



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:08 PM UTC

PDB ID : 6U2L / pdb_00006u2l
EMDB ID : EMD-20623
Title : EM structure of MPEG-1 (L425K, beta conformation) soluble pre-pore complex
Authors : Pang, S.S.; Bayly-Jones, C.
Deposited on : 2019-08-20
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

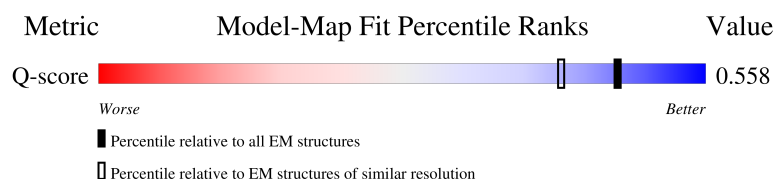
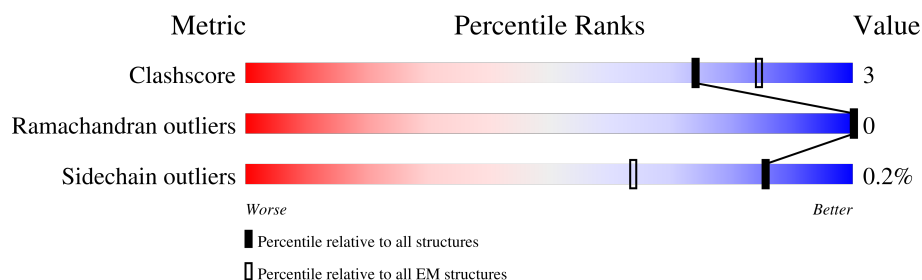
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	642	 7% 86% 9% 5%
1	AA	642	 6% 86% 9% 5%
1	B	642	 7% 83% 12% 5%
1	BB	642	 7% 86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	C	642	
1	CC	642	
1	D	642	
1	DD	642	
1	E	642	
1	EE	642	
1	F	642	
1	FF	642	
1	G	642	
1	GG	642	
1	H	642	
1	HH	642	
1	I	642	
1	II	642	
1	J	642	
1	JJ	642	
1	K	642	
1	KK	642	
1	L	642	
1	LL	642	
1	M	642	
1	MM	642	
1	N	642	
1	NN	642	
1	O	642	

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Mol	Chain	Length	Quality of chain
1	OO	642	
1	P	642	
1	PP	642	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	
2	a	2	
2	b	2	
2	c	2	
2	d	2	
2	e	2	
2	f	2	
2	g	2	
2	h	2	
2	i	2	
2	j	2	
2	k	2	
2	l	2	

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Mol	Chain	Length	Quality of chain	
2	m	2	50%	
				50%
2	n	2	50%	
				50%
2	o	2	50%	
				50%
2	p	2	50%	
				50%
2	q	2	50%	
				50%
2	r	2	50%	
				50%
2	s	2	50%	
				50%
2	t	2	50%	
				50%
2	u	2	50%	
				50%
2	v	2	50%	
				50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 153756 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 Macrophage-expressed gene 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	B	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	C	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	D	613	Total	C	N	O	S	0	0
			4762	3008	819	907	28		
1	E	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	F	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	G	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	H	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	I	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	J	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	K	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	L	613	Total	C	N	O	S	0	0
			4762	3008	819	907	28		
1	M	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	N	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	O	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	P	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	AA	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BB	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	CC	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	DD	613	Total	C	N	O	S	0	0
			4762	3008	819	907	28		
1	EE	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	FF	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	GG	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	HH	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	II	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	JJ	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	KK	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	LL	613	Total	C	N	O	S	0	0
			4762	3008	819	907	28		
1	MM	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	NN	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	OO	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		
1	PP	613	Total	C	N	O	S	0	0
			4763	3008	819	908	28		

