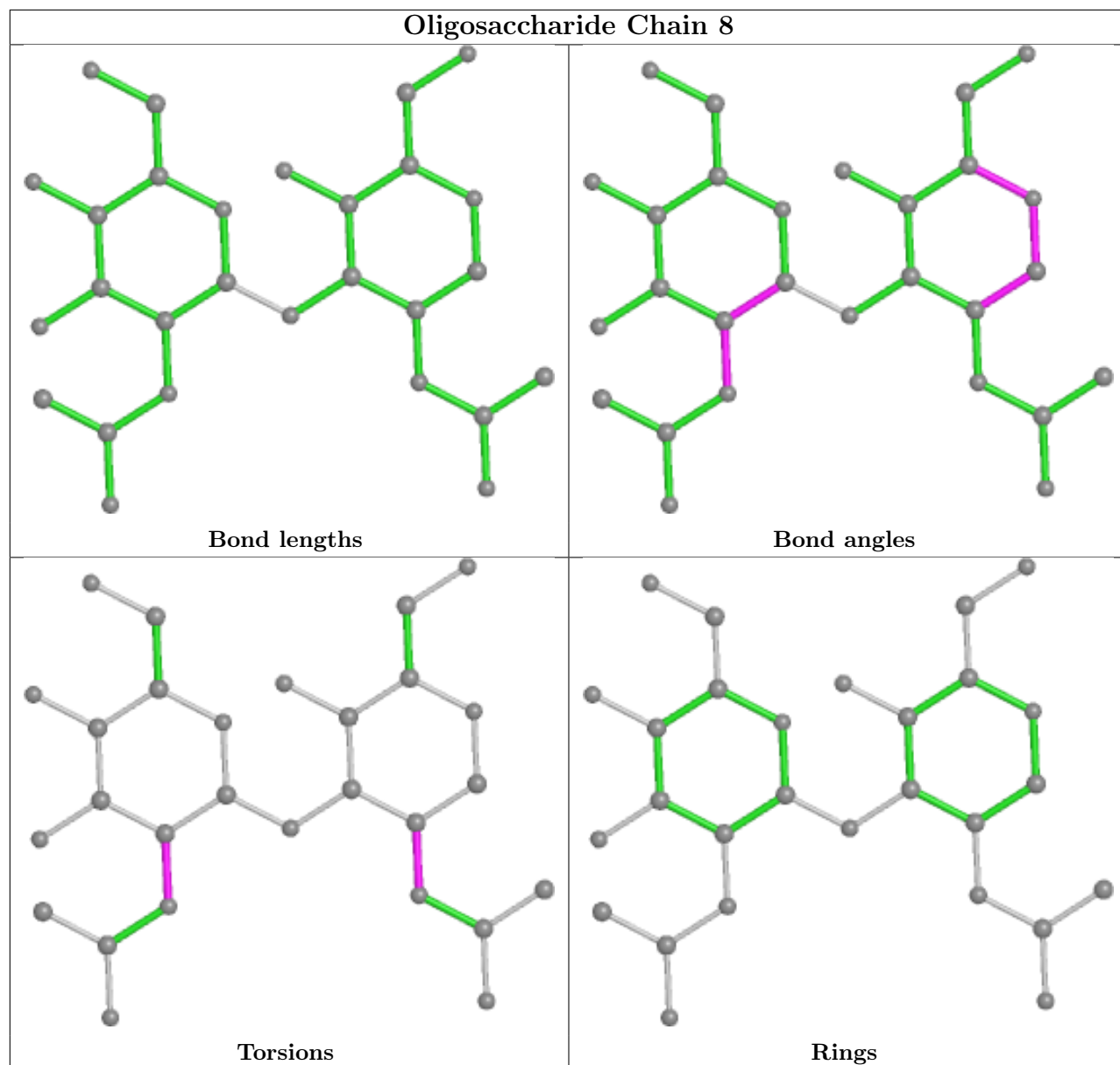


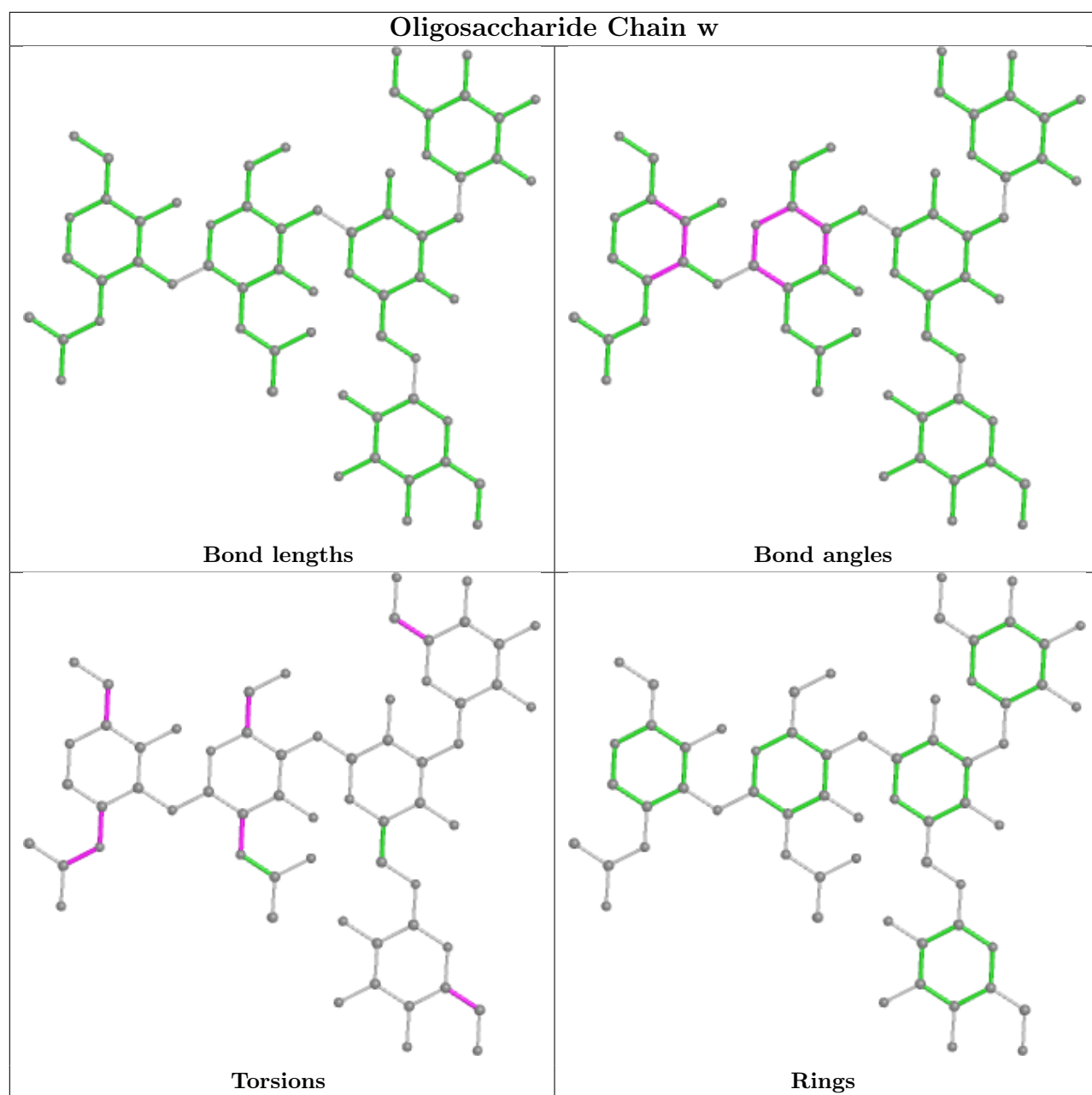


