



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 02:56 am GMT

PDB ID : 6QXP
Title : Protein peptide complex
Authors : Moussu, S.; Caroline, C.; Santos-Fernandez, G.; Wehrle, S.; Grossniklaus, U.;
Santiago, J.
Deposited on : 2019-03-07
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

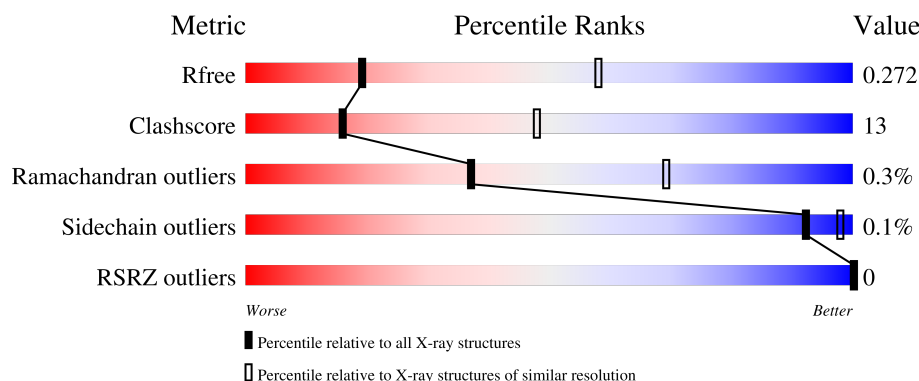
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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














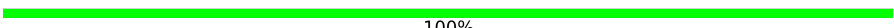
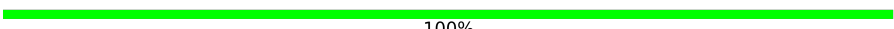
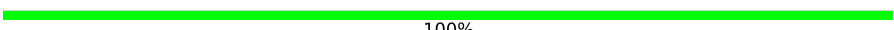
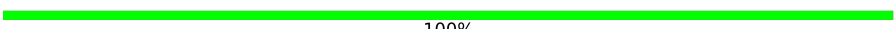


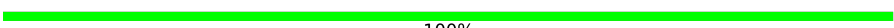

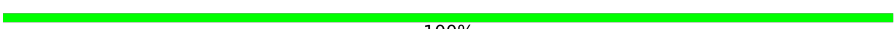
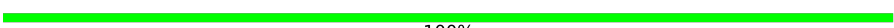
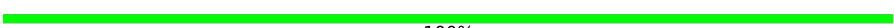
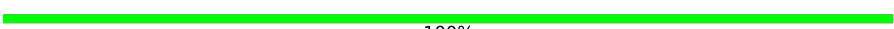


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	 68% 27% 5%
1	B	361	 62% 29% 9%
1	C	361	 68% 26% 5%
1	D	361	 68% 25% 7%
1	E	361	 68% 27% 5%



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Mol	Chain	Length	Quality of chain
1	F	361	
1	G	361	
1	H	361	
2	I	56	
2	J	56	
2	K	56	
2	L	56	
2	M	56	
2	N	56	
2	O	56	
2	P	56	
3	Q	3	
3	R	3	
3	T	3	
3	V	3	
3	X	3	
3	a	3	
3	f	3	
4	S	4	
5	U	2	
5	W	2	
5	Y	2	
5	c	2	
5	d	2	
5	e	2	

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Mol	Chain	Length	Quality of chain	
6	Z	4		
6	b	4		

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Leucine-rich repeat extensin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2616	1657	441	500	18			
1	B	328	Total	C	N	O	S	0	0	0
			2515	1593	422	482	18			
1	C	343	Total	C	N	O	S	0	0	0
			2636	1671	445	502	18			
1	D	336	Total	C	N	O	S	0	0	0
			2557	1619	429	491	18			
1	E	344	Total	C	N	O	S	0	0	0
			2624	1667	438	501	18			
1	F	336	Total	C	N	O	S	0	0	0
			2573	1633	429	494	17			
1	G	342	Total	C	N	O	S	0	0	0
			2616	1659	441	498	18			
1	H	325	Total	C	N	O	S	0	0	0
			2487	1577	415	479	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP O48809
A	387	GLU	-	expression tag	UNP O48809
A	388	ASN	-	expression tag	UNP O48809
A	389	LEU	-	expression tag	UNP O48809
B	386	LEU	-	expression tag	UNP O48809
B	387	GLU	-	expression tag	UNP O48809
B	388	ASN	-	expression tag	UNP O48809
B	389	LEU	-	expression tag	UNP O48809
C	386	LEU	-	expression tag	UNP O48809
C	387	GLU	-	expression tag	UNP O48809
C	388	ASN	-	expression tag	UNP O48809
C	389	LEU	-	expression tag	UNP O48809
D	386	LEU	-	expression tag	UNP O48809

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Chain	Residue	Modelled	Actual	Comment	Reference
D	387	GLU	-	expression tag	UNP O48809
D	388	ASN	-	expression tag	UNP O48809
D	389	LEU	-	expression tag	UNP O48809
E	385	LEU	-	expression tag	UNP O48809
E	386	GLU	-	expression tag	UNP O48809
E	387	ASN	-	expression tag	UNP O48809
E	388	LEU	-	expression tag	UNP O48809
F	386	LEU	-	expression tag	UNP O48809
F	387	GLU	-	expression tag	UNP O48809
F	388	ASN	-	expression tag	UNP O48809
F	389	LEU	-	expression tag	UNP O48809
G	386	LEU	-	expression tag	UNP O48809
G	387	GLU	-	expression tag	UNP O48809
G	388	ASN	-	expression tag	UNP O48809
G	389	LEU	-	expression tag	UNP O48809
H	386	LEU	-	expression tag	UNP O48809
H	387	GLU	-	expression tag	UNP O48809
H	388	ASN	-	expression tag	UNP O48809
H	389	LEU	-	expression tag	UNP O48809

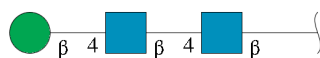
- Molecule 2 is a protein called Protein RALF-like 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	47	Total	C	N	O	S	0	0	0
			370	226	76	64	4			
2	J	46	Total	C	N	O	S	0	0	0
			373	229	77	63	4			
2	K	45	Total	C	N	O	S	0	0	0
			353	217	69	63	4			
2	L	47	Total	C	N	O	S	0	0	0
			364	223	73	64	4			
2	M	47	Total	C	N	O	S	0	0	0
			371	226	76	65	4			
2	N	46	Total	C	N	O	S	0	0	0
			359	220	72	63	4			
2	O	47	Total	C	N	O	S	0	0	0
			364	223	73	64	4			
2	P	45	Total	C	N	O	S	0	0	0
			342	211	65	62	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1052	MET	-	initiating methionine	UNP Q9FZA0
I	1053	GLY	-	expression tag	UNP Q9FZA0
J	1052	MET	-	initiating methionine	UNP Q9FZA0
J	1053	GLY	-	expression tag	UNP Q9FZA0
K	1052	MET	-	initiating methionine	UNP Q9FZA0
K	1053	GLY	-	expression tag	UNP Q9FZA0
L	1052	MET	-	initiating methionine	UNP Q9FZA0
L	1053	GLY	-	expression tag	UNP Q9FZA0
M	1052	MET	-	initiating methionine	UNP Q9FZA0
M	1053	GLY	-	expression tag	UNP Q9FZA0
N	1052	MET	-	initiating methionine	UNP Q9FZA0
N	1053	GLY	-	expression tag	UNP Q9FZA0
O	1052	MET	-	initiating methionine	UNP Q9FZA0
O	1053	GLY	-	expression tag	UNP Q9FZA0
P	1052	MET	-	initiating methionine	UNP Q9FZA0
P	1053	GLY	-	expression tag	UNP Q9FZA0

- Molecule 3 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				ZeroOcc	AltConf	Trace
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	V	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	f	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



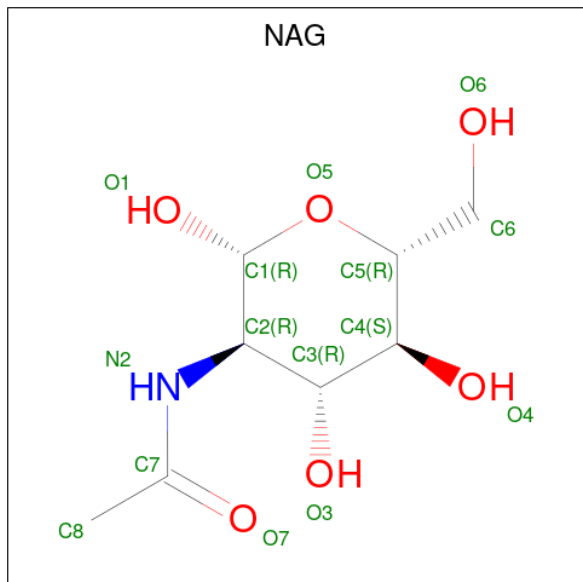
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	c	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	e	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 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				ZeroOcc	AltConf	Trace
6	Z	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	b	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

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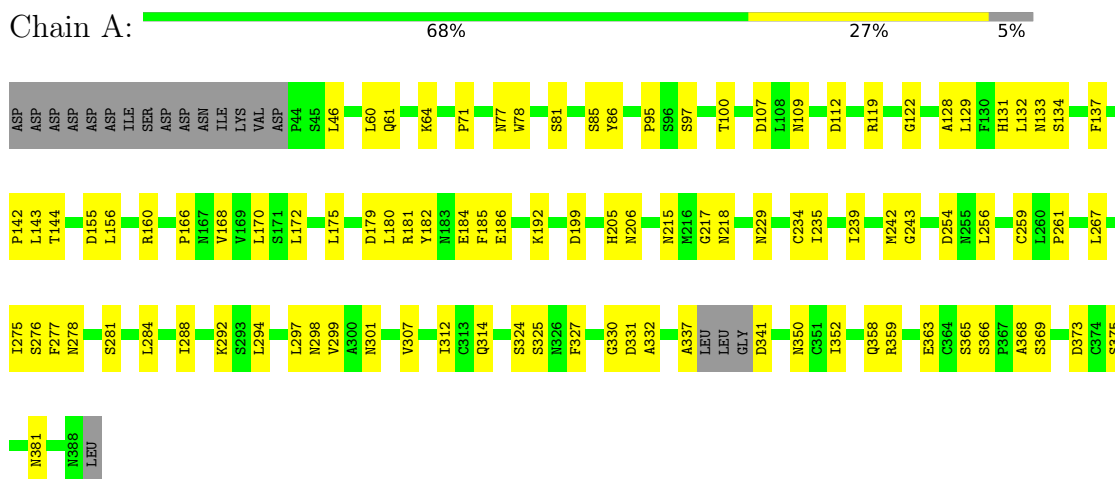
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	C	N	O	0	0
			14	8	1	5		