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	LYS	LEU	engineered mutation	UNP Q2M385
A	637	HIS	-	expression tag	UNP Q2M385
A	638	HIS	-	expression tag	UNP Q2M385
A	639	HIS	-	expression tag	UNP Q2M385
A	640	HIS	-	expression tag	UNP Q2M385
A	641	HIS	-	expression tag	UNP Q2M385
A	642	HIS	-	expression tag	UNP Q2M385
B	425	LYS	LEU	engineered mutation	UNP Q2M385
B	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
B	638	HIS	-	expression tag	UNP Q2M385
B	639	HIS	-	expression tag	UNP Q2M385
B	640	HIS	-	expression tag	UNP Q2M385
B	641	HIS	-	expression tag	UNP Q2M385
B	642	HIS	-	expression tag	UNP Q2M385
C	425	LYS	LEU	engineered mutation	UNP Q2M385
C	637	HIS	-	expression tag	UNP Q2M385
C	638	HIS	-	expression tag	UNP Q2M385
C	639	HIS	-	expression tag	UNP Q2M385
C	640	HIS	-	expression tag	UNP Q2M385
C	641	HIS	-	expression tag	UNP Q2M385
C	642	HIS	-	expression tag	UNP Q2M385
D	425	LYS	LEU	engineered mutation	UNP Q2M385
D	637	HIS	-	expression tag	UNP Q2M385
D	638	HIS	-	expression tag	UNP Q2M385
D	639	HIS	-	expression tag	UNP Q2M385
D	640	HIS	-	expression tag	UNP Q2M385
D	641	HIS	-	expression tag	UNP Q2M385
D	642	HIS	-	expression tag	UNP Q2M385
E	425	LYS	LEU	engineered mutation	UNP Q2M385
E	637	HIS	-	expression tag	UNP Q2M385
E	638	HIS	-	expression tag	UNP Q2M385
E	639	HIS	-	expression tag	UNP Q2M385
E	640	HIS	-	expression tag	UNP Q2M385
E	641	HIS	-	expression tag	UNP Q2M385
E	642	HIS	-	expression tag	UNP Q2M385
F	425	LYS	LEU	engineered mutation	UNP Q2M385
F	637	HIS	-	expression tag	UNP Q2M385
F	638	HIS	-	expression tag	UNP Q2M385
F	639	HIS	-	expression tag	UNP Q2M385
F	640	HIS	-	expression tag	UNP Q2M385
F	641	HIS	-	expression tag	UNP Q2M385
F	642	HIS	-	expression tag	UNP Q2M385
G	425	LYS	LEU	engineered mutation	UNP Q2M385
G	637	HIS	-	expression tag	UNP Q2M385
G	638	HIS	-	expression tag	UNP Q2M385
G	639	HIS	-	expression tag	UNP Q2M385
G	640	HIS	-	expression tag	UNP Q2M385
G	641	HIS	-	expression tag	UNP Q2M385
G	642	HIS	-	expression tag	UNP Q2M385
H	425	LYS	LEU	engineered mutation	UNP Q2M385
H	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
H	638	HIS	-	expression tag	UNP Q2M385
H	639	HIS	-	expression tag	UNP Q2M385
H	640	HIS	-	expression tag	UNP Q2M385
H	641	HIS	-	expression tag	UNP Q2M385
H	642	HIS	-	expression tag	UNP Q2M385
I	425	LYS	LEU	engineered mutation	UNP Q2M385
I	637	HIS	-	expression tag	UNP Q2M385
I	638	HIS	-	expression tag	UNP Q2M385
I	639	HIS	-	expression tag	UNP Q2M385
I	640	HIS	-	expression tag	UNP Q2M385
I	641	HIS	-	expression tag	UNP Q2M385
I	642	HIS	-	expression tag	UNP Q2M385
J	425	LYS	LEU	engineered mutation	UNP Q2M385
J	637	HIS	-	expression tag	UNP Q2M385
J	638	HIS	-	expression tag	UNP Q2M385
J	639	HIS	-	expression tag	UNP Q2M385
J	640	HIS	-	expression tag	UNP Q2M385
J	641	HIS	-	expression tag	UNP Q2M385
J	642	HIS	-	expression tag	UNP Q2M385
K	425	LYS	LEU	engineered mutation	UNP Q2M385
K	637	HIS	-	expression tag	UNP Q2M385
K	638	HIS	-	expression tag	UNP Q2M385
K	639	HIS	-	expression tag	UNP Q2M385
K	640	HIS	-	expression tag	UNP Q2M385
K	641	HIS	-	expression tag	UNP Q2M385
K	642	HIS	-	expression tag	UNP Q2M385
L	425	LYS	LEU	engineered mutation	UNP Q2M385
L	637	HIS	-	expression tag	UNP Q2M385
L	638	HIS	-	expression tag	UNP Q2M385
L	639	HIS	-	expression tag	UNP Q2M385
L	640	HIS	-	expression tag	UNP Q2M385
L	641	HIS	-	expression tag	UNP Q2M385
L	642	HIS	-	expression tag	UNP Q2M385
M	425	LYS	LEU	engineered mutation	UNP Q2M385
M	637	HIS	-	expression tag	UNP Q2M385
M	638	HIS	-	expression tag	UNP Q2M385
M	639	HIS	-	expression tag	UNP Q2M385
M	640	HIS	-	expression tag	UNP Q2M385
M	641	HIS	-	expression tag	UNP Q2M385
M	642	HIS	-	expression tag	UNP Q2M385
N	425	LYS	LEU	engineered mutation	UNP Q2M385
N	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
N	638	HIS	-	expression tag	UNP Q2M385
N	639	HIS	-	expression tag	UNP Q2M385
N	640	HIS	-	expression tag	UNP Q2M385
N	641	HIS	-	expression tag	UNP Q2M385
N	642	HIS	-	expression tag	UNP Q2M385
O	425	LYS	LEU	engineered mutation	UNP Q2M385
O	637	HIS	-	expression tag	UNP Q2M385
O	638	HIS	-	expression tag	UNP Q2M385
O	639	HIS	-	expression tag	UNP Q2M385
O	640	HIS	-	expression tag	UNP Q2M385
O	641	HIS	-	expression tag	UNP Q2M385
O	642	HIS	-	expression tag	UNP Q2M385
P	425	LYS	LEU	engineered mutation	UNP Q2M385
P	637	HIS	-	expression tag	UNP Q2M385
P	638	HIS	-	expression tag	UNP Q2M385
P	639	HIS	-	expression tag	UNP Q2M385
P	640	HIS	-	expression tag	UNP Q2M385