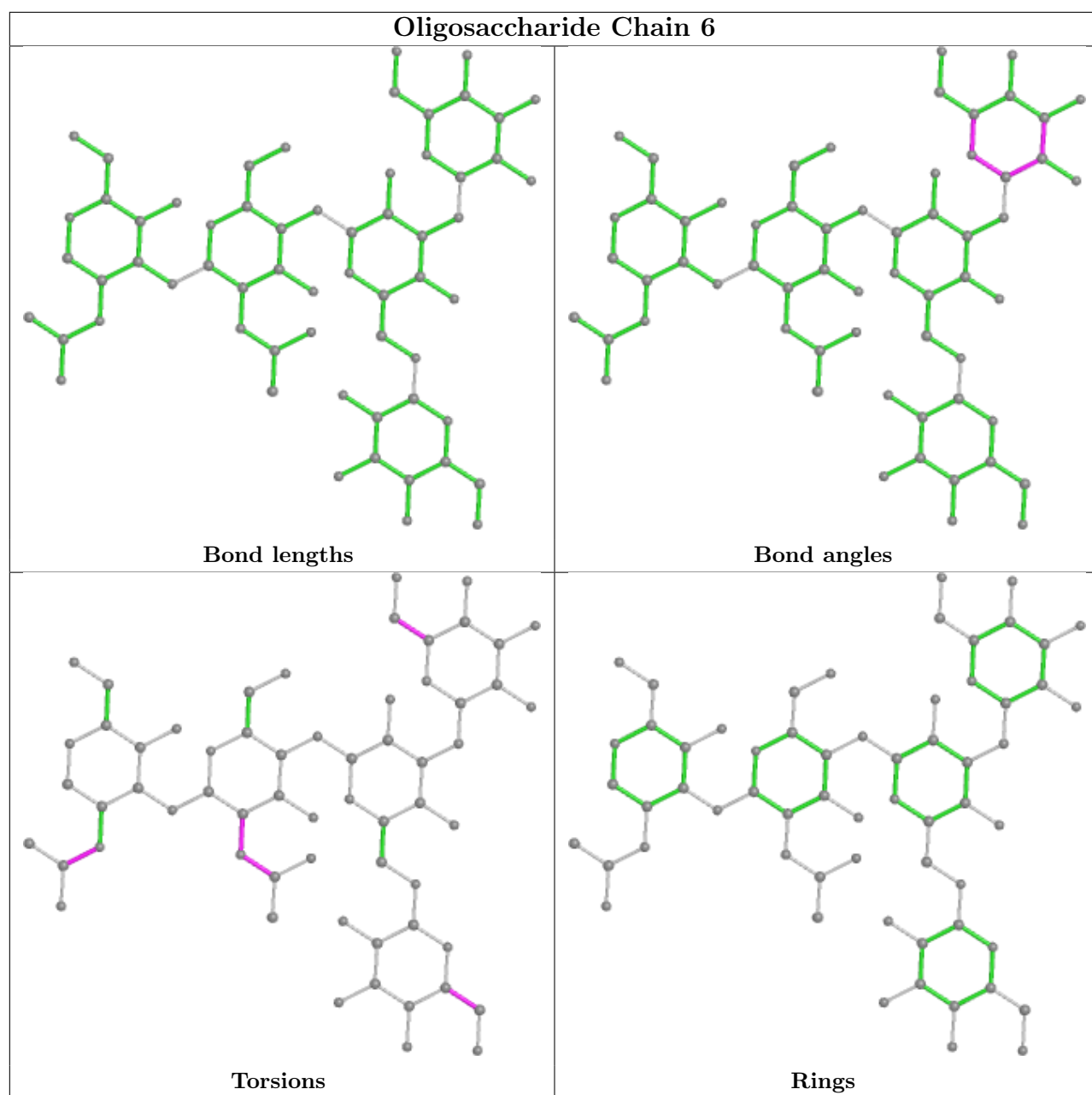


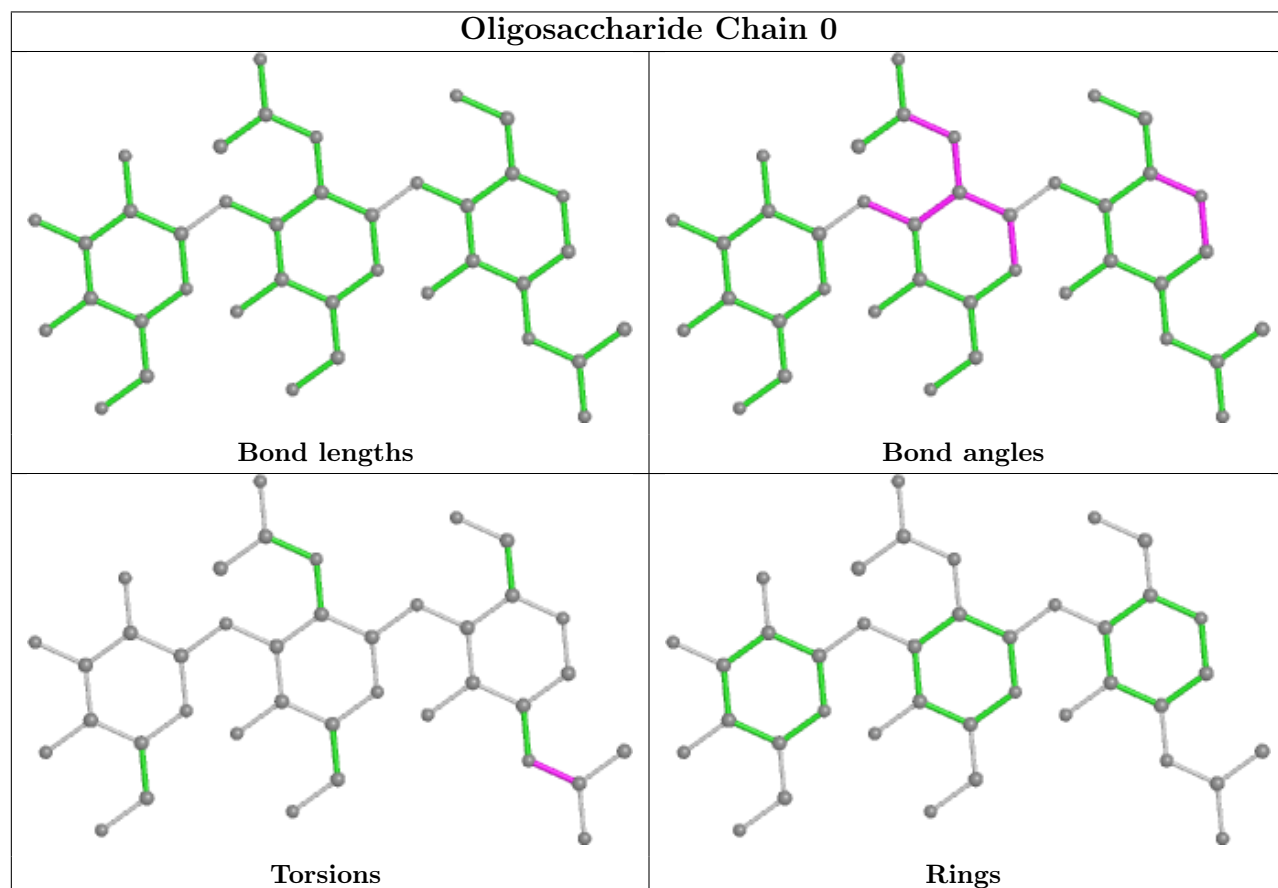
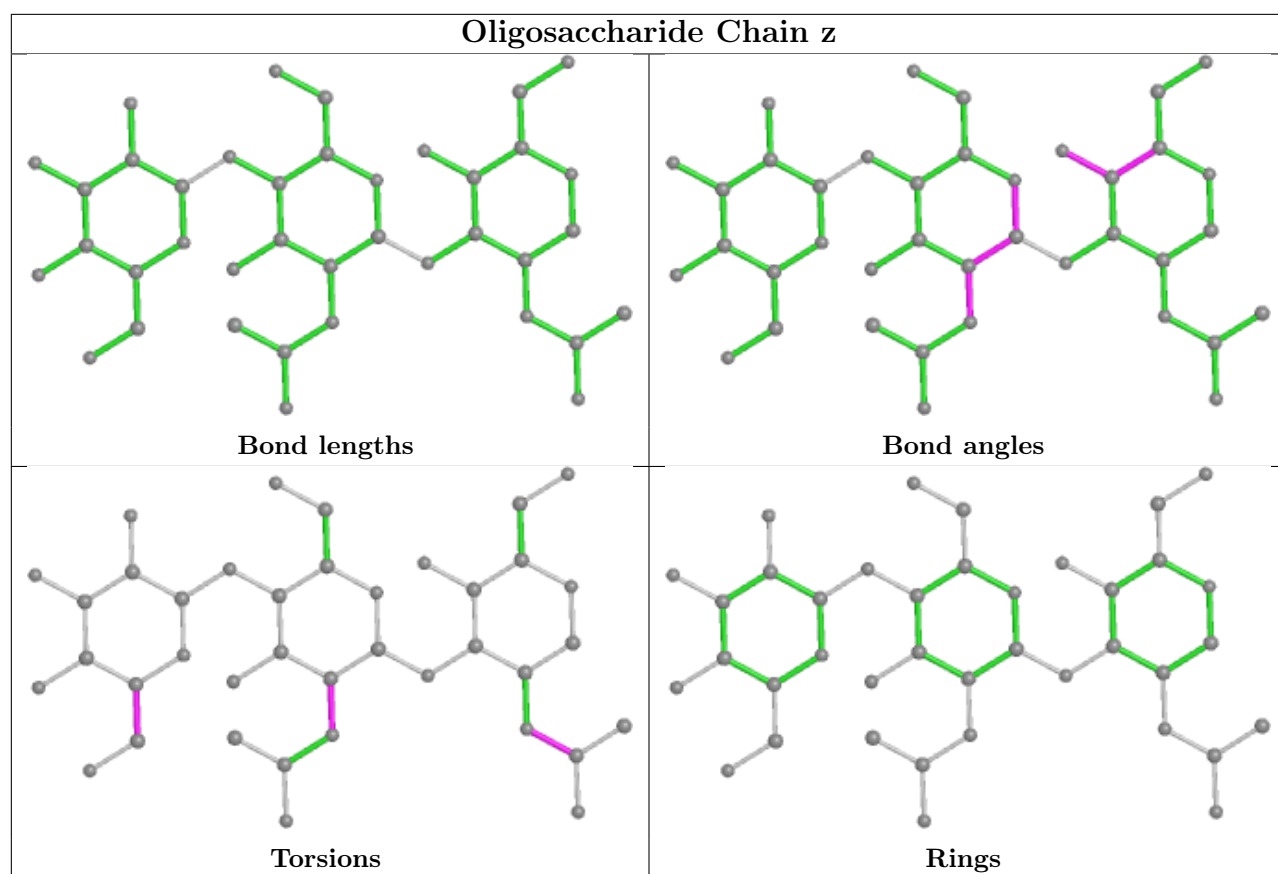