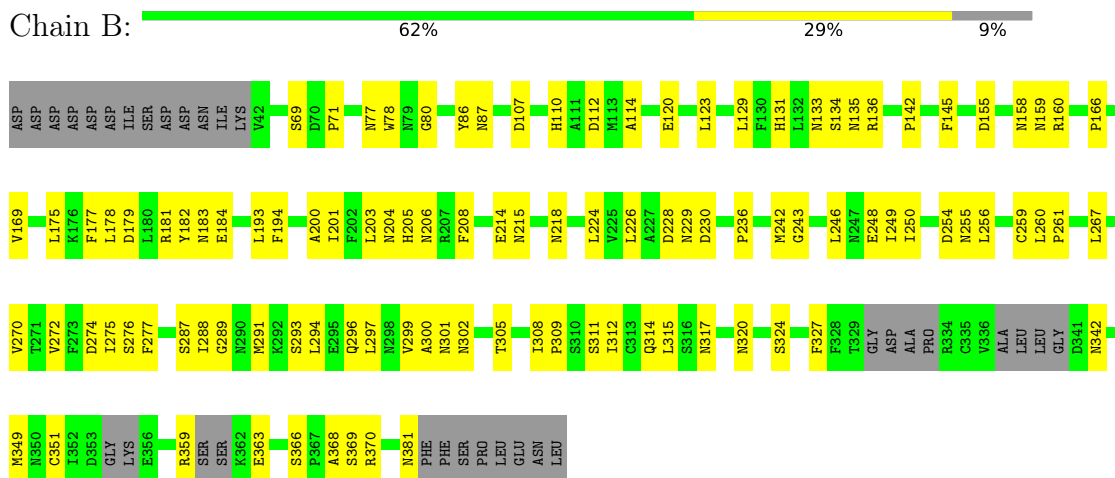
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Leucine-rich repeat extensin-like protein 2



- Molecule 1: Leucine-rich repeat extensin-like protein 2



- Molecule 1: Leucine-rich repeat extensin-like protein 2



- Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain D:  68% 25% 7%

- Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain E:  68% 27% 5%

- Molecule 1: Leucine-rich repeat extensin-like protein 2

Chain F:  71% 22% 7%

- Molecule 1: Leucine-rich repeat extensin-like protein 2

LEU	N388	L260	F152	ASP
	P261	P261	S157	ASP
	L267	L267	R158	ASP
	V270	N159	R160	ASP
	T271	F161	G163	ILE
	V272	R279	V168	SER
	R279	L280	L172	ASP
	S281	L284	L175	ASN
	L284	L288	R181	ILE
	L288	K292	Y182	LYS
ASP	S293	L294	F185	VAL
	E295	E295	S191	ASP
	Q296	L297	F194	ASP
	L297	R298	D199	ASP
	R298	V299	N204	ASP
	V299	G305	H205	ASP
	G306	V307	N206	ASP
	V307	Q314	N215	ASP
	Q314	N317	M216	ASP
	N317	G330	G217	ASP
ASP	G330	D331	N218	ASP
	D331	C335	S219	ASP
	C335	V336	P220	ASP
	V336	A337	V221	ASP
	A337	L338	L224	ASP
	L338	GLY	L226	ASP
	GLY	N342	A227	ASP
	N342	T352	N229	ASP
	T352	K355	C234	ASP
	K355	R359	L235	ASP
ASP	R359	E363	P236	ASP
	E363	C364	I239	ASP
	C364	S365	L249	ASP
	S365	S366	L280	ASP
	S366	P367	D254	ASP
	P367	A368	N255	ASP
	A368	G369	G258	ASP
	G369		C250	ASP
				ASP
				ASP

VAL	T264	P166	ASP
ALA	G265	M167	ASP
LEU	G266	V168	ASP
LEU	L267	V169	ASP
GLY			ASP
D341	V270	L172	ASP
	T271	P173	ILE
V345	V272	S174	SER
		L175	ASP
M349	S276	D179	ASP
N350	F277	L180	ASN
C351	N278	R181	ILE
I352	R279	V182	LYS
	L280	M183	VAL
K355	S281	E184	D43
		F185	L60
Q358	P285		
R359		S188	P71
F377	T289		
G378	N291	D196	N77
CYS	K292		W78
ASN	S293	F202	N79
ASN	L294	L203	G80
PHE	E295	N204	
PHI	Q296	H205	S85
SER	L297	N206	Y86
PRO		R207	
LEU	A300	F208	I89
GLU	R301	K209	
ASN	N302	T210	A92
LEU	R303	G211	
			H110
G306	G306	E214	A111
V307	V307	N215	D112
I308	I308	M216	
		G217	L124
	I312	N218	
			L127
L315	L315	V225	A128
S316	S316		L129
N317	N317	D228	F130
L318	L318	M229	H131
E319	E319	D230	L132
N320	N320	L231	N133
F321	F321	I235	S134
T322	T322	P236	N135
S324	S324		R136
S325	S325		F137
N326	N326	E247	
F327	F327		L143
F328	F328		
T329	T329	N255	K149
GLY	GLY	L256	
ASP	ASP	T257	D155
ALA	ALA	G258	
PRO	PRO	C259	N158
ARG	ARG	L260	N159
CYS	CYS	P261	F165

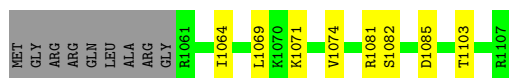
Met	Arg	Arg	Arg	Leu	Ala	Arg	Gly	I1061	I1064	L1069	K1070	K1071	V1074	P1075	C1076	R1081	S1082	Y1083	Y1084	N1092	Y1095	A1101	I1102	R1107
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MET	GLY	ARG	ARG	GLN	LEU	ALA	LEU	ARG	GLY	R1061	I1064	L1069	K1070	K1071	V1074	P1075	C1076	L1081	S1082	Y1083	R1089	N1092	I1102	Y1106	ARG
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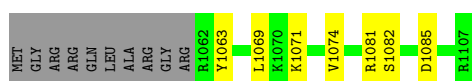
- Molecule 2: Protein RALF-like 4



- Molecule 2: Protein RALF-like 4



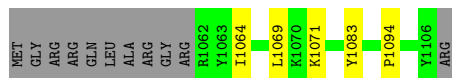
- Molecule 2: Protein RALF-like 4



- Molecule 2: Protein RALF-like 4



- Molecule 2: Protein RALF-like 4



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



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

Chain R:  100%

WAG1
WAG2
BMA3

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

Chain T:  100%

WAG1
WAG2
BMA3

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

Chain V:  100%

WAG1
WAG2
BMA3

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

Chain X:  67% 33%

WAG1
WAG2
BMA3

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

Chain a:  67% 33%

WAG1
WAG2
BMA3

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

Chain f:  100%

WAG1
WAG2
BMA3

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

Chain S:  75% 25%

WAG1
WAG2
BMA3
MAN4

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

Chain U:  100%



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

Chain W:  100%



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

Chain Y:  100%



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

Chain c:  100%



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

Chain d:  100%



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

Chain e:  100%



- Molecule 6: 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

Chain Z:  75% 25%



- Molecule 6: 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

Chain b:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	119.99Å 119.99Å 305.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 3.20 59.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.99-3.20) 100.0 (59.99-3.20)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.19Å)	Xtriage
Refinement program	PHENIX v1.14	Depositor
R, R_{free}	0.227 , 0.274 0.223 , 0.272	Depositor DCC
R_{free} test set	3561 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24293	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/2675	0.50	0/3629
1	B	0.26	0/2567	0.51	0/3480
1	C	0.27	0/2695	0.52	0/3655
1	D	0.26	0/2612	0.49	0/3545
1	E	0.26	0/2683	0.51	1/3642 (0.0%)
1	F	0.27	0/2631	0.50	0/3570
1	G	0.27	0/2675	0.48	0/3629
1	H	0.26	0/2542	0.52	0/3449
2	I	0.27	0/378	0.45	0/509
2	J	0.31	0/381	0.48	0/510
2	K	0.34	0/361	0.50	0/486
2	L	0.25	0/372	0.41	0/502
2	M	0.26	0/379	0.45	0/510
2	N	0.25	0/367	0.42	0/495
2	O	0.26	0/372	0.45	0/502
2	P	0.27	0/350	0.42	0/474
All	All	0.27	0/24040	0.50	1/32587 (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	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	351	CYS	CA-CB-SG	5.43	123.78	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	335	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2525	80	0
1	B	2515	0	2428	87	1
1	C	2636	0	2560	75	1
1	D	2557	0	2467	69	0
1	E	2624	0	2536	74	0
1	F	2573	0	2483	60	0
1	G	2616	0	2532	69	0
1	H	2487	0	2407	85	0
2	I	370	0	331	17	0
2	J	373	0	353	14	0
2	K	353	0	319	11	0
2	L	364	0	320	8	0
2	M	371	0	334	16	0
2	N	359	0	318	8	0
2	O	364	0	320	12	0
2	P	342	0	294	5	0
3	Q	39	0	34	0	0
3	R	39	0	34	0	0
3	T	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	1	0
3	a	39	0	34	0	0
3	f	39	0	34	0	0
4	S	50	0	43	0	0
5	U	28	0	25	0	0
5	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
6	Z	50	0	43	0	0
6	b	50	0	43	0	0
7	A	42	0	39	0	0
7	D	28	0	26	0	0
7	E	42	0	39	0	0
7	F	28	0	26	0	0
7	G	28	0	26	0	0
7	H	14	0	13	0	0
All	All	24293	0	23213	615	1

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 13.

The worst 5 of 615 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:D:282:GLY:HA2	1:D:372:VAL:HG21	1.41	1.01
1:H:208:PHE:HB2	1:H:229:ASN:HD21	1.24	0.97
1:G:204:ASN:HD21	1:G:225:VAL:HG12	1.31	0.95
1:B:351:CYS:SG	1:B:359:ARG:NH2	2.43	0.92
1:E:111:ALA:O	1:E:135:ASN:ND2	2.09	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:SER:OG	1:C:342:ASN:OD1[4_654]	1.98	0.22

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 X-ray entries followed by that with respect to entries of similar resolution.