P	641	HIS	-	expression tag	UNP Q2M385
P	642	HIS	-	expression tag	UNP Q2M385
AA	425	LYS	LEU	engineered mutation	UNP Q2M385
AA	637	HIS	-	expression tag	UNP Q2M385
AA	638	HIS	-	expression tag	UNP Q2M385
AA	639	HIS	-	expression tag	UNP Q2M385
AA	640	HIS	-	expression tag	UNP Q2M385
AA	641	HIS	-	expression tag	UNP Q2M385
AA	642	HIS	-	expression tag	UNP Q2M385
BB	425	LYS	LEU	engineered mutation	UNP Q2M385
BB	637	HIS	-	expression tag	UNP Q2M385
BB	638	HIS	-	expression tag	UNP Q2M385
BB	639	HIS	-	expression tag	UNP Q2M385
BB	640	HIS	-	expression tag	UNP Q2M385
BB	641	HIS	-	expression tag	UNP Q2M385
BB	642	HIS	-	expression tag	UNP Q2M385
CC	425	LYS	LEU	engineered mutation	UNP Q2M385
CC	637	HIS	-	expression tag	UNP Q2M385
CC	638	HIS	-	expression tag	UNP Q2M385
CC	639	HIS	-	expression tag	UNP Q2M385
CC	640	HIS	-	expression tag	UNP Q2M385
CC	641	HIS	-	expression tag	UNP Q2M385
CC	642	HIS	-	expression tag	UNP Q2M385
DD	425	LYS	LEU	engineered mutation	UNP Q2M385
DD	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	638	HIS	-	expression tag	UNP Q2M385
DD	639	HIS	-	expression tag	UNP Q2M385
DD	640	HIS	-	expression tag	UNP Q2M385
DD	641	HIS	-	expression tag	UNP Q2M385
DD	642	HIS	-	expression tag	UNP Q2M385
EE	425	LYS	LEU	engineered mutation	UNP Q2M385
EE	637	HIS	-	expression tag	UNP Q2M385
EE	638	HIS	-	expression tag	UNP Q2M385
EE	639	HIS	-	expression tag	UNP Q2M385
EE	640	HIS	-	expression tag	UNP Q2M385
EE	641	HIS	-	expression tag	UNP Q2M385
EE	642	HIS	-	expression tag	UNP Q2M385
FF	425	LYS	LEU	engineered mutation	UNP Q2M385
FF	637	HIS	-	expression tag	UNP Q2M385
FF	638	HIS	-	expression tag	UNP Q2M385
FF	639	HIS	-	expression tag	UNP Q2M385
FF	640	HIS	-	expression tag	UNP Q2M385
FF	641	HIS	-	expression tag	UNP Q2M385
FF	642	HIS	-	expression tag	UNP Q2M385
GG	425	LYS	LEU	engineered mutation	UNP Q2M385
GG	637	HIS	-	expression tag	UNP Q2M385
GG	638	HIS	-	expression tag	UNP Q2M385
GG	639	HIS	-	expression tag	UNP Q2M385
GG	640	HIS	-	expression tag	UNP Q2M385
GG	641	HIS	-	expression tag	UNP Q2M385
GG	642	HIS	-	expression tag	UNP Q2M385
HH	425	LYS	LEU	engineered mutation	UNP Q2M385
HH	637	HIS	-	expression tag	UNP Q2M385
HH	638	HIS	-	expression tag	UNP Q2M385
HH	639	HIS	-	expression tag	UNP Q2M385
HH	640	HIS	-	expression tag	UNP Q2M385
HH	641	HIS	-	expression tag	UNP Q2M385
HH	642	HIS	-	expression tag	UNP Q2M385
II	425	LYS	LEU	engineered mutation	UNP Q2M385
II	637	HIS	-	expression tag	UNP Q2M385
II	638	HIS	-	expression tag	UNP Q2M385
II	639	HIS	-	expression tag	UNP Q2M385
II	640	HIS	-	expression tag	UNP Q2M385
II	641	HIS	-	expression tag	UNP Q2M385
II	642	HIS	-	expression tag	UNP Q2M385
JJ	425	LYS	LEU	engineered mutation	UNP Q2M385
JJ	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
JJ	638	HIS	-	expression tag	UNP Q2M385
JJ	639	HIS	-	expression tag	UNP Q2M385
JJ	640	HIS	-	expression tag	UNP Q2M385
JJ	641	HIS	-	expression tag	UNP Q2M385
JJ	642	HIS	-	expression tag	UNP Q2M385
KK	425	LYS	LEU	engineered mutation	UNP Q2M385
KK	637	HIS	-	expression tag	UNP Q2M385
KK	638	HIS	-	expression tag	UNP Q2M385
KK	639	HIS	-	expression tag	UNP Q2M385
KK	640	HIS	-	expression tag	UNP Q2M385
KK	641	HIS	-	expression tag	UNP Q2M385
KK	642	HIS	-	expression tag	UNP Q2M385
LL	425	LYS	LEU	engineered mutation	UNP Q2M385
LL	637	HIS	-	expression tag	UNP Q2M385
LL	638	HIS	-	expression tag	UNP Q2M385
LL	639	HIS	-	expression tag	UNP Q2M385
LL	640	HIS	-	expression tag	UNP Q2M385
LL	641	HIS	-	expression tag	UNP Q2M385
LL	642	HIS	-	expression tag	UNP Q2M385
MM	425	LYS	LEU	engineered mutation	UNP Q2M385
MM	637	HIS	-	expression tag	UNP Q2M385
MM	638	HIS	-	expression tag	UNP Q2M385
MM	639	HIS	-	expression tag	UNP Q2M385
MM	640	HIS	-	expression tag	UNP Q2M385
MM	641	HIS	-	expression tag	UNP Q2M385
MM	642	HIS	-	expression tag	UNP Q2M385
NN	425	LYS	LEU	engineered mutation	UNP Q2M385
NN	637	HIS	-	expression tag	UNP Q2M385
NN	638	HIS	-	expression tag	UNP Q2M385
NN	639	HIS	-	expression tag	UNP Q2M385
NN	640	HIS	-	expression tag	UNP Q2M385
NN	641	HIS	-	expression tag	UNP Q2M385
NN	642	HIS	-	expression tag	UNP Q2M385
OO	425	LYS	LEU	engineered mutation	UNP Q2M385
OO	637	HIS	-	expression tag	UNP Q2M385
OO	638	HIS	-	expression tag	UNP Q2M385
OO	639	HIS	-	expression tag	UNP Q2M385
OO	640	HIS	-	expression tag	UNP Q2M385
OO	641	HIS	-	expression tag	UNP Q2M385
OO	642	HIS	-	expression tag	UNP Q2M385
PP	425	LYS	LEU	engineered mutation	UNP Q2M385
PP	637	HIS	-	expression tag	UNP Q2M385