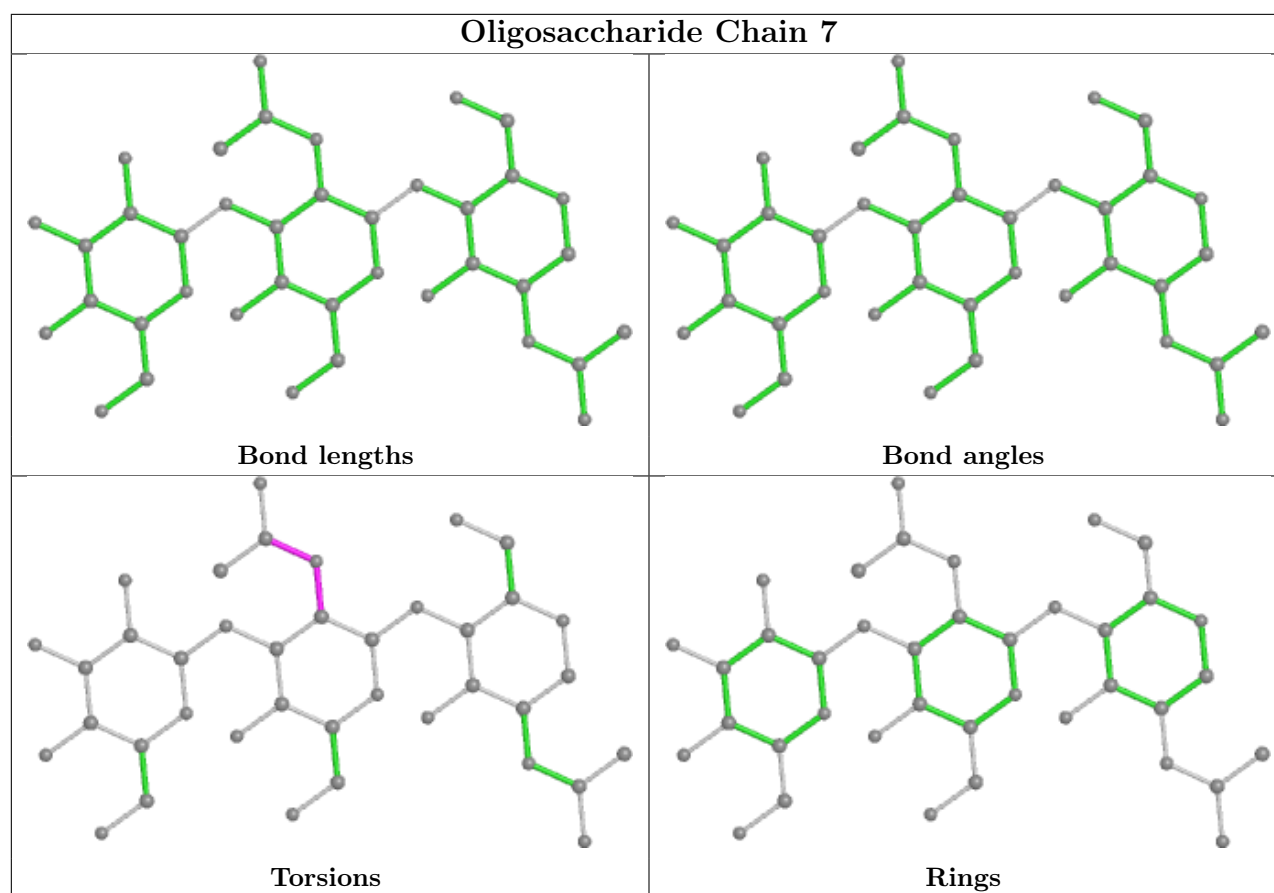












5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 90 are monoatomic - leaving 46 for Mogul analysis.

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	$\# Z > 2$
17	NAG	A	4703	1	14,14,15	0.39	0	17,19,21	0.42	0
17	NAG	B	4704	1	14,14,15	0.90	0	17,19,21	0.98	0
18	A2G	B	4715	1	14,14,15	0.45	0	17,19,21	0.68	0
17	NAG	A	4702	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
18	A2G	B	4712	1	14,14,15	0.46	0	17,19,21	1.41	4 (23%)
17	NAG	B	4708	1	14,14,15	0.50	0	17,19,21	1.01	1 (5%)
18	A2G	A	4719	1	14,14,15	0.50	0	17,19,21	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	A	4706	1	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
17	NAG	A	4711	1	14,14,15	0.39	0	17,19,21	1.19	2 (11%)
18	A2G	A	4712	1	14,14,15	0.47	0	17,19,21	1.73	3 (17%)
17	NAG	A	4705	1	14,14,15	0.51	0	17,19,21	2.13	2 (11%)
17	NAG	A	4707	1	14,14,15	0.40	0	17,19,21	1.36	4 (23%)
18	A2G	B	4716	1	14,14,15	0.51	0	17,19,21	1.11	2 (11%)
18	A2G	A	4720	1	14,14,15	0.46	0	17,19,21	0.51	0
18	A2G	A	4718	1	14,14,15	0.52	0	17,19,21	1.56	3 (17%)
17	NAG	B	4707	1	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
17	NAG	B	4710	1	14,14,15	0.43	0	17,19,21	0.80	0
18	A2G	A	4713	1	14,14,15	0.56	0	17,19,21	0.58	0
17	NAG	B	4703	1	14,14,15	0.40	0	17,19,21	0.41	0
17	NAG	A	4708	1	14,14,15	0.41	0	17,19,21	0.31	0
17	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	0.65	0
18	A2G	A	4716	1	14,14,15	0.99	1 (7%)	17,19,21	1.33	2 (11%)
18	A2G	B	4723	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)
17	NAG	A	4704	1	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
17	NAG	B	4702	1	14,14,15	0.40	0	17,19,21	0.47	0
17	NAG	B	4701	1	14,14,15	0.40	0	17,19,21	0.63	0
17	NAG	B	4711	1	14,14,15	0.43	0	17,19,21	0.67	0
18	A2G	A	4721	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
17	NAG	A	4710	1	14,14,15	0.40	0	17,19,21	0.59	0
18	A2G	A	4723	1	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
18	A2G	B	4722	1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
18	A2G	B	4719	1	14,14,15	0.39	0	17,19,21	1.07	1 (5%)
17	NAG	B	4706	1	14,14,15	0.40	0	17,19,21	0.39	0
18	A2G	B	4713	1	14,14,15	0.52	0	17,19,21	0.65	0
18	A2G	A	4714	1	14,14,15	0.48	0	17,19,21	0.91	1 (5%)
18	A2G	A	4715	1	14,14,15	0.50	0	17,19,21	1.37	1 (5%)
17	NAG	B	4705	1	14,14,15	0.40	0	17,19,21	0.69	0
18	A2G	B	4714	1	14,14,15	0.89	1 (7%)	17,19,21	0.86	1 (5%)
18	A2G	B	4718	1	14,14,15	0.50	0	17,19,21	0.88	0
18	A2G	B	4721	1	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
18	A2G	B	4720	1	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
18	A2G	B	4717	1	14,14,15	0.38	0	17,19,21	0.76	0
17	NAG	B	4709	1	14,14,15	0.98	1 (7%)	17,19,21	0.92	1 (5%)
18	A2G	A	4717	1	14,14,15	0.40	0	17,19,21	0.64	0
18	A2G	A	4722	1	14,14,15	0.51	0	17,19,21	1.55	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	A	4709	1	14,14,15	0.41	0	17,19,21	0.30	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
17	NAG	A	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4704	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4708	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4719	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4706	1	-	1/6/23/26	0/1/1/1
17	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4712	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4705	1	-	3/6/23/26	0/1/1/1
17	NAG	A	4707	1	-	2/6/23/26	0/1/1/1
18	A2G	B	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4718	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4707	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4710	1	-	2/6/23/26	0/1/1/1
18	A2G	A	4713	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4708	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4716	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4723	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4704	1	-	2/6/23/26	0/1/1/1
17	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4701	1	-	3/6/23/26	0/1/1/1
17	NAG	B	4711	1	-	4/6/23/26	0/1/1/1
18	A2G	A	4721	1	-	0/6/23/26	0/1/1/1
17	NAG	A	4710	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4723	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4722	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4719	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4713	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4714	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4715	1	-	0/6/23/26	0/1/1/1
17	NAG	B	4705	1	-	3/6/23/26	0/1/1/1
18	A2G	B	4714	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4718	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4721	1	-	1/6/23/26	0/1/1/1
18	A2G	B	4720	1	-	0/6/23/26	0/1/1/1
18	A2G	B	4717	1	-	1/6/23/26	0/1/1/1
17	NAG	B	4709	1	-	1/6/23/26	0/1/1/1
18	A2G	A	4717	1	-	0/6/23/26	0/1/1/1
18	A2G	A	4722	1	-	2/6/23/26	0/1/1/1
17	NAG	A	4709	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	4709	NAG	O5-C5	2.43	1.48	1.43
18	A	4716	A2G	O5-C5	2.12	1.47	1.43
18	B	4714	A2G	O5-C5	2.07	1.47	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4705	NAG	O5-C1-C2	6.32	121.26	111.29
17	A	4705	NAG	C1-O5-C5	5.74	119.97	112.19
18	A	4712	A2G	C1-C2-N2	4.51	118.19	110.49
18	A	4715	A2G	C1-C2-N2	4.21	117.67	110.49
18	A	4718	A2G	C2-N2-C7	4.01	128.61	122.90
18	B	4722	A2G	C2-N2-C7	3.88	128.43	122.90
18	A	4722	A2G	C2-N2-C7	3.78	128.29	122.90
18	A	4723	A2G	C1-C2-N2	3.76	116.92	110.49
18	A	4722	A2G	C1-C2-N2	3.75	116.89	110.49
17	A	4704	NAG	C1-O5-C5	3.74	117.26	112.19
18	A	4718	A2G	C1-C2-N2	3.74	116.88	110.49
18	B	4712	A2G	O5-C1-C2	3.48	116.79	111.29
17	A	4707	NAG	C1-O5-C5	3.43	116.84	112.19
18	A	4712	A2G	C2-N2-C7	3.42	127.77	122.90
17	A	4711	NAG	C1-O5-C5	3.32	116.69	112.19
18	A	4716	A2G	C2-N2-C7	3.22	127.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	4702	NAG	C1-O5-C5	3.03	116.30	112.19
17	B	4708	NAG	C1-O5-C5	2.99	116.24	112.19
18	B	4712	A2G	C1-O5-C5	-2.89	108.27	112.19
18	A	4712	A2G	O5-C1-C2	2.88	115.84	111.29
18	B	4719	A2G	O5-C1-C2	2.87	115.82	111.29
18	B	4722	A2G	C1-C2-N2	2.86	115.38	110.49
18	A	4719	A2G	O5-C1-C2	2.82	115.75	111.29
17	B	4709	NAG	C1-O5-C5	2.80	115.98	112.19
17	A	4711	NAG	O5-C1-C2	2.79	115.69	111.29
18	B	4716	A2G	C1-O5-C5	-2.78	108.43	112.19
18	A	4716	A2G	O5-C5-C6	2.73	111.48	107.20
18	A	4714	A2G	O5-C1-C2	2.71	115.57	111.29
18	A	4721	A2G	C1-C2-N2	2.56	114.87	110.49
18	B	4716	A2G	O5-C5-C6	2.47	111.07	107.20
18	B	4721	A2G	O5-C5-C6	2.44	111.02	107.20
17	B	4707	NAG	C1-O5-C5	2.41	115.45	112.19
18	B	4720	A2G	C1-O5-C5	-2.37	108.98	112.19
18	B	4712	A2G	O5-C5-C6	2.37	110.92	107.20
17	A	4707	NAG	O5-C1-C2	2.37	115.03	111.29
18	B	4723	A2G	C1-O5-C5	-2.32	109.05	112.19
18	B	4722	A2G	C1-O5-C5	-2.28	109.10	112.19
18	A	4718	A2G	O3-C3-C2	2.16	113.94	109.47
17	A	4706	NAG	C2-N2-C7	2.16	125.98	122.90
18	A	4722	A2G	O3-C3-C2	2.14	113.89	109.47
18	B	4721	A2G	C1-O5-C5	-2.12	109.33	112.19
18	B	4714	A2G	C1-O5-C5	2.02	114.93	112.19
18	B	4712	A2G	O3-C3-C2	2.02	113.64	109.47
18	A	4719	A2G	C1-O5-C5	-2.02	109.46	112.19
17	A	4707	NAG	O5-C5-C6	2.01	110.36	107.20
17	A	4707	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	4705	NAG	C3-C2-N2-C7
17	A	4705	NAG	C8-C7-N2-C2
17	A	4705	NAG	O7-C7-N2-C2
17	A	4708	NAG	C8-C7-N2-C2
17	A	4708	NAG	O7-C7-N2-C2
17	B	4711	NAG	C8-C7-N2-C2
17	B	4711	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
18	A	4718	A2G	C3-C2-N2-C7
18	A	4722	A2G	C3-C2-N2-C7
17	A	4709	NAG	C8-C7-N2-C2
17	A	4709	NAG	O7-C7-N2-C2
17	B	4701	NAG	C8-C7-N2-C2
17	B	4705	NAG	C8-C7-N2-C2
17	B	4711	NAG	C1-C2-N2-C7
17	A	4707	NAG	O5-C5-C6-O6
17	B	4701	NAG	O7-C7-N2-C2
17	B	4705	NAG	O7-C7-N2-C2
18	B	4723	A2G	O5-C5-C6-O6
18	B	4716	A2G	O5-C5-C6-O6
17	B	4710	NAG	C4-C5-C6-O6
17	B	4701	NAG	C1-C2-N2-C7
17	B	4705	NAG	C1-C2-N2-C7
17	B	4711	NAG	O5-C5-C6-O6
17	A	4707	NAG	C4-C5-C6-O6
18	A	4719	A2G	C1-C2-N2-C7
18	B	4721	A2G	O5-C5-C6-O6
18	A	4722	A2G	O5-C5-C6-O6
18	B	4714	A2G	O5-C5-C6-O6
18	B	4718	A2G	O5-C5-C6-O6
18	B	4712	A2G	O5-C5-C6-O6
18	A	4712	A2G	C3-C2-N2-C7
18	B	4722	A2G	C3-C2-N2-C7
17	B	4710	NAG	O5-C5-C6-O6
18	B	4712	A2G	C1-C2-N2-C7
17	A	4704	NAG	C1-C2-N2-C7
17	A	4706	NAG	C3-C2-N2-C7
18	A	4716	A2G	C3-C2-N2-C7
17	B	4709	NAG	O5-C5-C6-O6
18	B	4719	A2G	C1-C2-N2-C7
18	B	4723	A2G	C4-C5-C6-O6
18	A	4712	A2G	C4-C5-C6-O6
18	B	4717	A2G	C4-C5-C6-O6
17	A	4704	NAG	C3-C2-N2-C7
18	A	4718	A2G	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	4707	NAG	1	0
17	A	4710	NAG	1	0