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	338/361 (94%)	305 (90%)	32 (10%)	1 (0%)	37	69
1	B	318/361 (88%)	289 (91%)	29 (9%)	0	100	100
1	C	339/361 (94%)	297 (88%)	40 (12%)	2 (1%)	22	57
1	D	330/361 (91%)	303 (92%)	27 (8%)	0	100	100
1	E	340/361 (94%)	301 (88%)	38 (11%)	1 (0%)	37	69
1	F	330/361 (91%)	305 (92%)	25 (8%)	0	100	100
1	G	338/361 (94%)	301 (89%)	33 (10%)	4 (1%)	11	43
1	H	321/361 (89%)	293 (91%)	28 (9%)	0	100	100
2	I	45/56 (80%)	42 (93%)	3 (7%)	0	100	100
2	J	44/56 (79%)	40 (91%)	4 (9%)	0	100	100
2	K	43/56 (77%)	38 (88%)	5 (12%)	0	100	100
2	L	45/56 (80%)	44 (98%)	1 (2%)	0	100	100
2	M	45/56 (80%)	41 (91%)	4 (9%)	0	100	100
2	N	44/56 (79%)	43 (98%)	1 (2%)	0	100	100
2	O	45/56 (80%)	42 (93%)	3 (7%)	0	100	100
2	P	43/56 (77%)	42 (98%)	1 (2%)	0	100	100
All	All	3008/3336 (90%)	2726 (91%)	274 (9%)	8 (0%)	37	69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	344	VAL
1	G	336	VAL
1	A	365	SER
1	E	112	ASP
1	G	335	CYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	298/320 (93%)	298 (100%)	0	100	100
1	B	288/320 (90%)	287 (100%)	1 (0%)	91	96
1	C	302/320 (94%)	302 (100%)	0	100	100
1	D	291/320 (91%)	291 (100%)	0	100	100
1	E	298/320 (93%)	298 (100%)	0	100	100
1	F	294/320 (92%)	294 (100%)	0	100	100
1	G	298/320 (93%)	298 (100%)	0	100	100
1	H	284/320 (89%)	283 (100%)	1 (0%)	89	94
2	I	35/48 (73%)	35 (100%)	0	100	100
2	J	37/48 (77%)	37 (100%)	0	100	100
2	K	35/48 (73%)	35 (100%)	0	100	100
2	L	34/48 (71%)	34 (100%)	0	100	100
2	M	36/48 (75%)	36 (100%)	0	100	100
2	N	34/48 (71%)	34 (100%)	0	100	100
2	O	34/48 (71%)	34 (100%)	0	100	100
2	P	32/48 (67%)	32 (100%)	0	100	100
All	All	2630/2944 (89%)	2628 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	342	ASN
1	H	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	77	ASN
1	G	204	ASN
1	F	218	ASN
1	F	350	ASN
1	G	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

45 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	$\# Z > 2$
3	NAG	Q	1	1,3	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.56	0
3	BMA	Q	3	3	11,11,12	0.69	0	15,15,17	0.75	0
3	NAG	R	1	1,3	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	R	2	3	14,14,15	0.28	0	17,19,21	0.40	0
3	BMA	R	3	3	11,11,12	0.65	0	15,15,17	0.86	0
4	NAG	S	1	1,4	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	S	2	4	14,14,15	0.19	0	17,19,21	0.44	0
4	BMA	S	3	4	11,11,12	0.75	0	15,15,17	0.88	0
4	MAN	S	4	4	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.53	0
3	BMA	T	3	3	11,11,12	0.72	0	15,15,17	0.72	0
5	NAG	U	1	1,5	14,14,15	0.30	0	17,19,21	0.42	0
5	NAG	U	2	5	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	V	1	1,3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	V	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	BMA	V	3	3	11,11,12	0.59	0	15,15,17	0.85	0
5	NAG	W	1	1,5	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	W	2	5	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	X	1	1,3	14,14,15	0.38	0	17,19,21	0.58	0
3	NAG	X	2	3	14,14,15	0.23	0	17,19,21	0.51	0
3	BMA	X	3	3	11,11,12	0.62	0	15,15,17	0.83	0
5	NAG	Y	1	1,5	14,14,15	0.41	0	17,19,21	0.42	0
5	NAG	Y	2	5	14,14,15	0.17	0	17,19,21	0.46	0
6	NAG	Z	1	1,6	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	Z	2	6	14,14,15	0.32	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	Z	3	6	11,11,12	0.67	0	15,15,17	0.70	0
6	MAN	Z	4	6	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
3	NAG	a	1	1,3	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	a	2	3	14,14,15	0.34	0	17,19,21	0.36	0
3	BMA	a	3	3	11,11,12	0.69	0	15,15,17	1.02	1 (6%)
6	NAG	b	1	1,6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	b	2	6	14,14,15	0.19	0	17,19,21	0.48	0
6	BMA	b	3	6	11,11,12	0.55	0	15,15,17	0.75	0
6	MAN	b	4	6	11,11,12	0.74	1 (9%)	15,15,17	1.09	2 (13%)
5	NAG	c	1	1,5	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	c	2	5	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	d	1	1,5	14,14,15	0.24	0	17,19,21	0.53	0
5	NAG	d	2	5	14,14,15	0.29	0	17,19,21	0.58	0
5	NAG	e	1	1,5	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	e	2	5	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	f	1	1,3	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	f	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	BMA	f	3	3	11,11,12	0.63	0	15,15,17	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	BMA	R	3	3	-	1/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
4	MAN	S	4	4	-	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	4	MAN	C1-C2	2.04	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	4	MAN	C1-O5-C5	2.75	115.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	4	MAN	C1-O5-C5	2.60	115.71	112.19
6	Z	4	MAN	O2-C2-C3	-2.19	105.75	110.14
4	S	4	MAN	O2-C2-C3	-2.10	105.92	110.14
6	b	4	MAN	O2-C2-C3	-2.07	105.98	110.14

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O5-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	f	3	BMA	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6

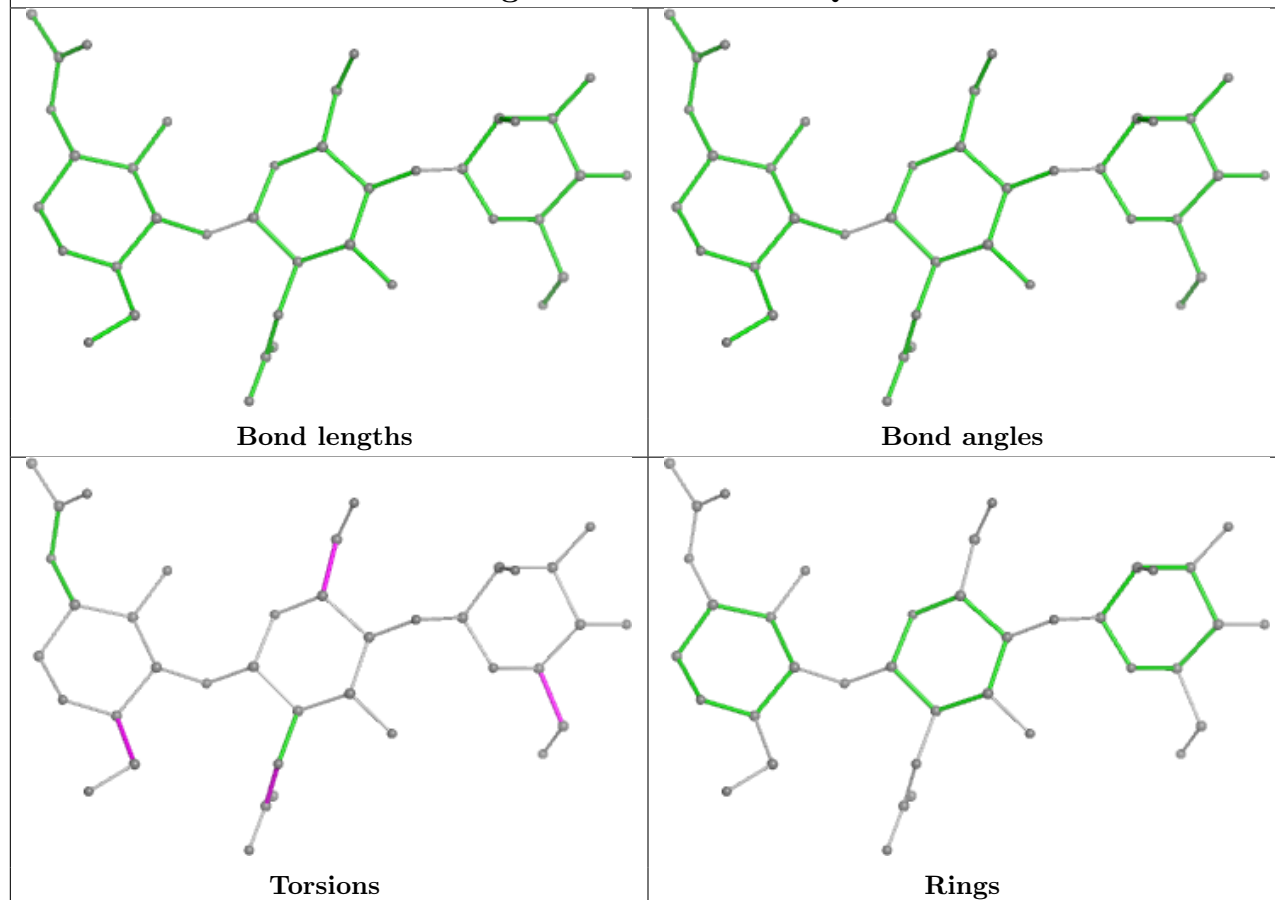
There are no ring outliers.

1 monomer is involved in 1 short contact:

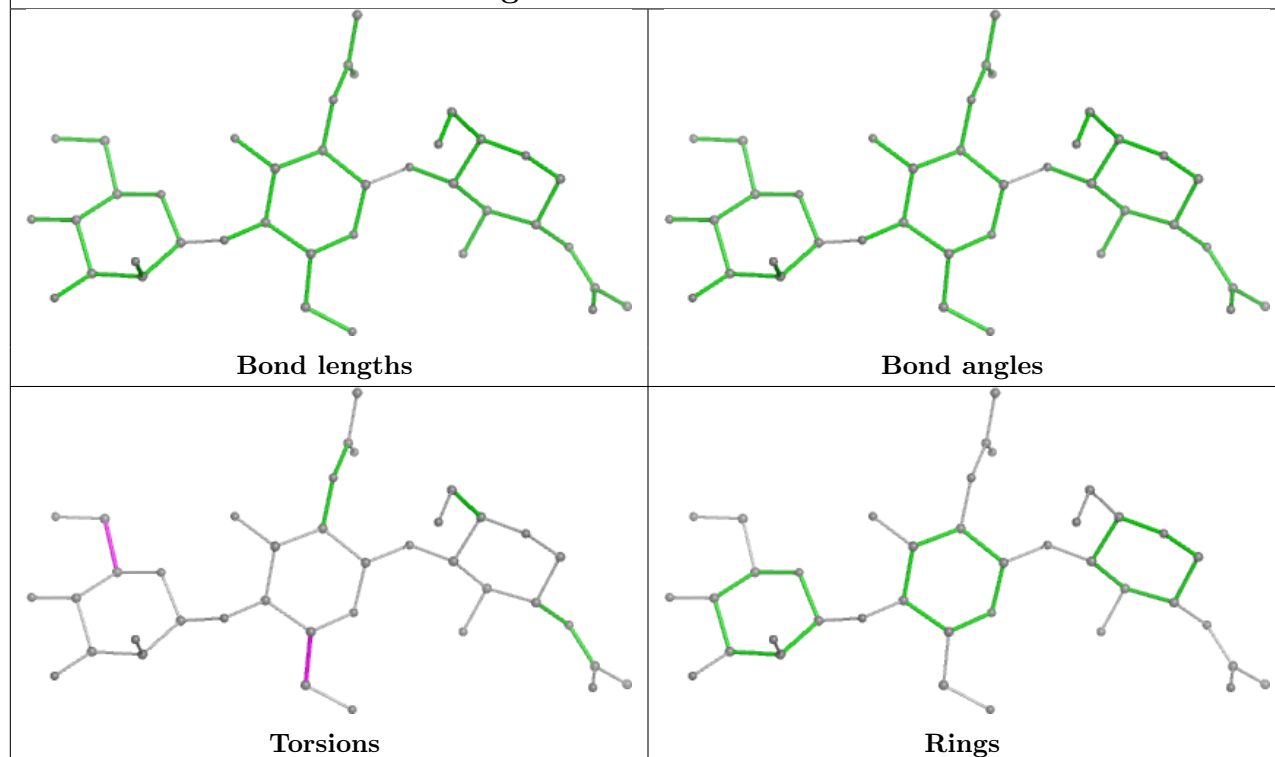
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0