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Chain	Residue	Modelled	Actual	Comment	Reference
PP	638	HIS	-	expression tag	UNP Q2M385
PP	639	HIS	-	expression tag	UNP Q2M385
PP	640	HIS	-	expression tag	UNP Q2M385
PP	641	HIS	-	expression tag	UNP Q2M385
PP	642	HIS	-	expression tag	UNP Q2M385

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



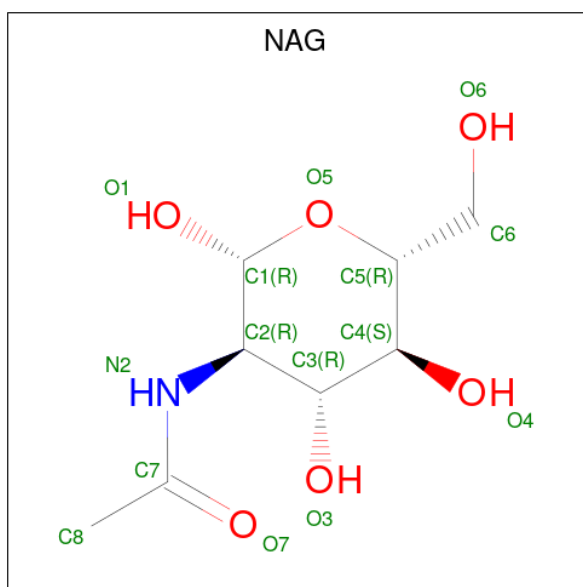
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	k	2	Total	C	N	O	0	0
			28	16	2	10		
2	l	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	p	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	t	2	Total	C	N	O	0	0
			28	16	2	10		
2	u	2	Total	C	N	O	0	0
			28	16	2	10		
2	v	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

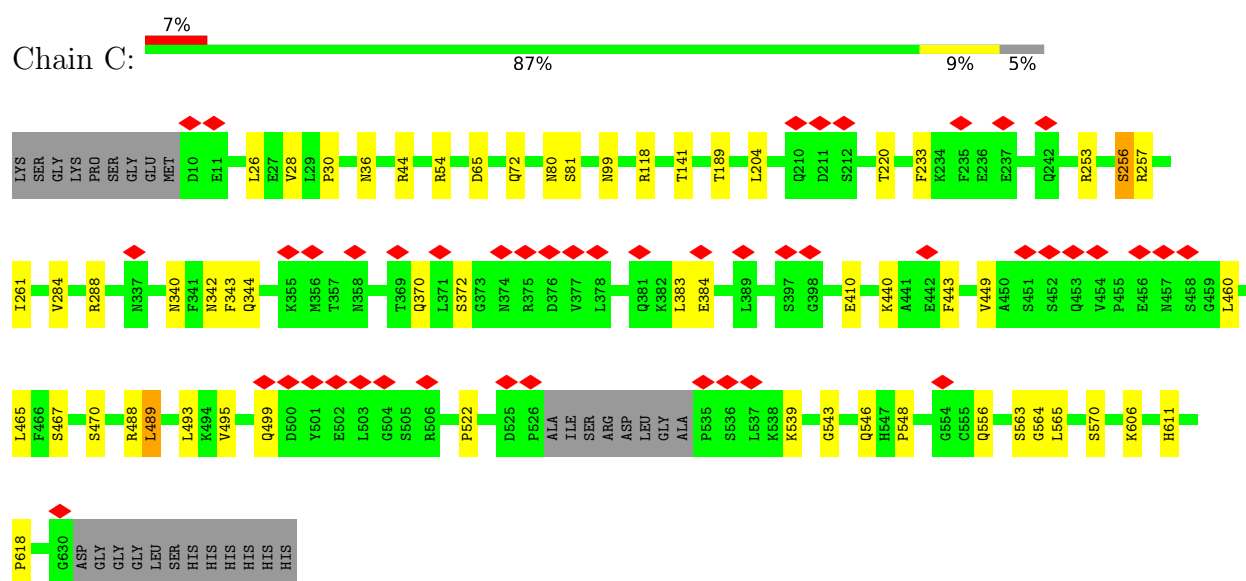


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	E	1	Total	C	N	O	0
			14	8	1	5	
3	F	1	Total	C	N	O	0
			14	8	1	5	
3	G	1	Total	C	N	O	0
			14	8	1	5	
3	H	1	Total	C	N	O	0
			14	8	1	5	
3	I	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	K	1	Total	C	N	O	0
			14	8	1	5	
3	L	1	Total	C	N	O	0
			14	8	1	5	
3	M	1	Total	C	N	O	0
			14	8	1	5	
3	N	1	Total	C	N	O	0
			14	8	1	5	