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.

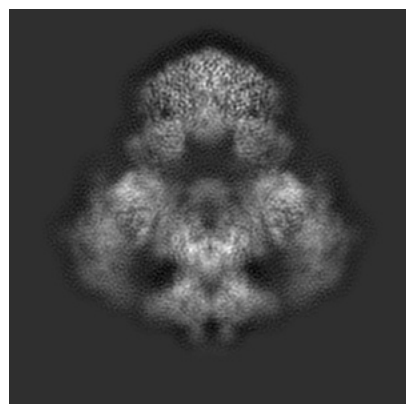
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36663. These allow visual inspection of the internal detail of the map and identification of artifacts.

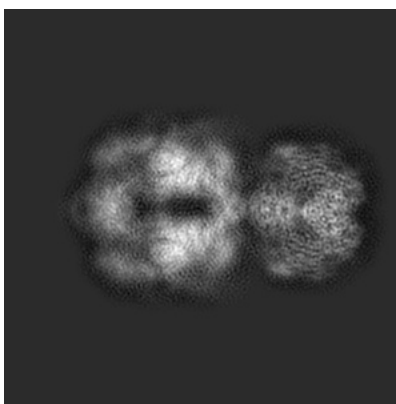
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

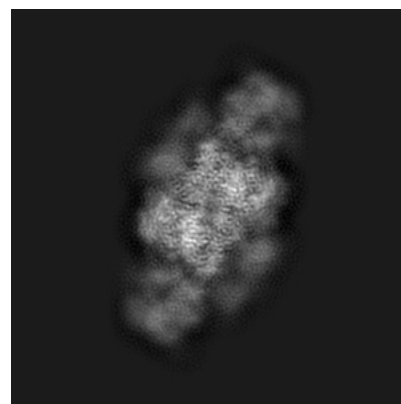
6.1.1 Primary map



X

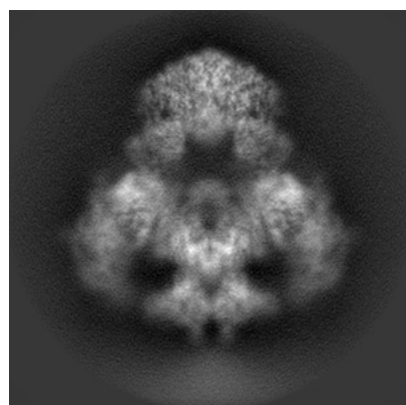


Y

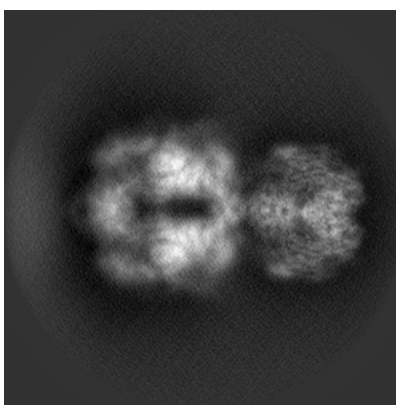


Z

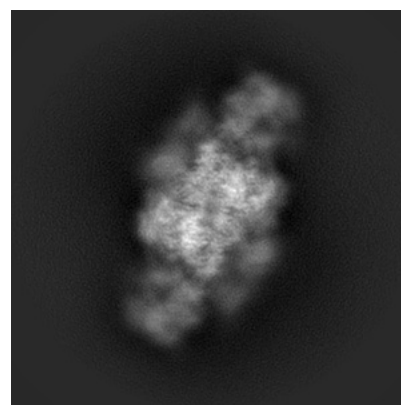
6.1.2 Raw map



X



Y

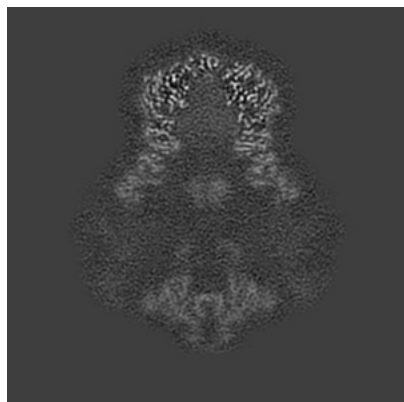


Z

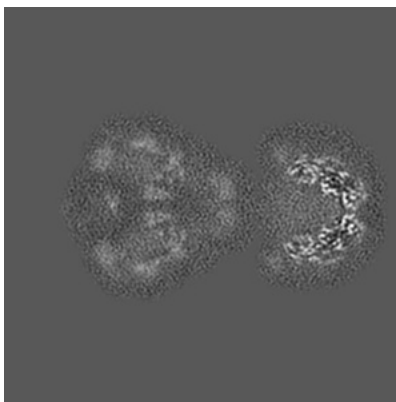
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