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

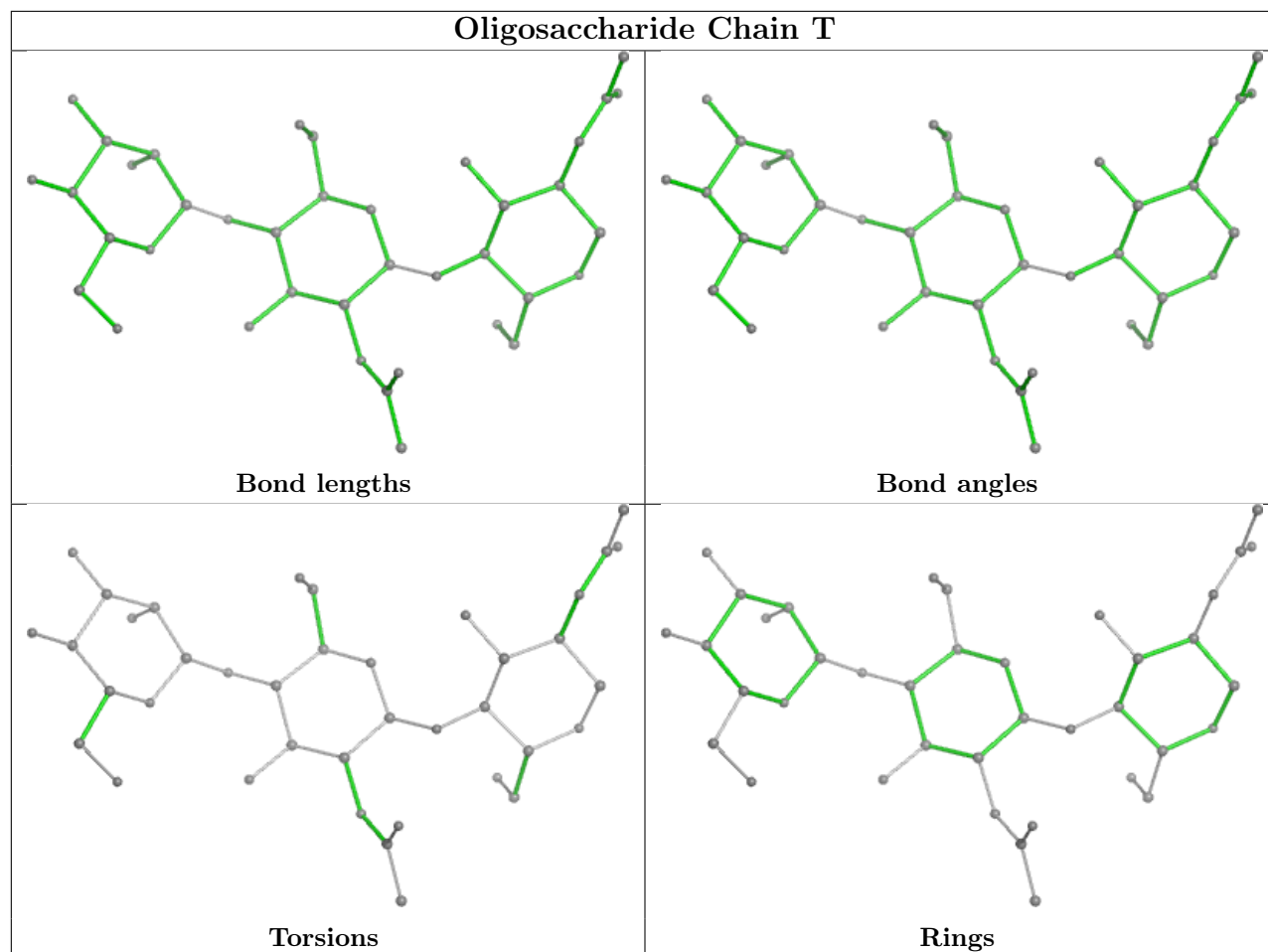
Oligosaccharide Chain Q



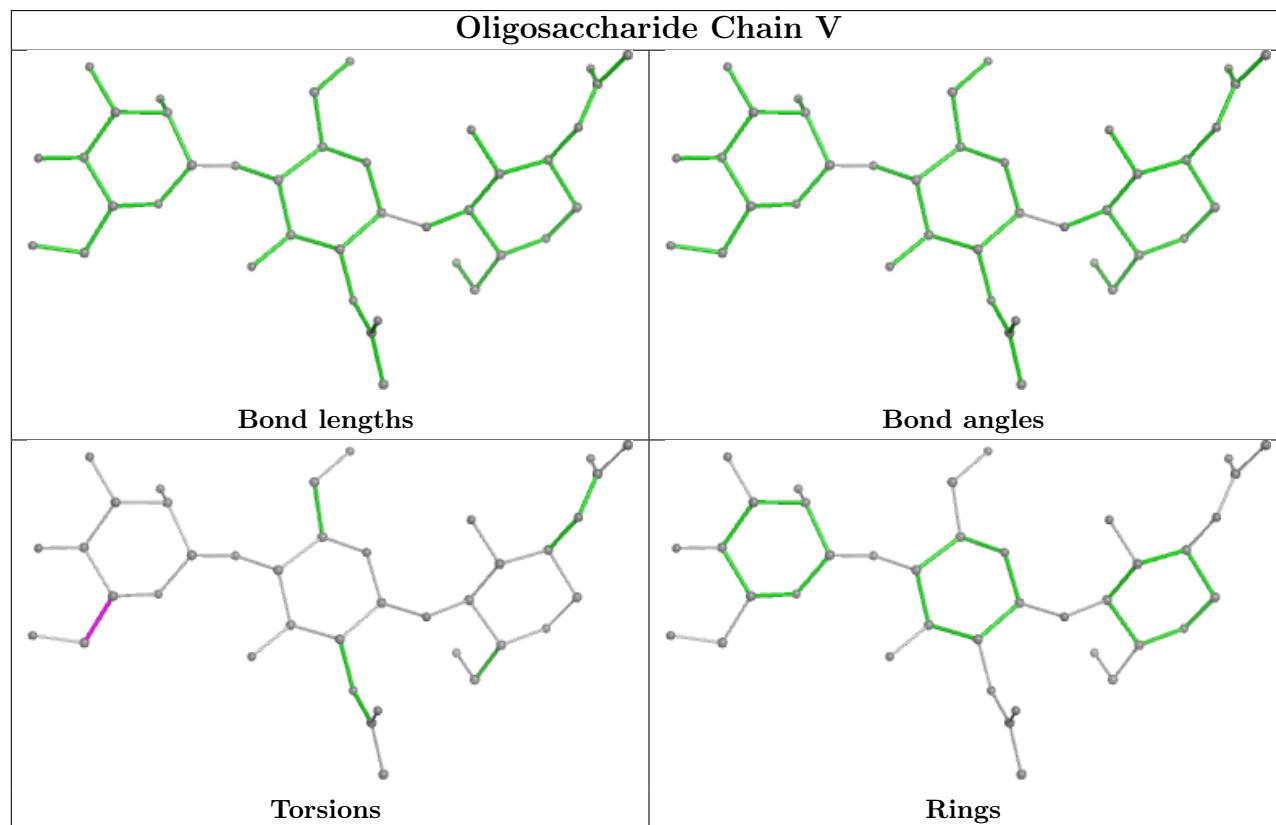
Oligosaccharide Chain R

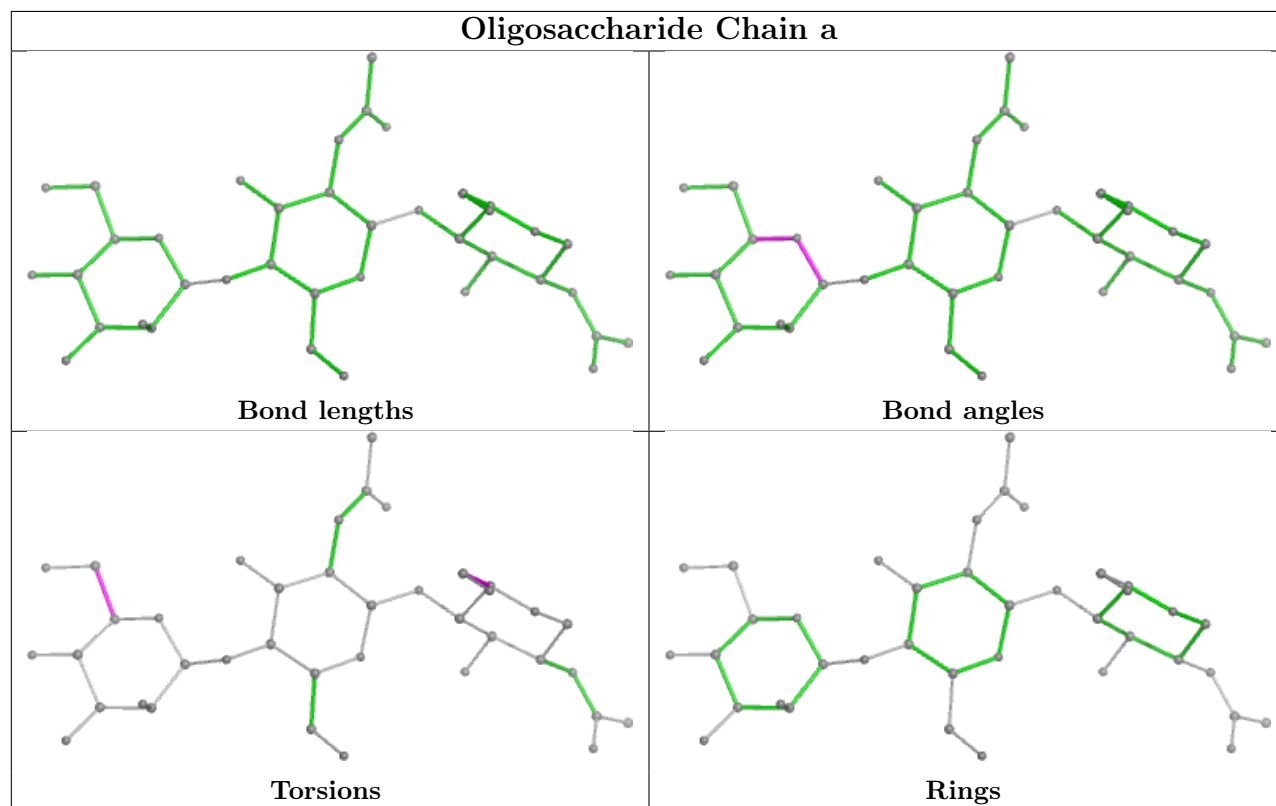
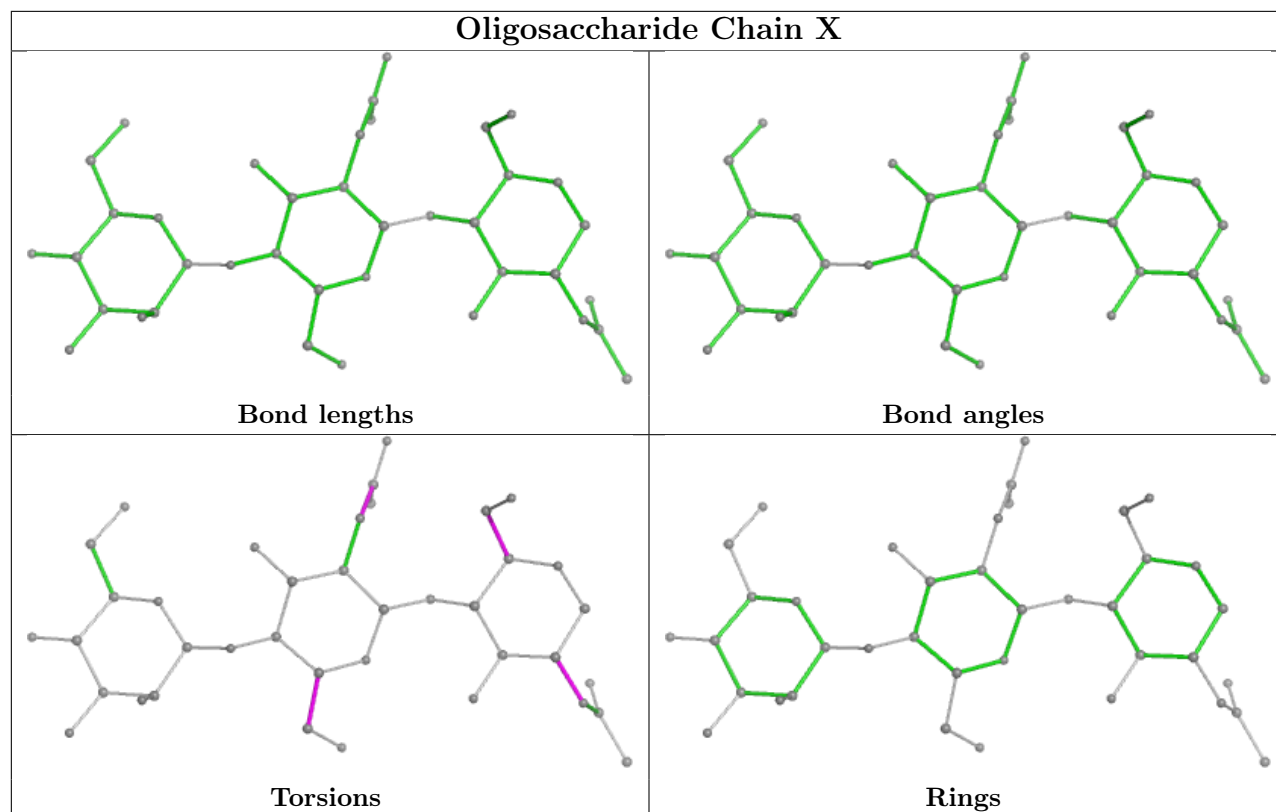