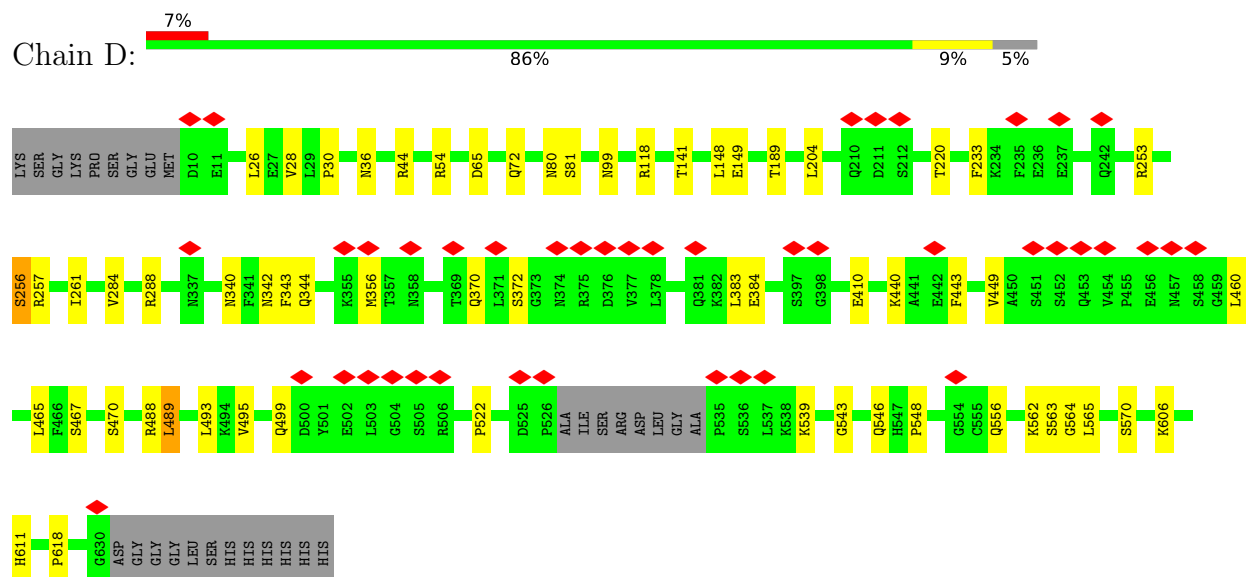
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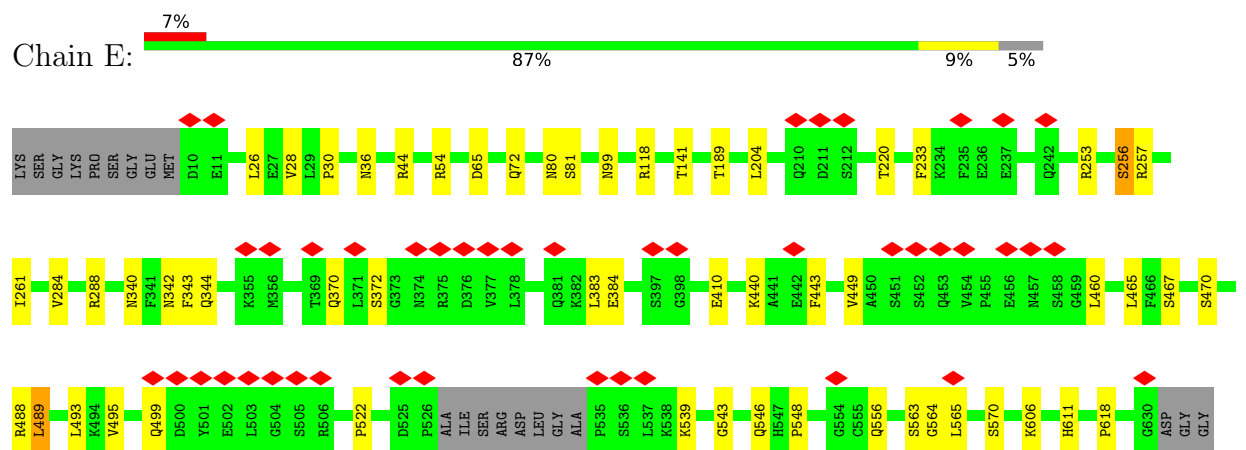
Mol	Chain	Residues	Atoms				AltConf
3	O	1	Total	C	N	O	0
			14	8	1	5	
3	P	1	Total	C	N	O	0
			14	8	1	5	
3	AA	1	Total	C	N	O	0
			14	8	1	5	
3	BB	1	Total	C	N	O	0
			14	8	1	5	
3	CC	1	Total	C	N	O	0
			14	8	1	5	
3	DD	1	Total	C	N	O	0
			14	8	1	5	
3	EE	1	Total	C	N	O	0
			14	8	1	5	
3	FF	1	Total	C	N	O	0
			14	8	1	5	
3	GG	1	Total	C	N	O	0
			14	8	1	5	
3	HH	1	Total	C	N	O	0
			14	8	1	5	
3	II	1	Total	C	N	O	0
			14	8	1	5	
3	JJ	1	Total	C	N	O	0
			14	8	1	5	
3	KK	1	Total	C	N	O	0
			14	8	1	5	
3	LL	1	Total	C	N	O	0
			14	8	1	5	
3	MM	1	Total	C	N	O	0
			14	8	1	5	
3	NN	1	Total	C	N	O	0
			14	8	1	5	
3	OO	1	Total	C	N	O	0
			14	8	1	5	
3	PP	1	Total	C	N	O	0
			14	8	1	5	

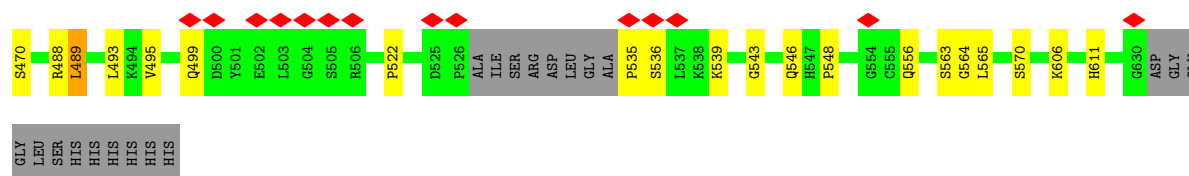


• Molecule 1: Macrophage-expressed gene 1 protein



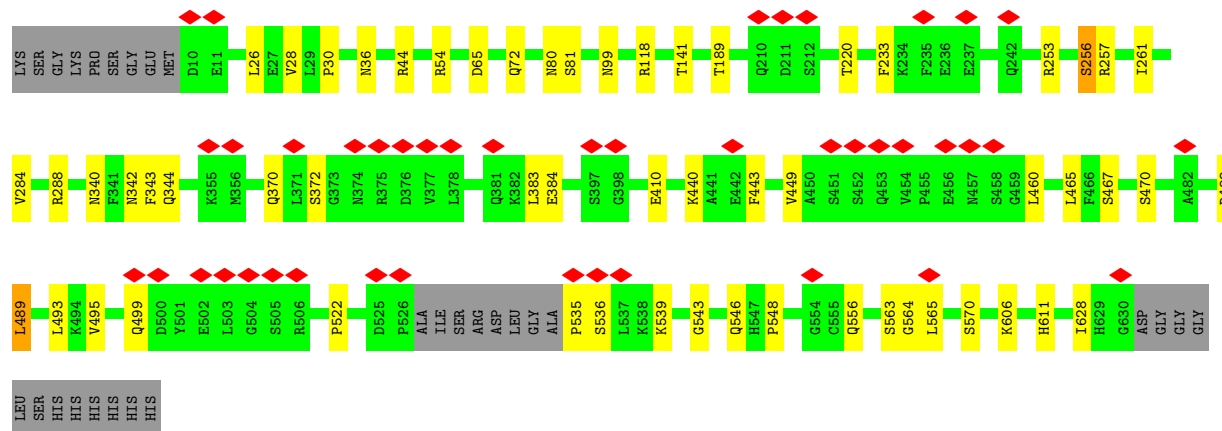
• Molecule 1: Macrophage-expressed gene 1 protein