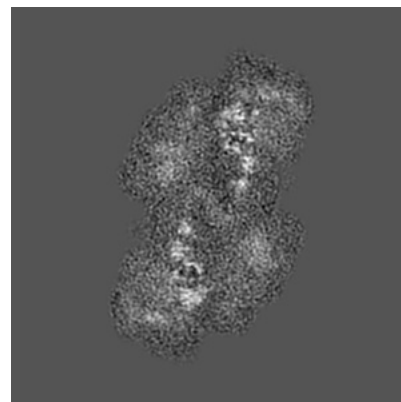
6.2.1 Primary map



X Index: 130

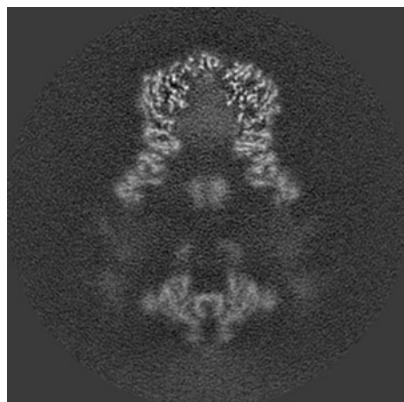


Y Index: 130

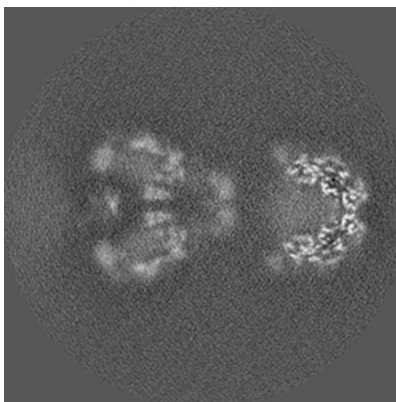


Z Index: 130

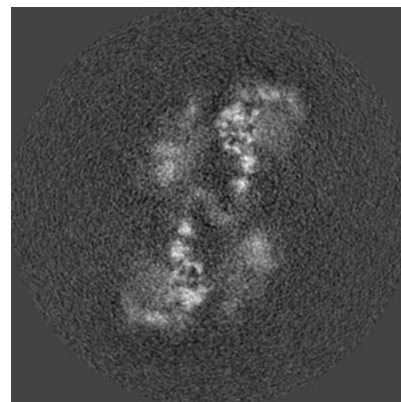
6.2.2 Raw map



X Index: 130



Y Index: 130

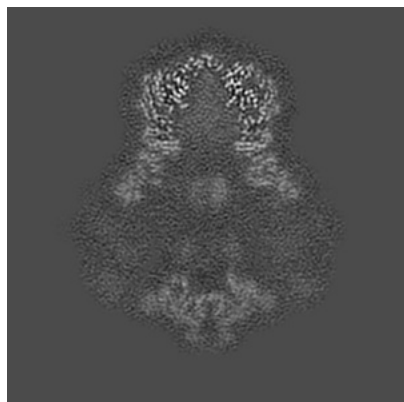


Z Index: 130

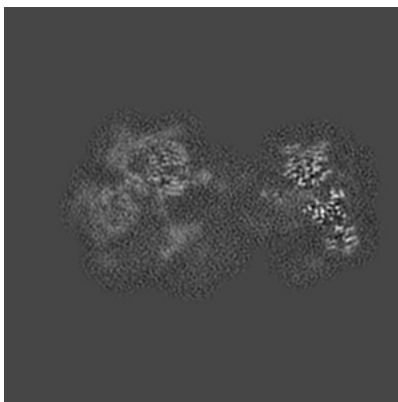
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

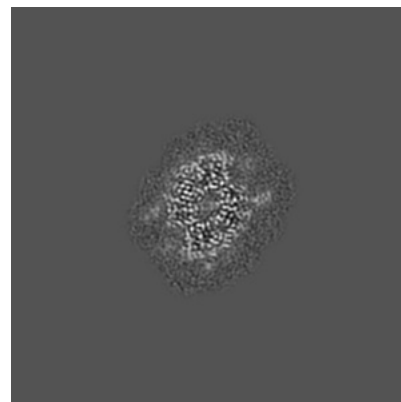
6.3.1 Primary map



X Index: 129

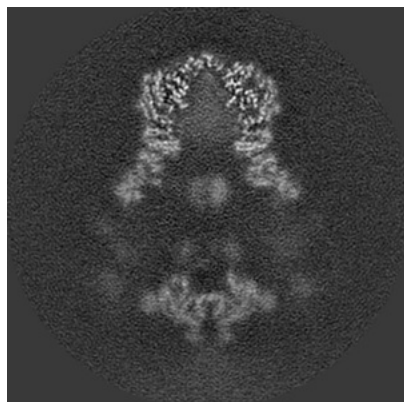


Y Index: 145

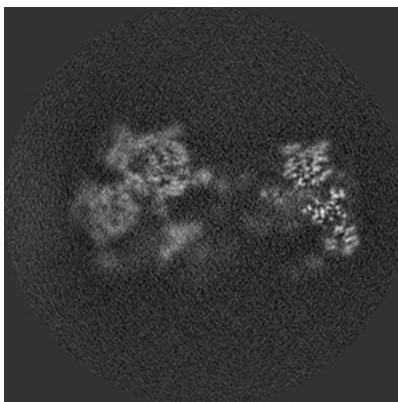


Z Index: 215

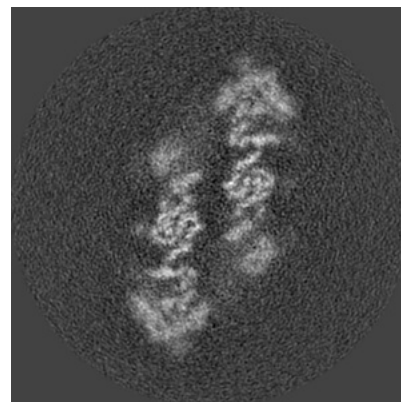
6.3.2 Raw map



X Index: 129



Y Index: 145

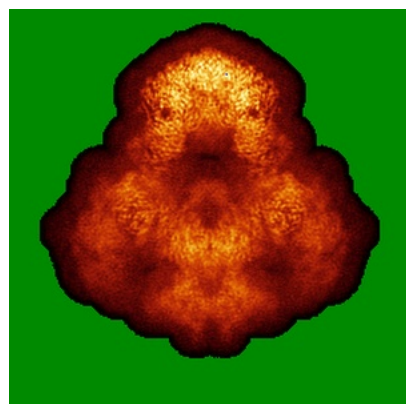


Z Index: 115

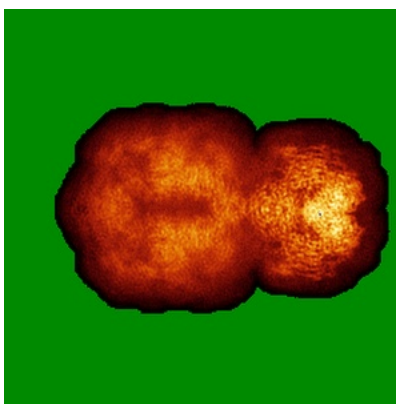
The images above show the largest variance slices of the map in three orthogonal directions.

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

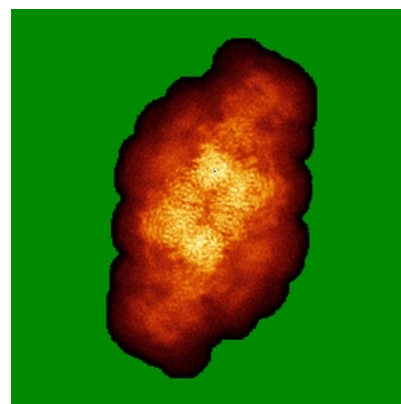
6.4.1 Primary map



X

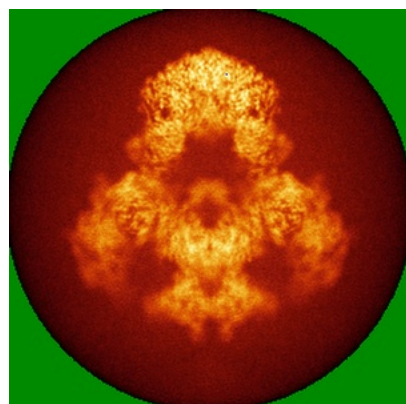


Y

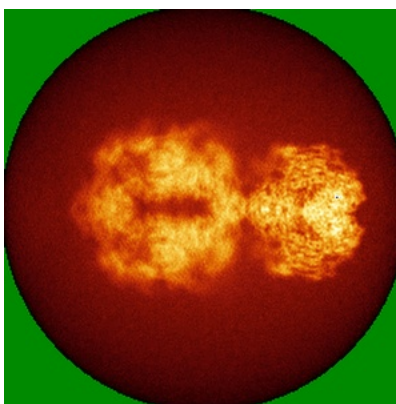


Z

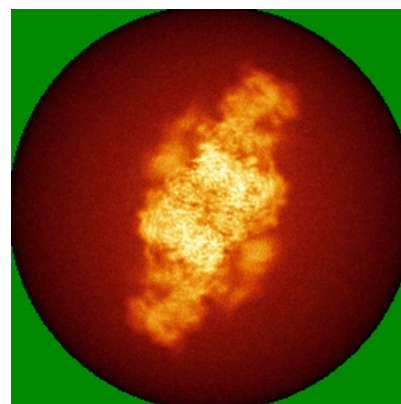
6.4.2 Raw map



X



Y

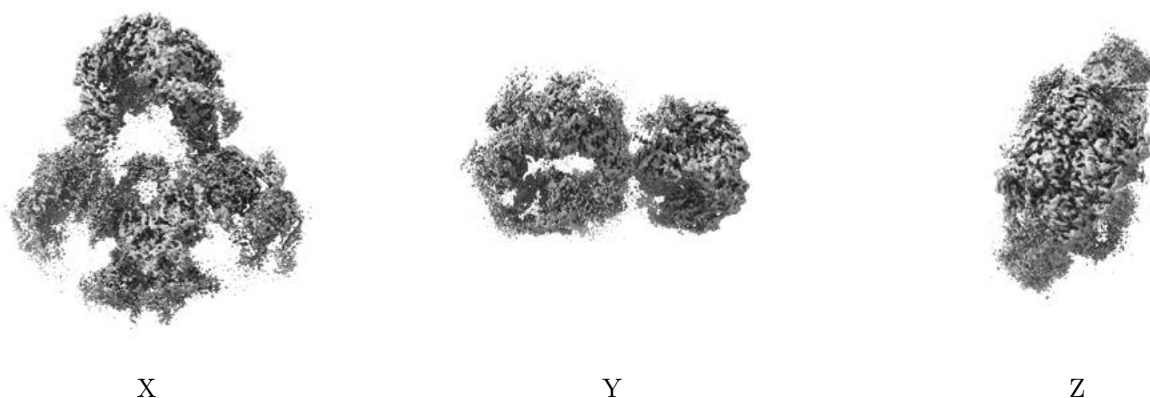


Z

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.