Oligosaccharide Chain T

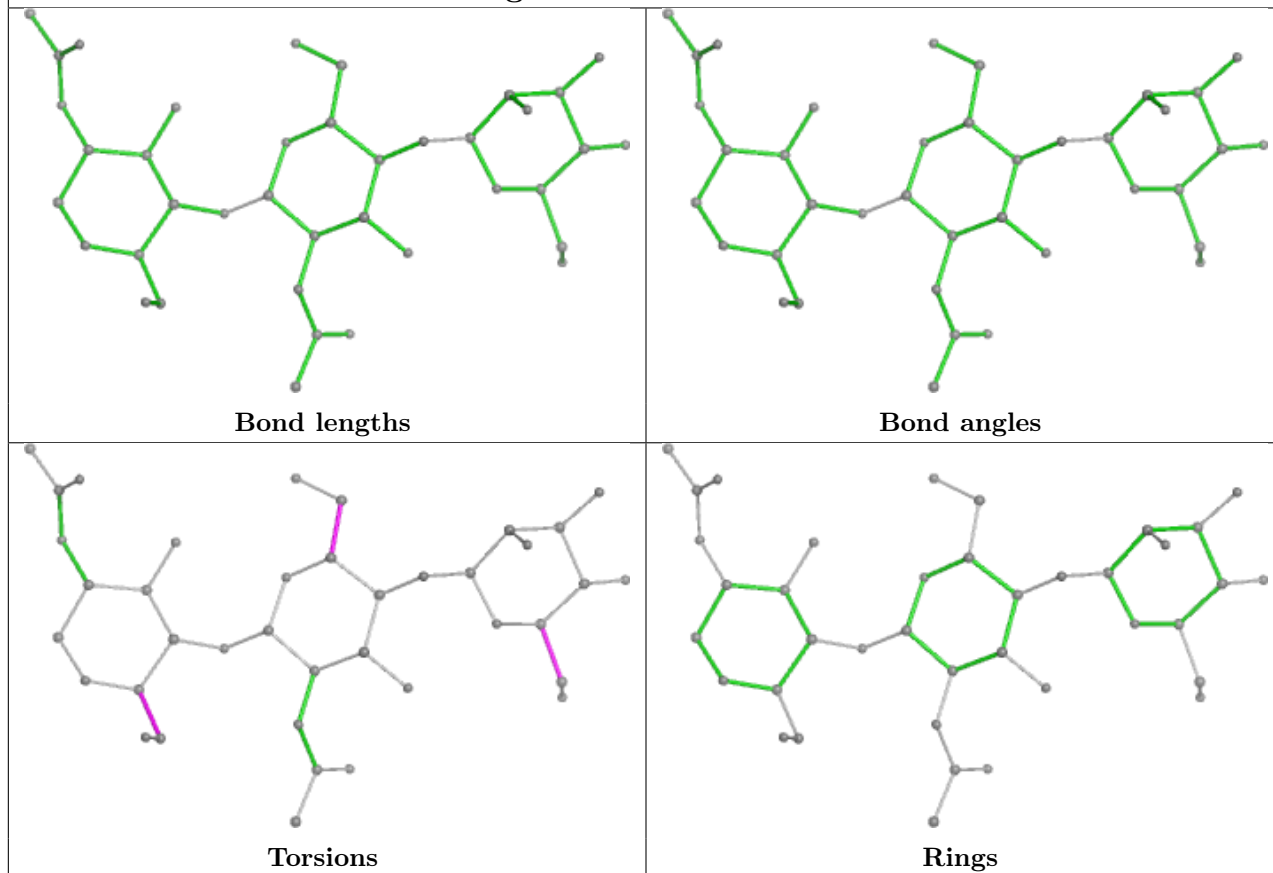


Oligosaccharide Chain V

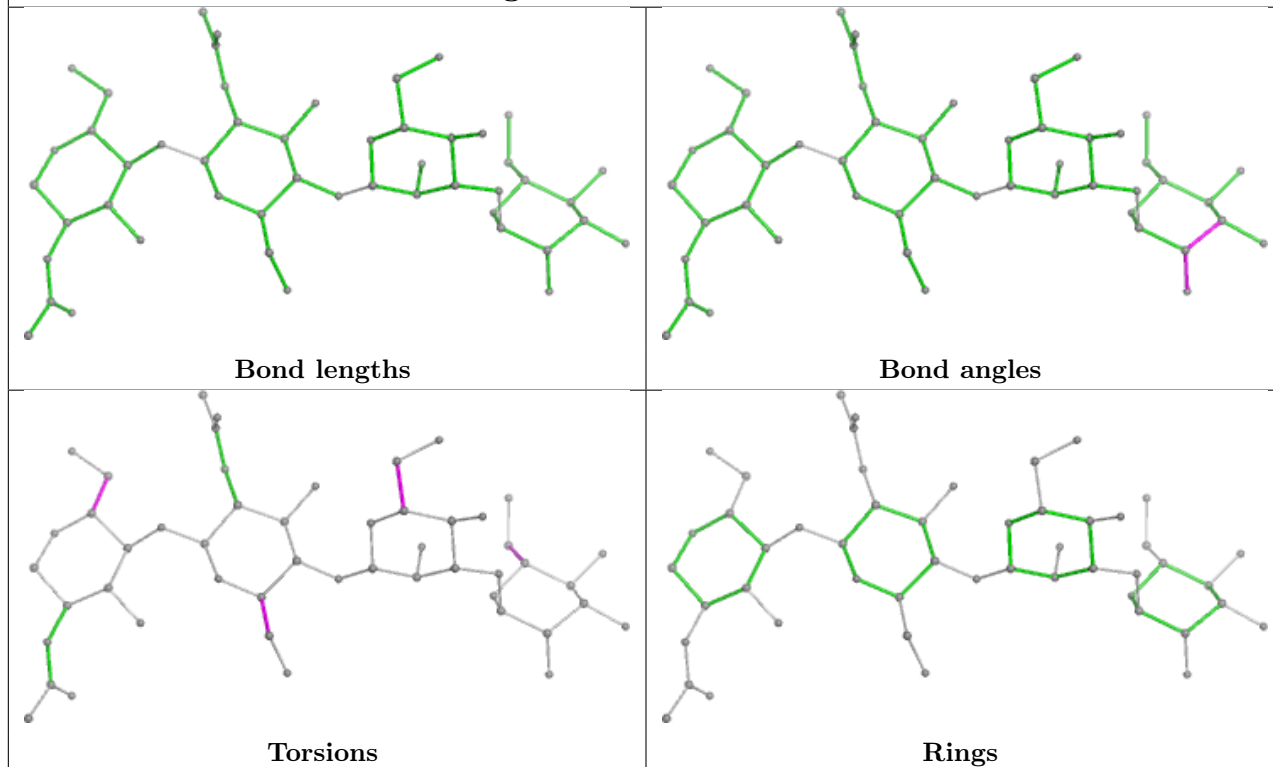


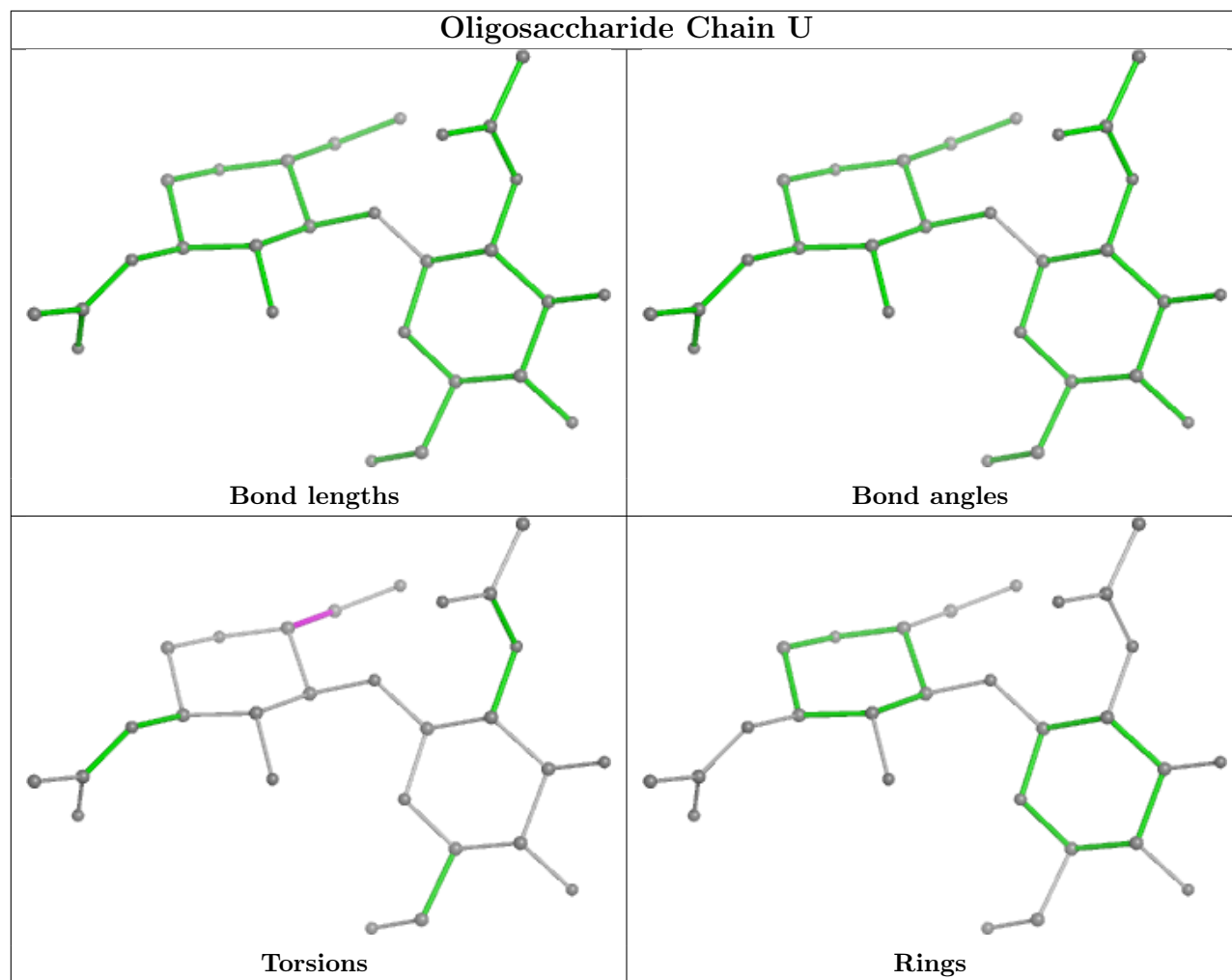


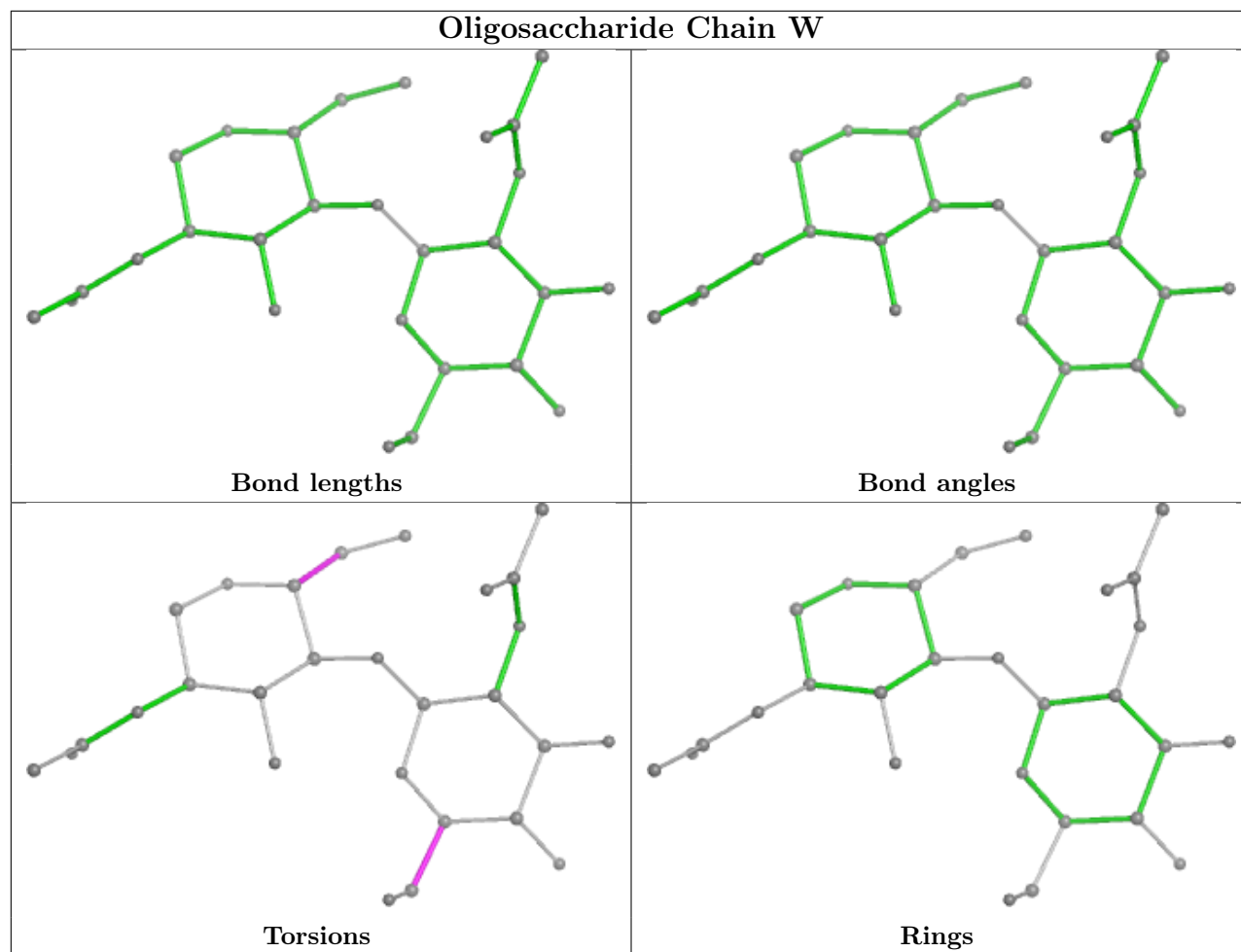
Oligosaccharide Chain f

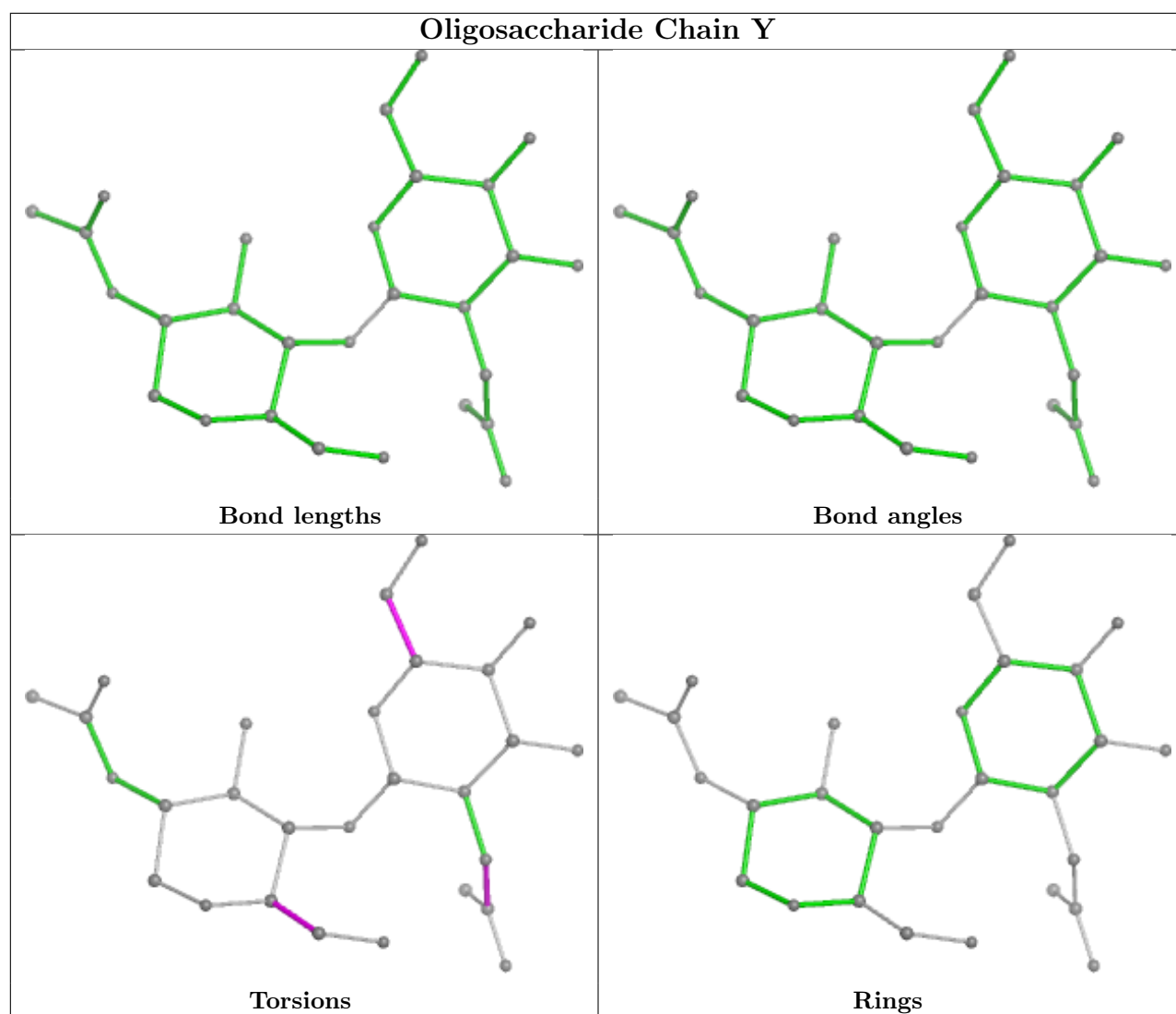


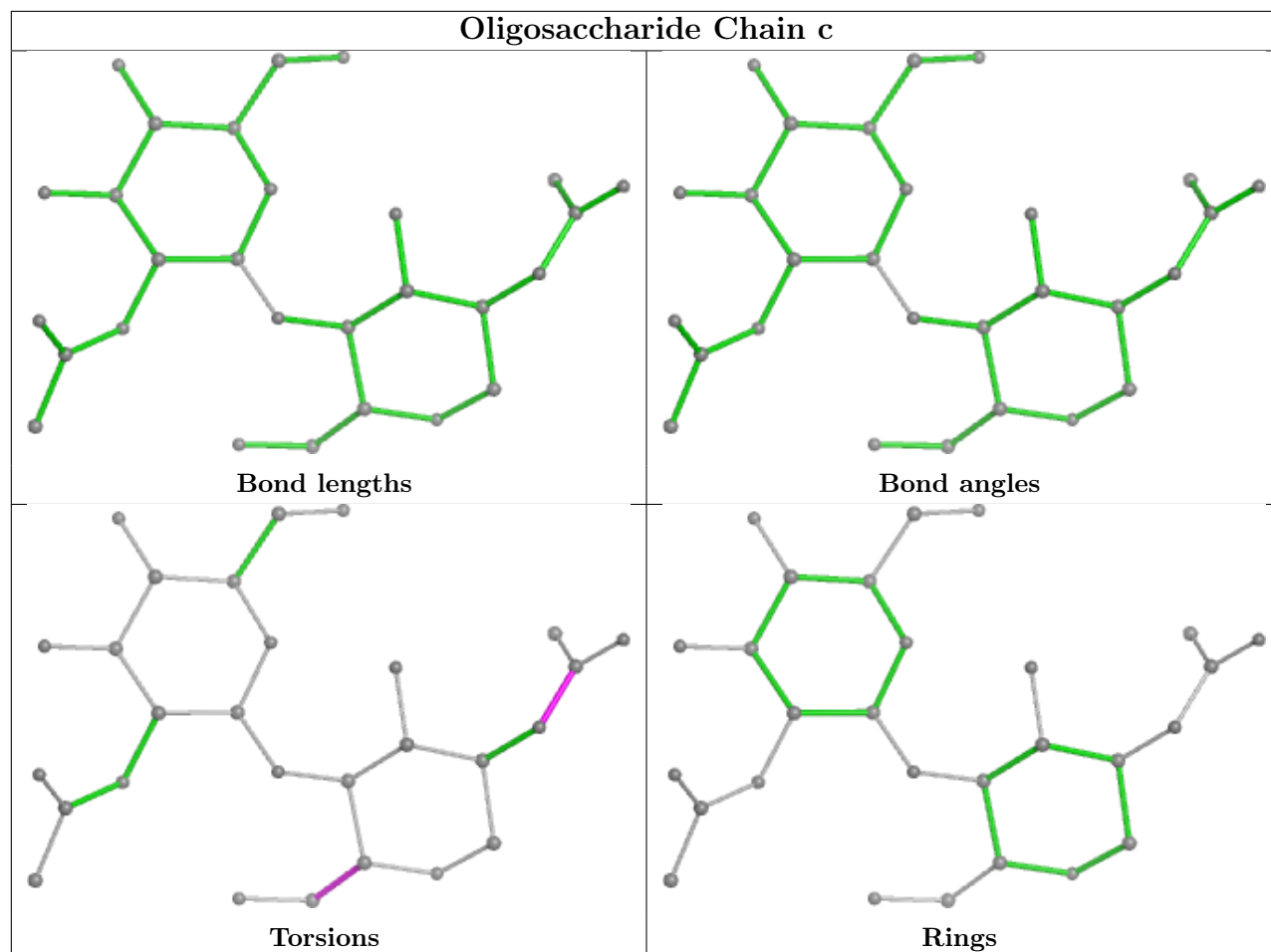
Oligosaccharide Chain S

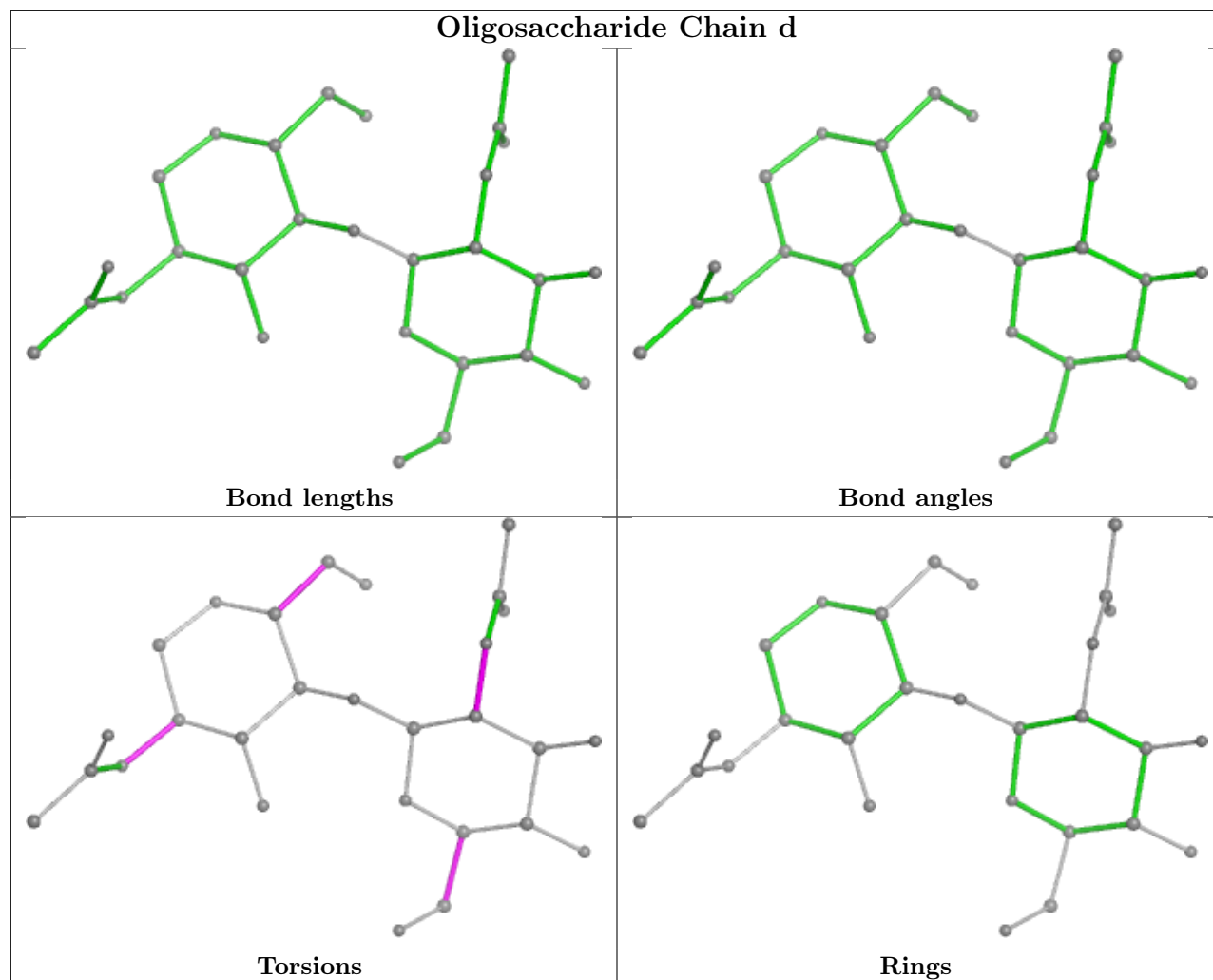


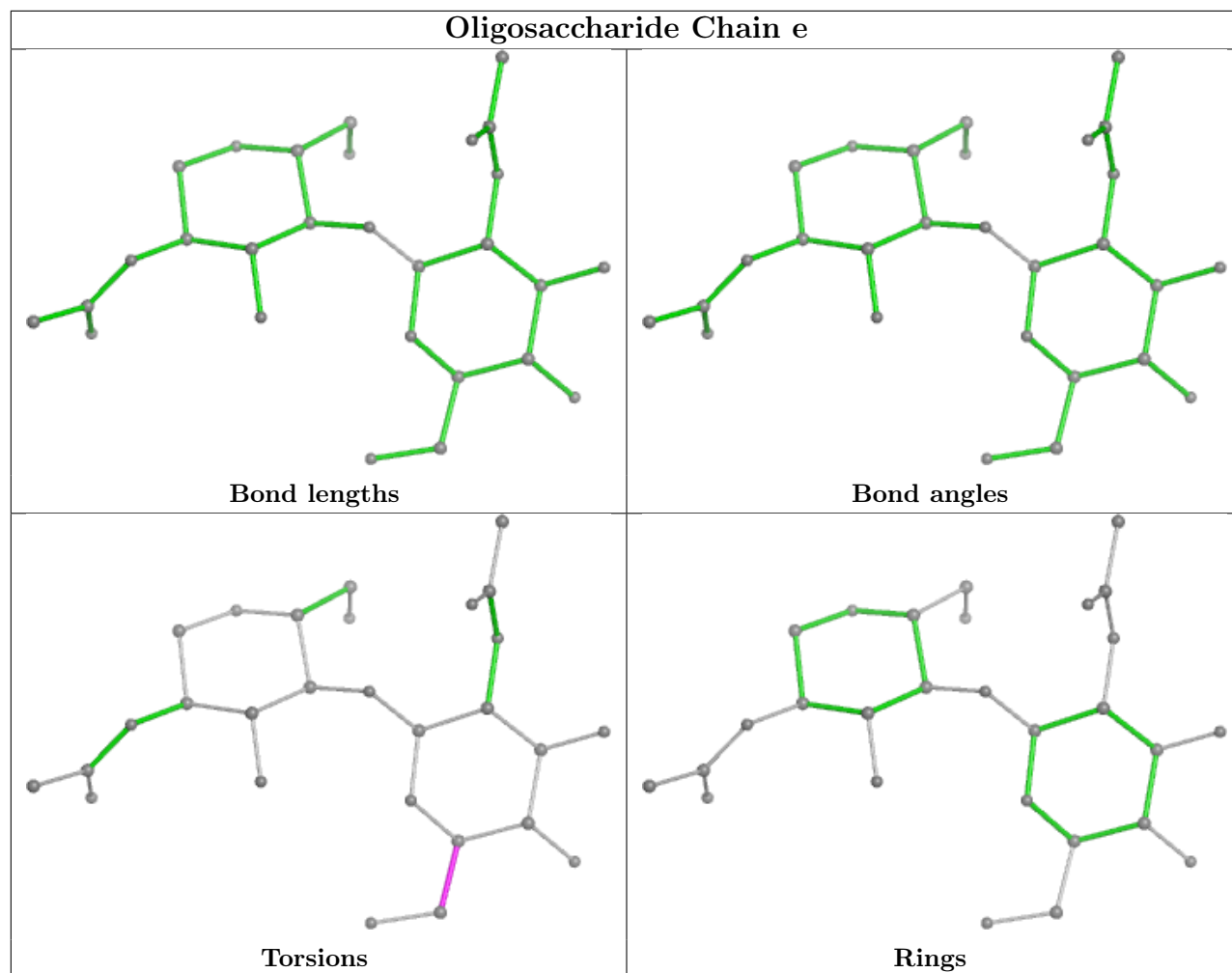


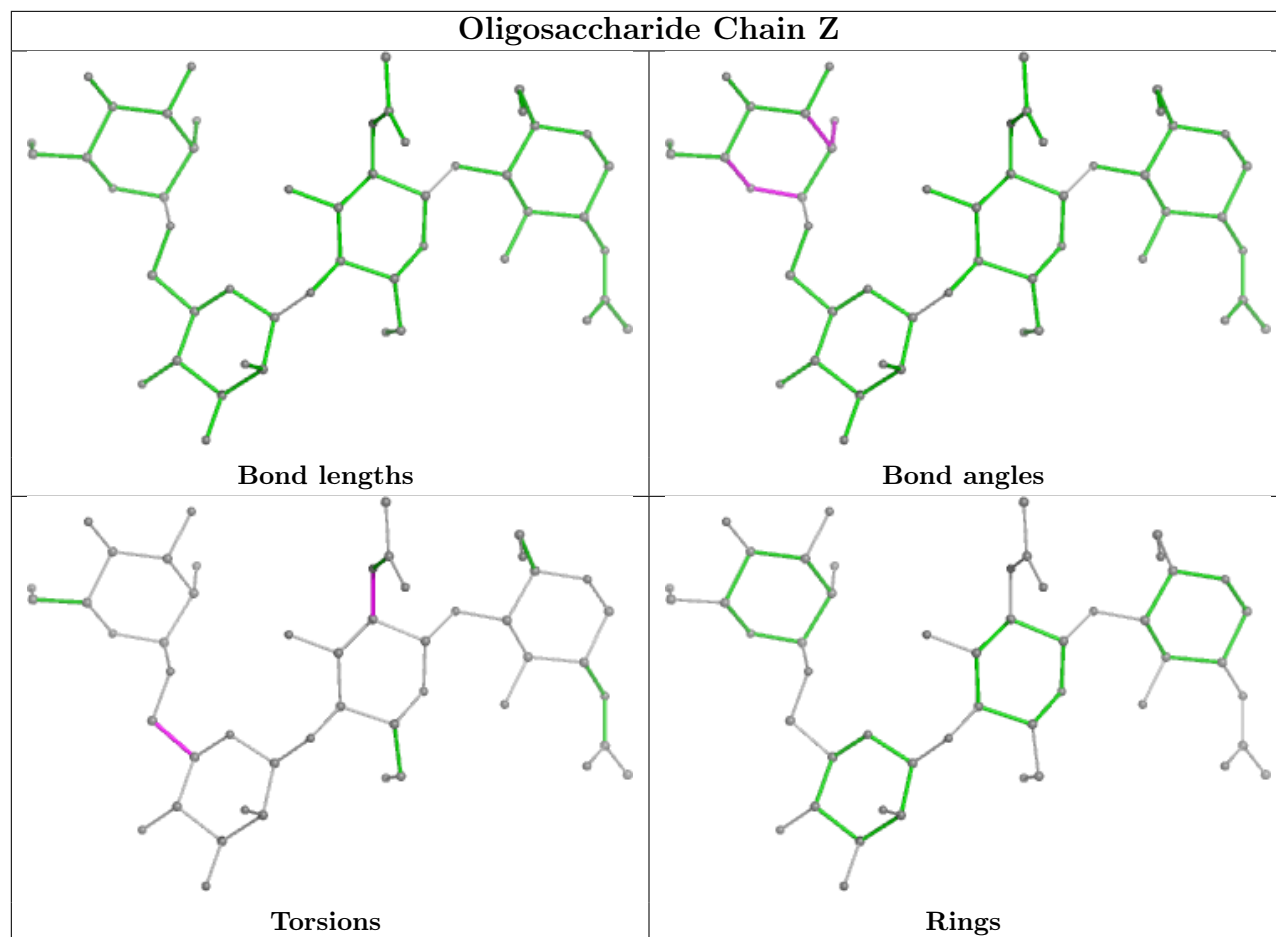


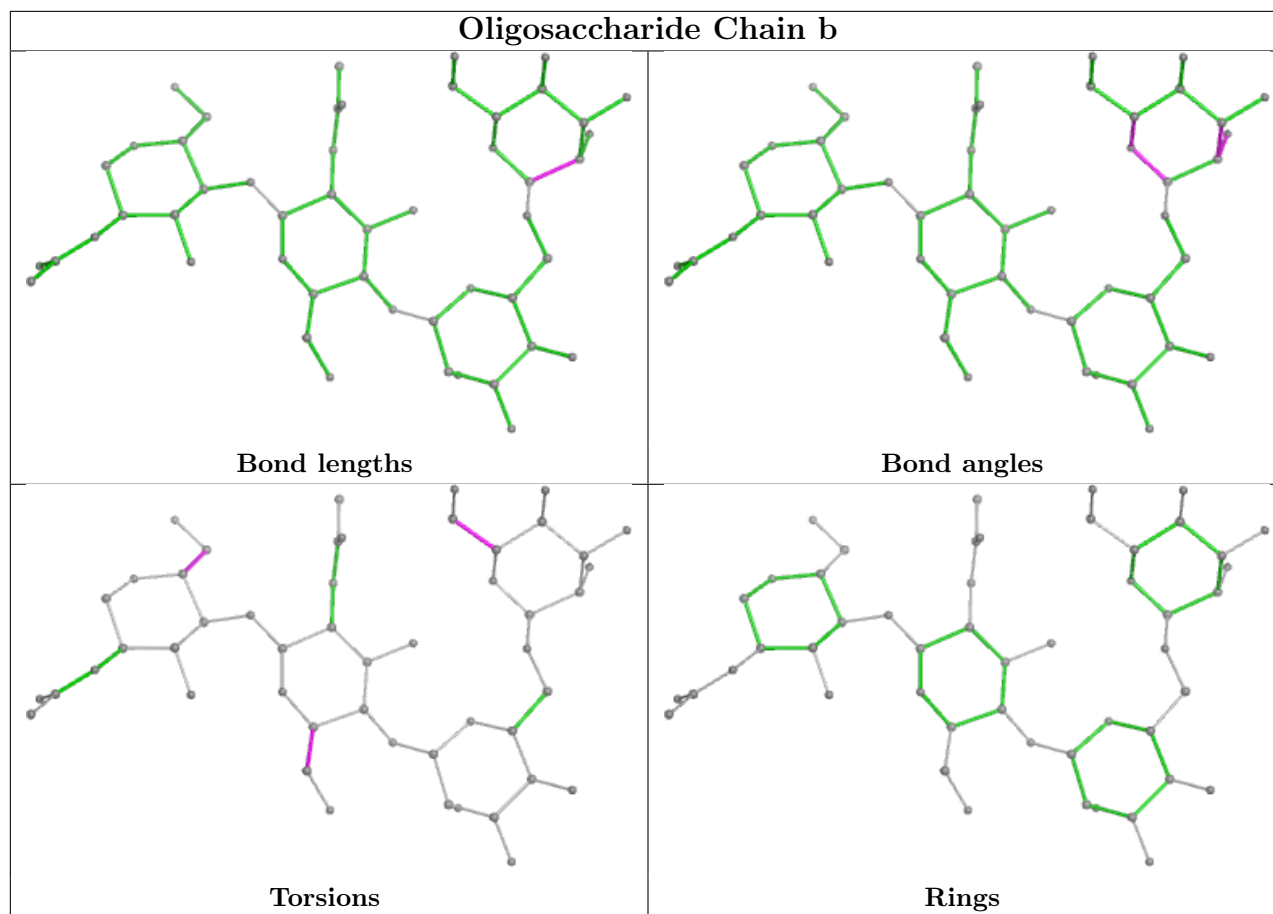












5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	G	405	1	14,14,15	0.35	0	17,19,21	0.61	0
7	NAG	F	406	1	14,14,15	0.40	0	17,19,21	0.47	0
7	NAG	H	404	1	14,14,15	0.27	0	17,19,21	0.48	0
7	NAG	D	404	1	14,14,15	0.27	0	17,19,21	0.39	0
7	NAG	A	409	1	14,14,15	0.37	0	17,19,21	0.48	0
7	NAG	G	408	1	14,14,15	0.34	0	17,19,21	0.45	0
7	NAG	F	405	1	14,14,15	0.30	0	17,19,21	0.44	0