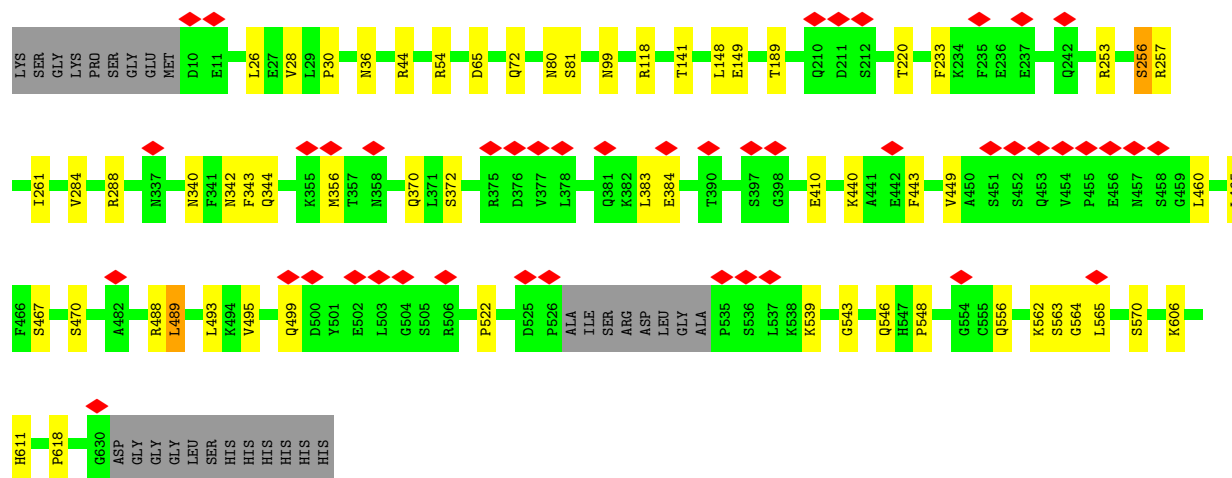
• Molecule 1: Macrophage-expressed gene 1 protein