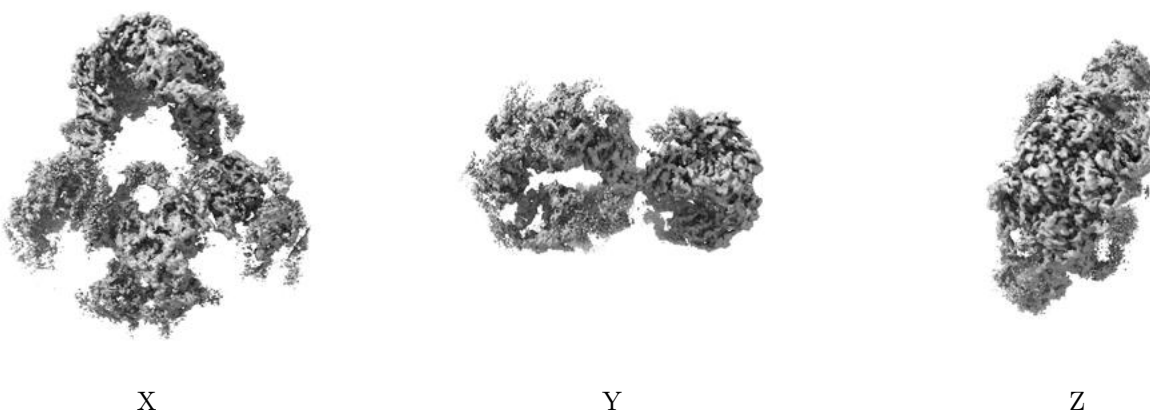
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0242. 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.

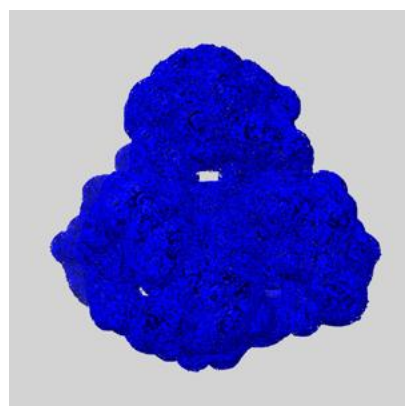
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

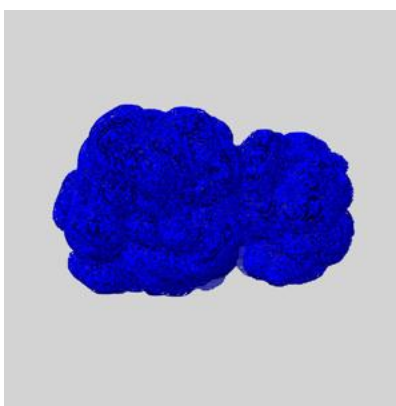
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

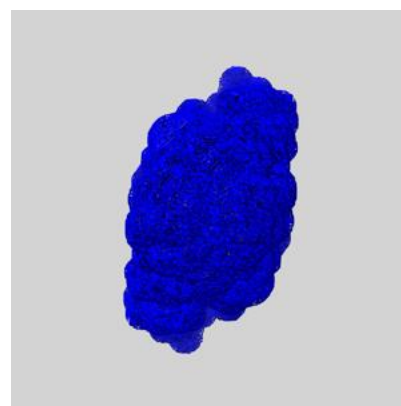
6.6.1 emd_36663_msk_1.map [i](#)



X



Y

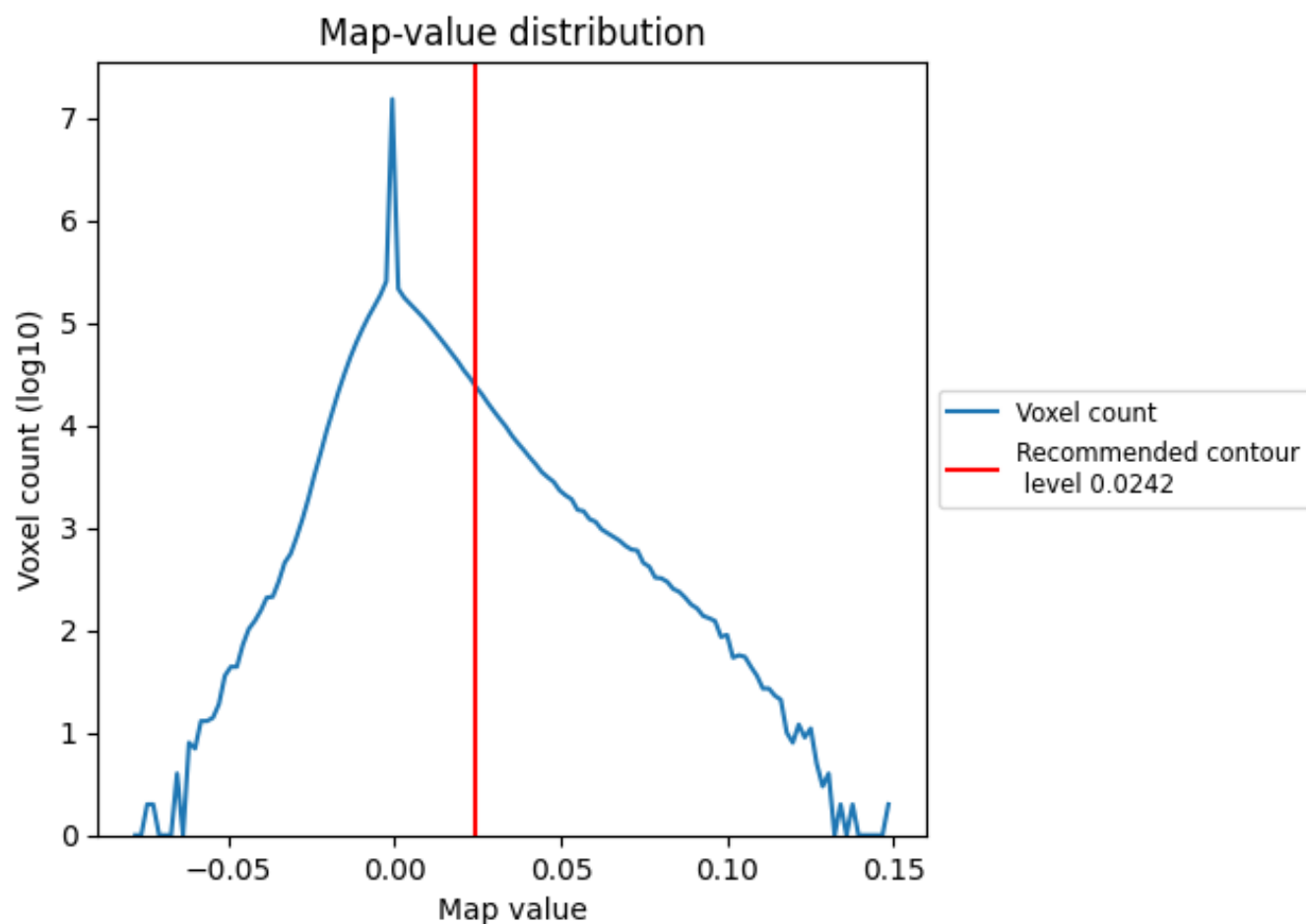


Z

7 Map analysis [i](#)

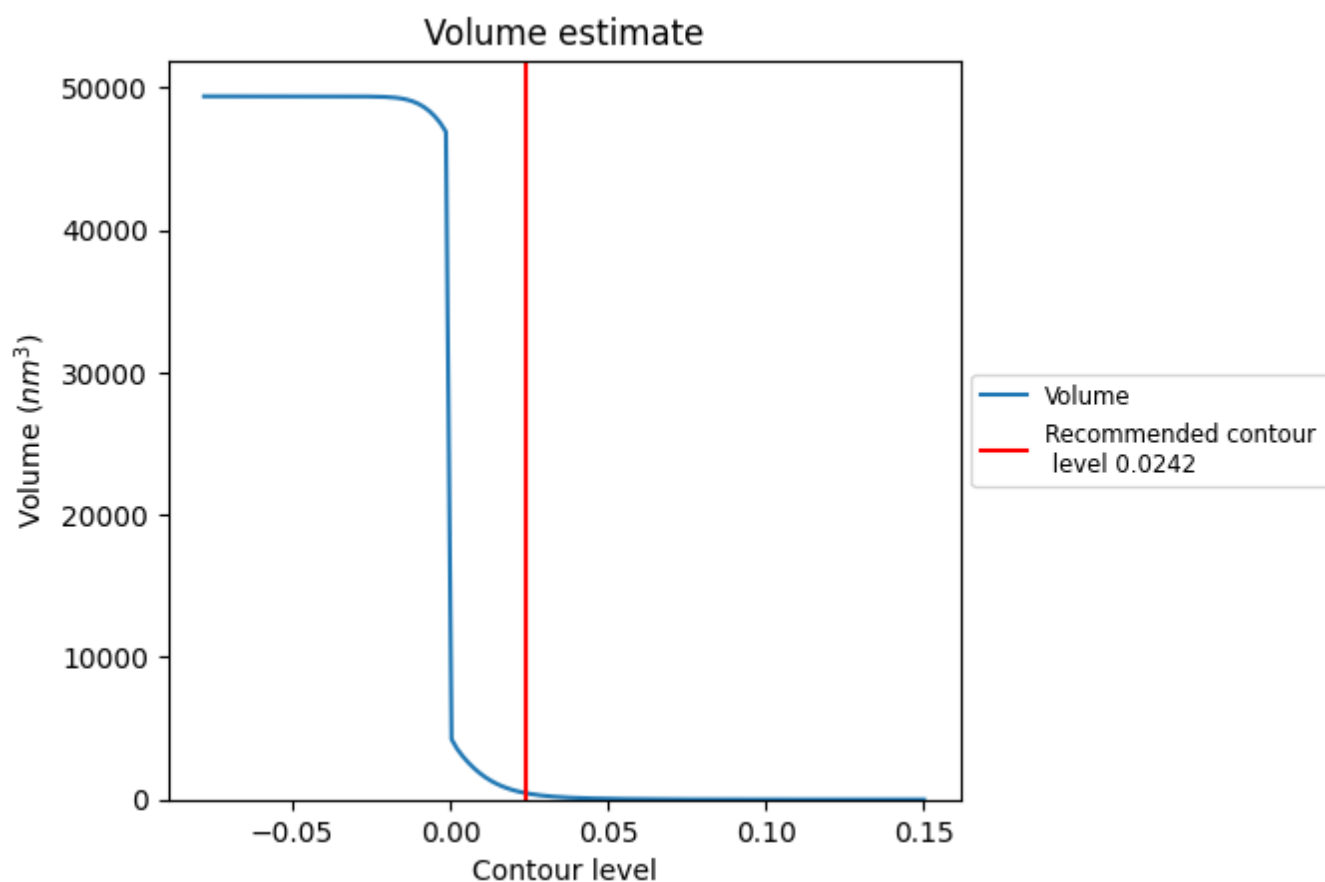
This section contains the results of statistical analysis of the map.