7	NAG	E	406	1	14,14,15	0.26	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	410	1	14,14,15	0.28	0	17,19,21	0.48	0
7	NAG	E	405	1	14,14,15	0.35	0	17,19,21	0.52	0
7	NAG	A	404	1	14,14,15	0.63	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	A	405	1	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	D	405	1	14,14,15	0.31	0	17,19,21	0.53	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
7	NAG	G	405	1	-	3/6/23/26	0/1/1/1
7	NAG	F	406	1	-	2/6/23/26	0/1/1/1
7	NAG	H	404	1	-	0/6/23/26	0/1/1/1
7	NAG	D	404	1	-	2/6/23/26	0/1/1/1
7	NAG	A	409	1	-	1/6/23/26	0/1/1/1
7	NAG	G	408	1	-	1/6/23/26	0/1/1/1
7	NAG	F	405	1	-	3/6/23/26	0/1/1/1
7	NAG	E	406	1	-	0/6/23/26	0/1/1/1
7	NAG	E	410	1	-	1/6/23/26	0/1/1/1
7	NAG	E	405	1	-	2/6/23/26	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
7	NAG	A	405	1	-	3/6/23/26	0/1/1/1
7	NAG	D	405	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	404	NAG	C1-C2	2.07	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	404	NAG	C1-O5-C5	3.54	116.99	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	404	NAG	O5-C5-C6-O6
7	A	405	NAG	O5-C5-C6-O6
7	E	405	NAG	O5-C5-C6-O6
7	G	405	NAG	O5-C5-C6-O6
7	F	405	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/361 (94%)	-1.21	0 100 100	39, 71, 118, 197	0
1	B	328/361 (90%)	-0.74	0 100 100	64, 122, 174, 233	0
1	C	343/361 (95%)	-1.27	0 100 100	38, 69, 117, 178	0
1	D	336/361 (93%)	-1.08	0 100 100	32, 82, 160, 196	0
1	E	344/361 (95%)	-1.31	0 100 100	34, 67, 113, 175	0
1	F	336/361 (93%)	-1.04	0 100 100	33, 82, 171, 241	0
1	G	342/361 (94%)	-1.22	0 100 100	36, 72, 115, 208	0
1	H	325/361 (90%)	-0.64	0 100 100	69, 123, 188, 257	0
2	I	47/56 (83%)	-1.22	0 100 100	46, 73, 112, 127	0
2	J	46/56 (82%)	-0.56	0 100 100	93, 134, 172, 265	0
2	K	45/56 (80%)	-1.02	0 100 100	57, 88, 126, 150	0
2	L	47/56 (83%)	-1.16	0 100 100	55, 78, 111, 120	0