Chain I: 7% 86% 9% 5%



• Molecule 1: Macrophage-expressed gene 1 protein

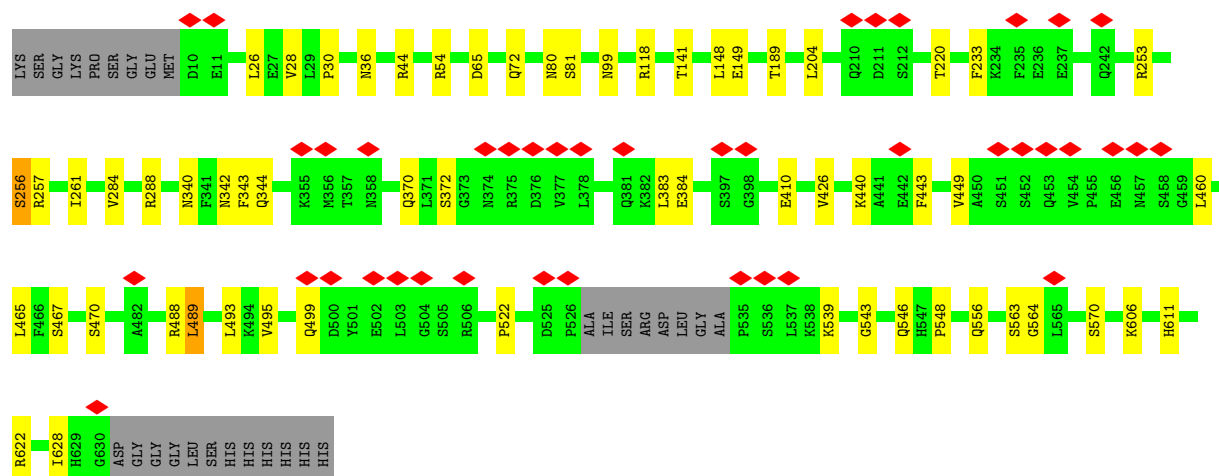
Chain J: 7% 86% 9% 5%



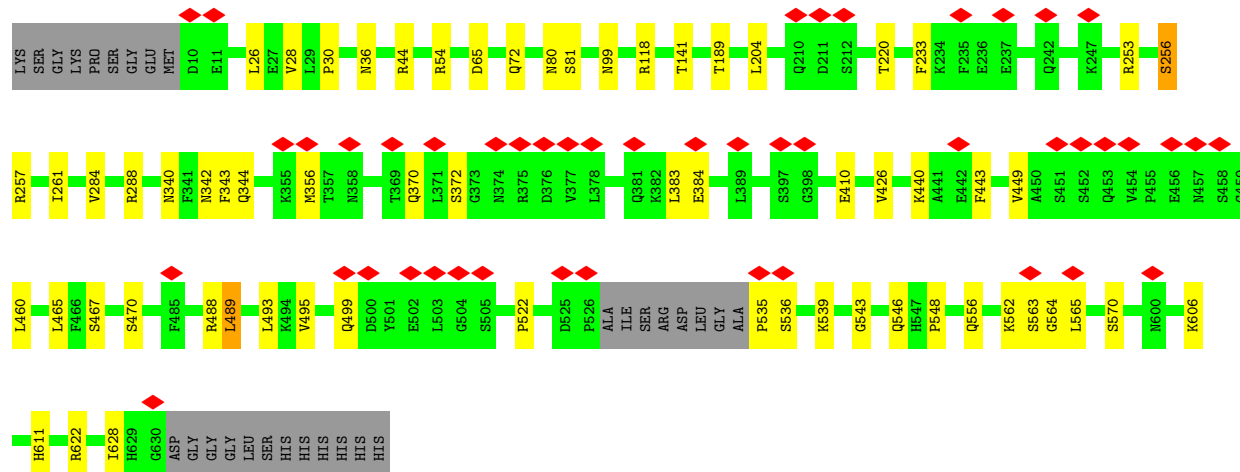
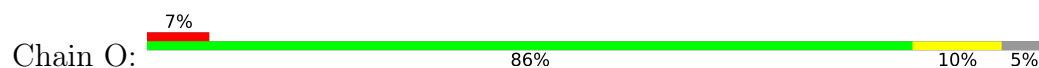
• Molecule 1: Macrophage-expressed gene 1 protein

Chain K: 7% 87% 9% 5%

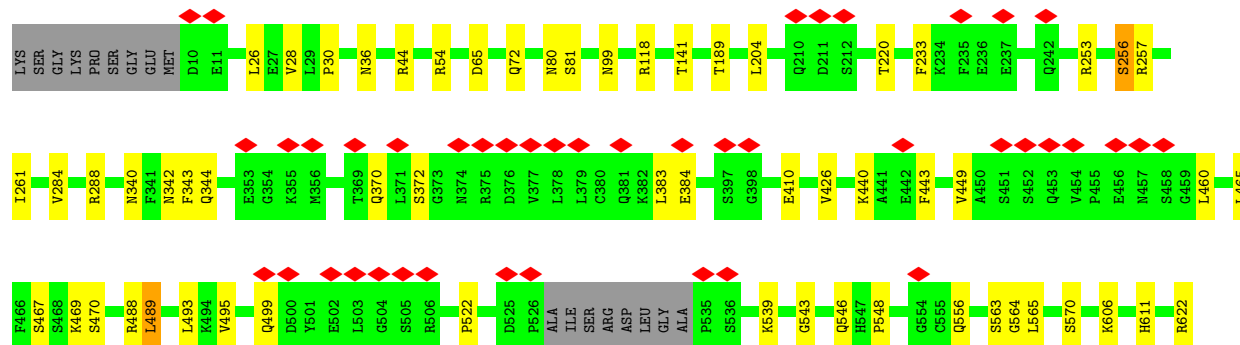
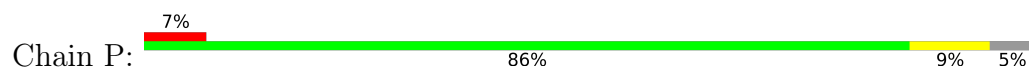


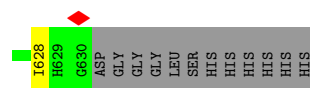


• Molecule 1: Macrophage-expressed gene 1 protein

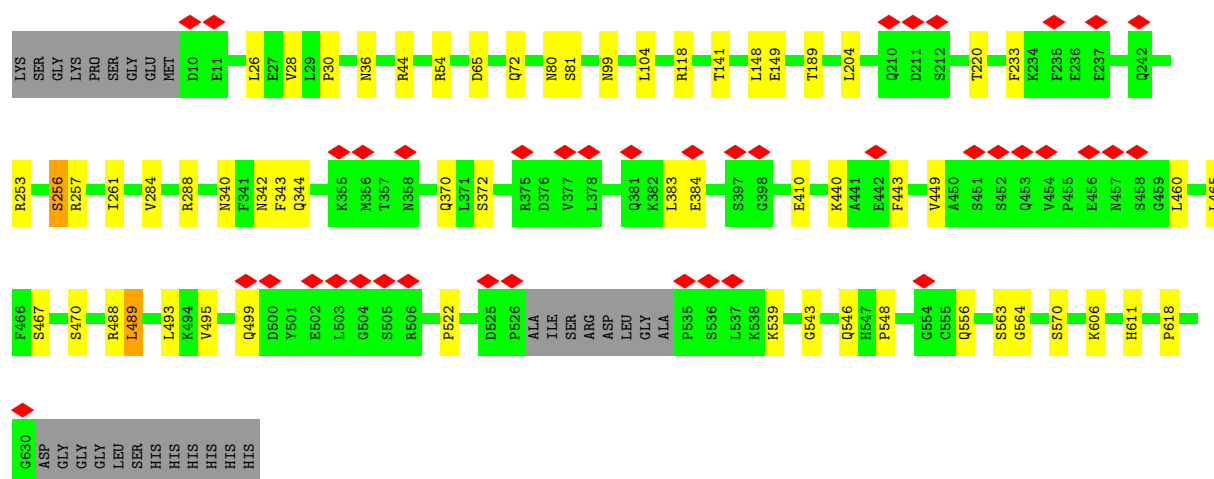
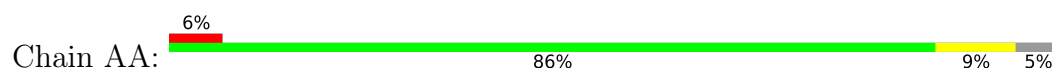