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.

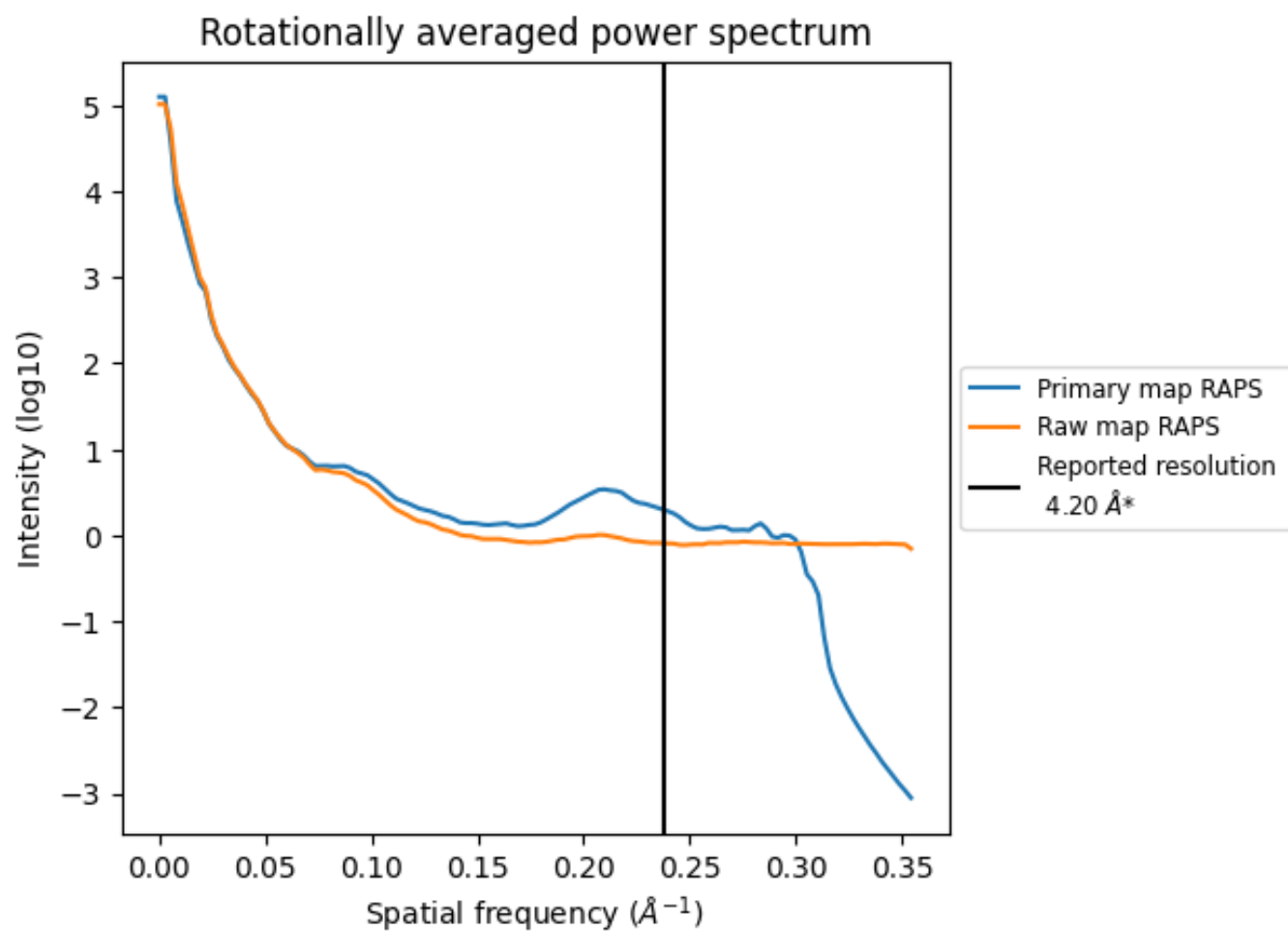
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 445 nm³; this corresponds to an approximate mass of 402 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

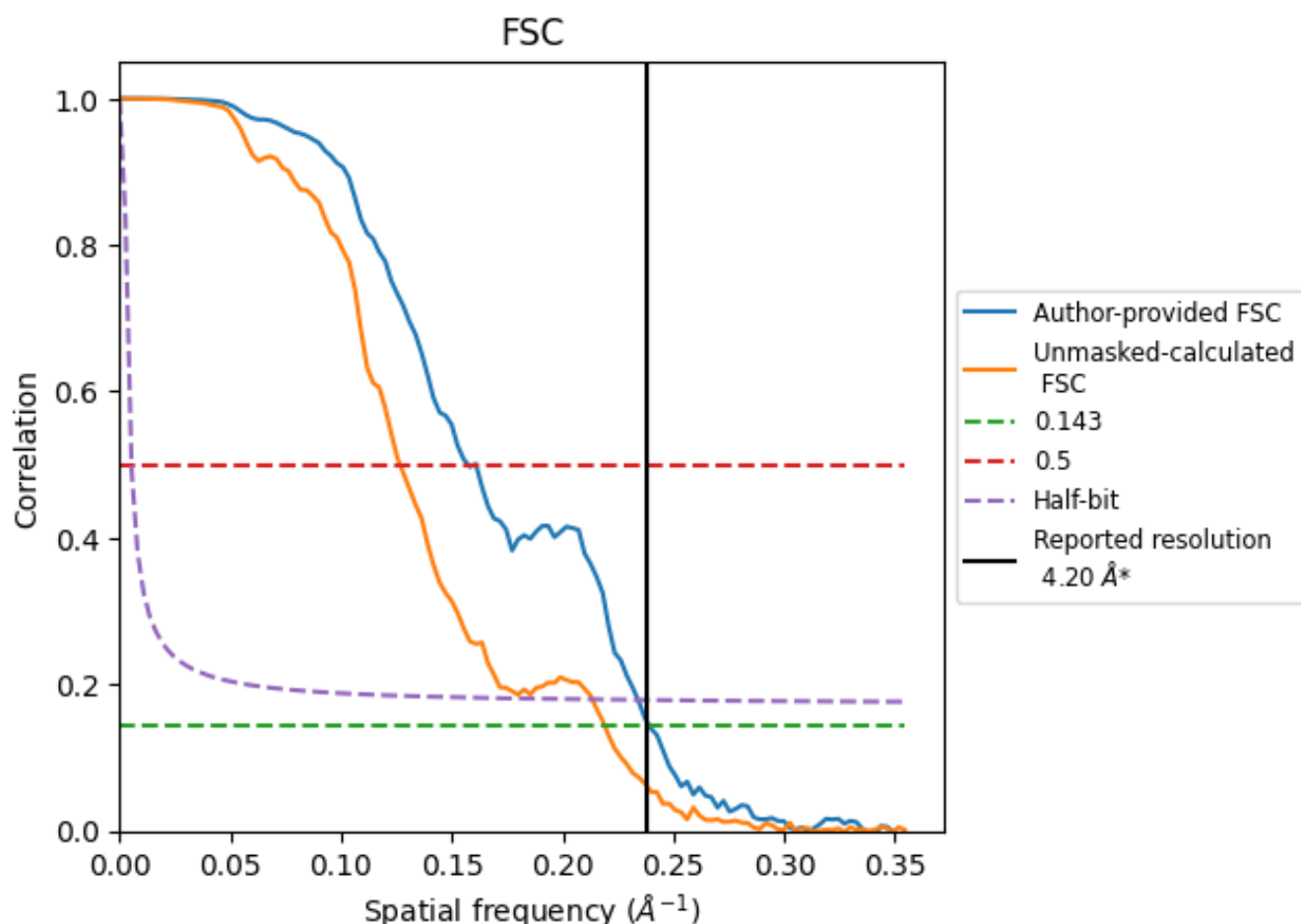


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

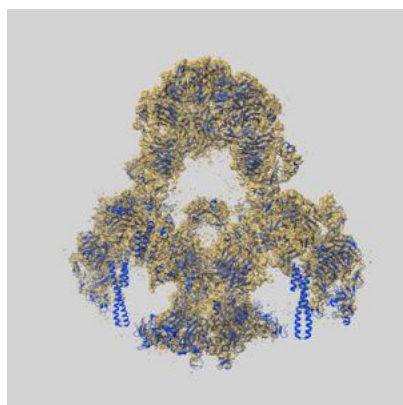
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.36	4.27
Unmasked-calculated*	4.57	7.90	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

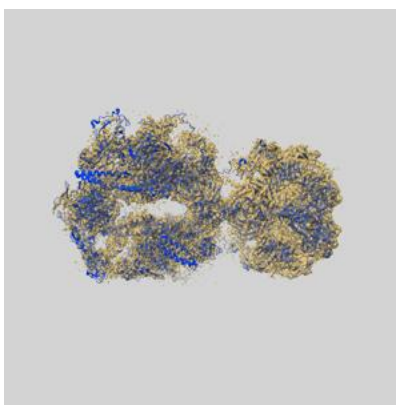
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36663 and PDB model 8JUT. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