2	M	47/56 (83%)	-1.01	0 100 100	61, 93, 136, 170	0
2	N	46/56 (82%)	-1.22	0 100 100	52, 76, 99, 131	0
2	O	47/56 (83%)	-1.25	0 100 100	50, 74, 117, 139	0
2	P	45/56 (80%)	-0.65	0 100 100	93, 125, 171, 192	0
All	All	3066/3336 (91%)	-1.06	0 100 100	32, 85, 162, 265	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	D	405	14/15	0.95	0.08	104,127,138,141	0
7	NAG	E	406	14/15	0.95	0.08	88,128,148,153	0
7	NAG	E	410	14/15	0.96	0.06	97,117,128,129	0
7	NAG	F	405	14/15	0.96	0.06	86,108,121,124	0
7	NAG	F	406	14/15	0.96	0.09	112,130,141,141	0
7	NAG	A	404	14/15	0.97	0.06	100,124,134,145	0
7	NAG	G	405	14/15	0.97	0.05	73,98,118,124	0
7	NAG	H	404	14/15	0.97	0.06	106,127,133,134	0
7	NAG	A	405	14/15	0.98	0.05	86,99,108,112	0
7	NAG	E	405	14/15	0.98	0.04	64,70,75,76	0
7	NAG	A	409	14/15	0.98	0.06	102,124,135,136	0
7	NAG	G	408	14/15	0.98	0.07	106,126,133,136	0
7	NAG	D	404	14/15	0.98	0.06	111,127,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.