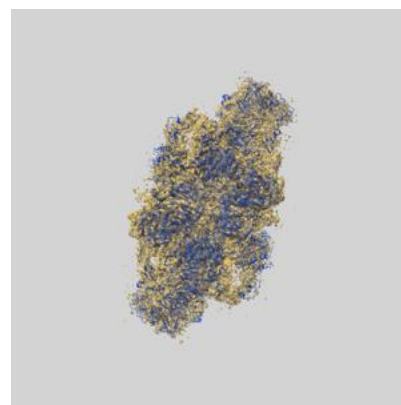
9.1 Map-model overlay [i](#)



X



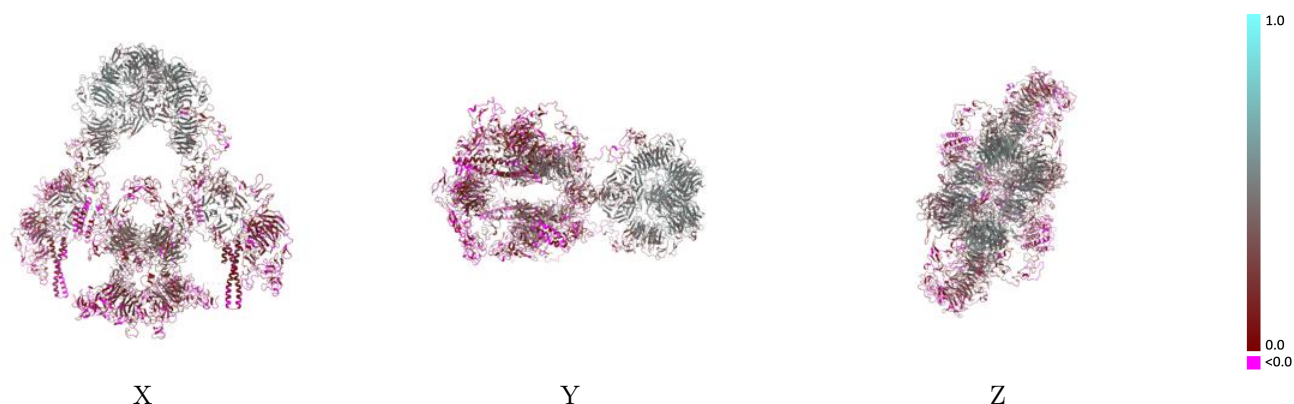
Y



Z

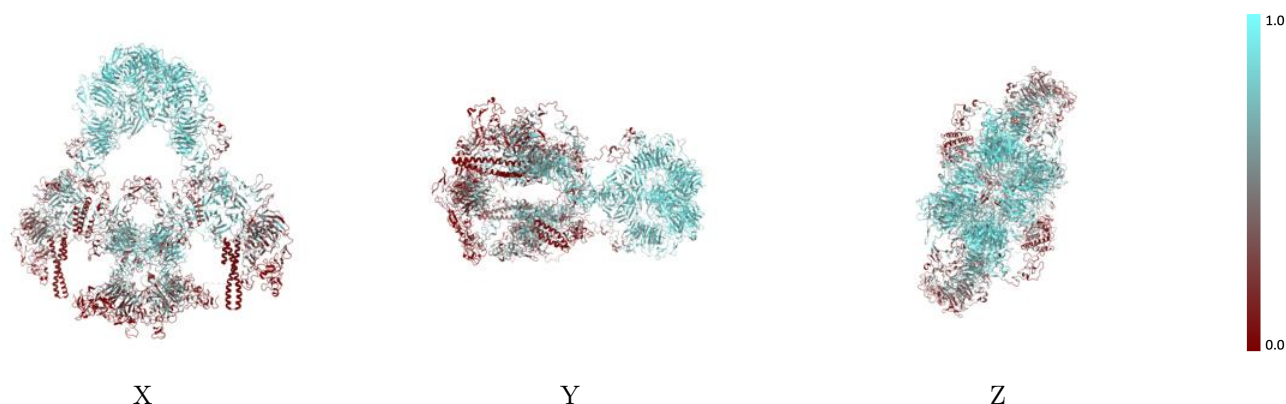
The images above show the 3D surface view of the map at the recommended contour level 0.0242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



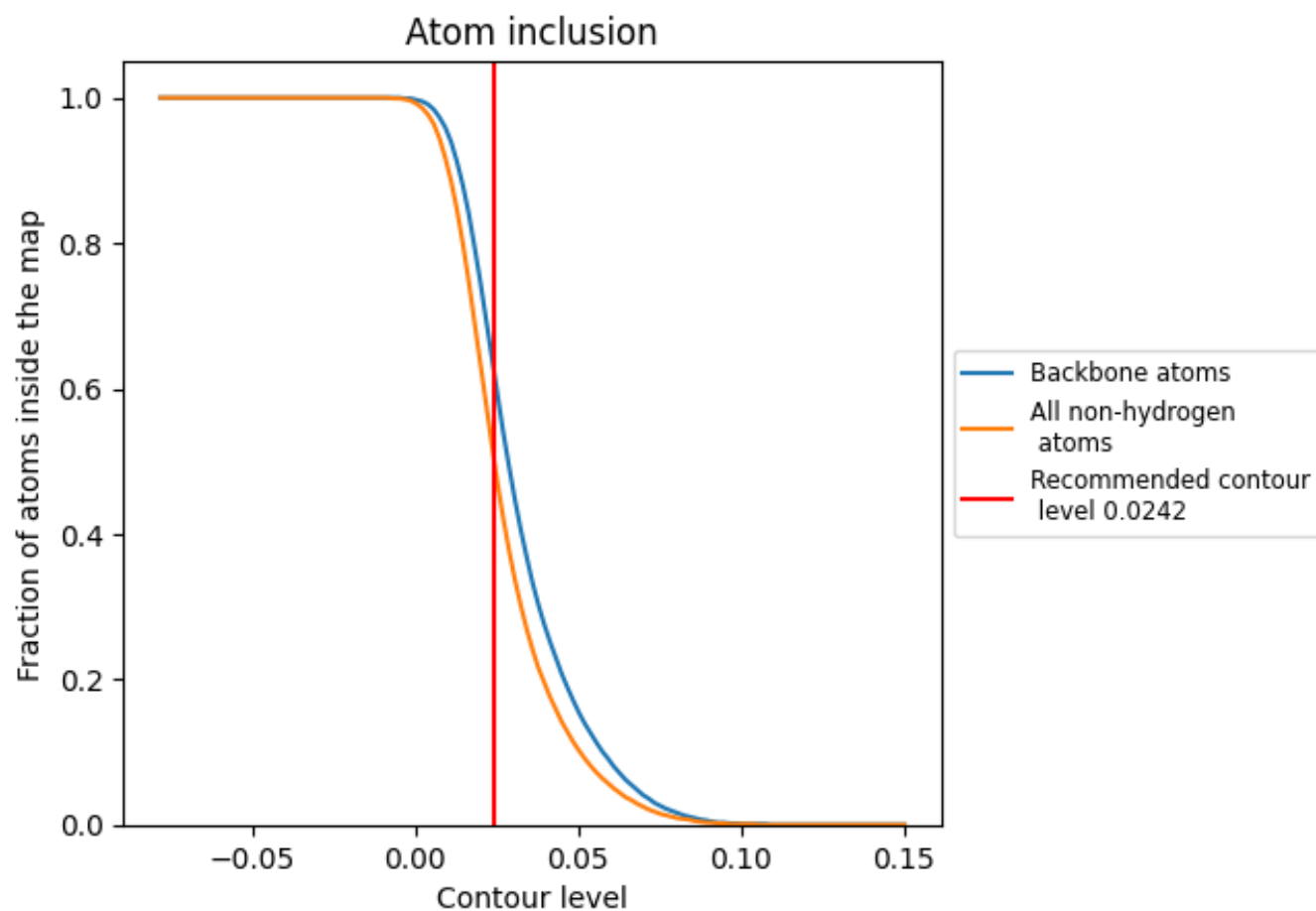
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0242).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.0242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.2660
0	 0.3850	 0.2180
1	 0.3440	 0.2710
2	 0.1540	 0.3230
3	 0.2050	 0.1120
4	 0.0820	 0.1020
5	 0.1640	 0.1380
6	 0.0000	 0.0090
7	 0.0260	 0.1010
8	 0.0000	 -0.0760
9	 0.0160	 0.0770
A	 0.5220	 0.2700
B	 0.5360	 0.2830
C	 0.1000	 0.0690
D	 0.0830	 0.0740
E	 0.0360	 0.0950
F	 0.0330	 0.1270
G	 0.1670	 0.0860
H	 0.6790	 0.3580
I	 0.8790	 0.4280
J	 0.4380	 0.2380
K	 0.5450	 0.3920
L	 0.5000	 0.3310
M	 0.7500	 0.4240
N	 0.2000	 0.2410
O	 0.8210	 0.4120
P	 0.8490	 0.4680
Q	 0.6250	 0.2130
R	 0.6360	 0.4410
S	 0.5360	 0.3240
T	 0.8570	 0.4090
U	 0.3610	 0.2860
V	 0.1790	 0.0880
W	 0.5130	 0.3470
X	 0.3570	 0.1840



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Chain	Atom inclusion	Q-score
Y	 0.3570	 0.2610
Z	 0.3440	 0.2510
a	 0.3570	 0.1800
b	 0.7210	 0.4070
c	 0.4290	 0.2360
d	 0.3930	 0.2950
e	 0.2050	 0.1320
f	 0.4100	 0.3070
g	 0.3770	 0.2160
h	 0.1280	 0.0990
i	 0.2050	 0.1630
j	 0.1310	 -0.0180
k	 0.1310	 0.1450
l	 0.0160	 0.0730
m	 0.0260	 0.1920
n	 0.0710	 -0.0280
o	 0.0710	 0.0970
p	 0.5130	 0.3370
q	 0.4290	 0.4120
r	 0.5640	 0.3000
s	 0.6070	 0.4470
t	 0.4640	 0.3800
u	 0.2460	 0.2960
v	 0.3930	 0.3110
w	 0.7210	 0.3990
x	 0.4290	 0.2300
y	 0.4290	 0.2700
z	 0.1030	 0.0360