• Molecule 1: Macrophage-expressed gene 1 protein

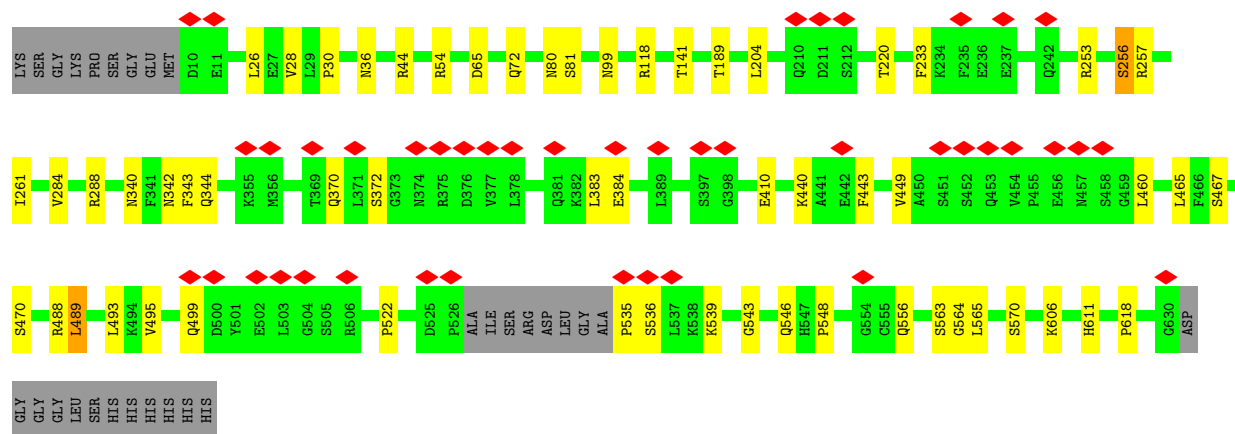
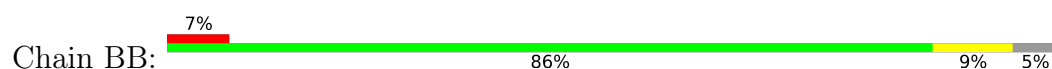




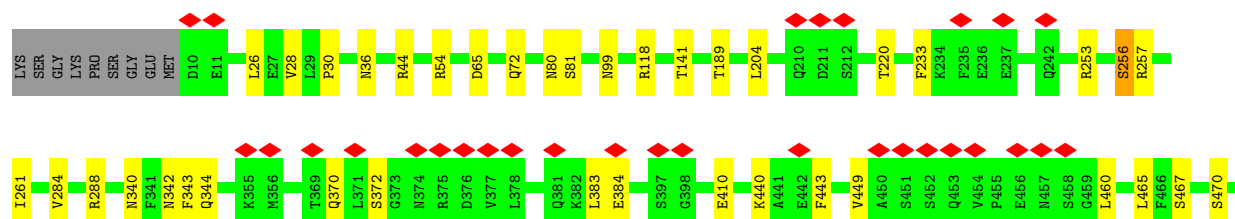
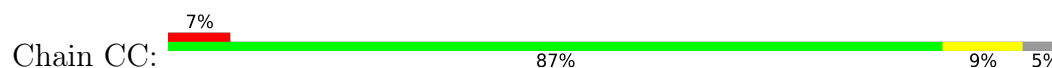
• Molecule 1: Macrophage-expressed gene 1 protein

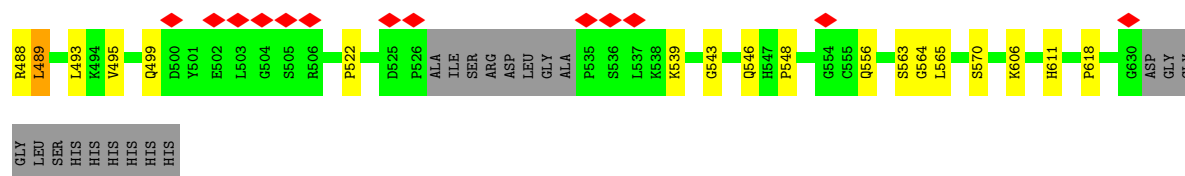


• Molecule 1: Macrophage-expressed gene 1 protein



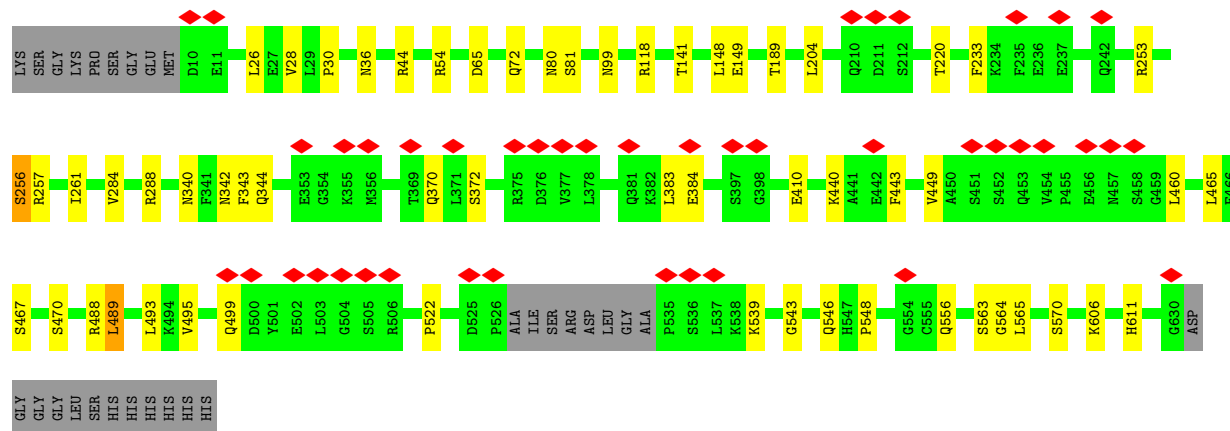
• Molecule 1: Macrophage-expressed gene 1 protein





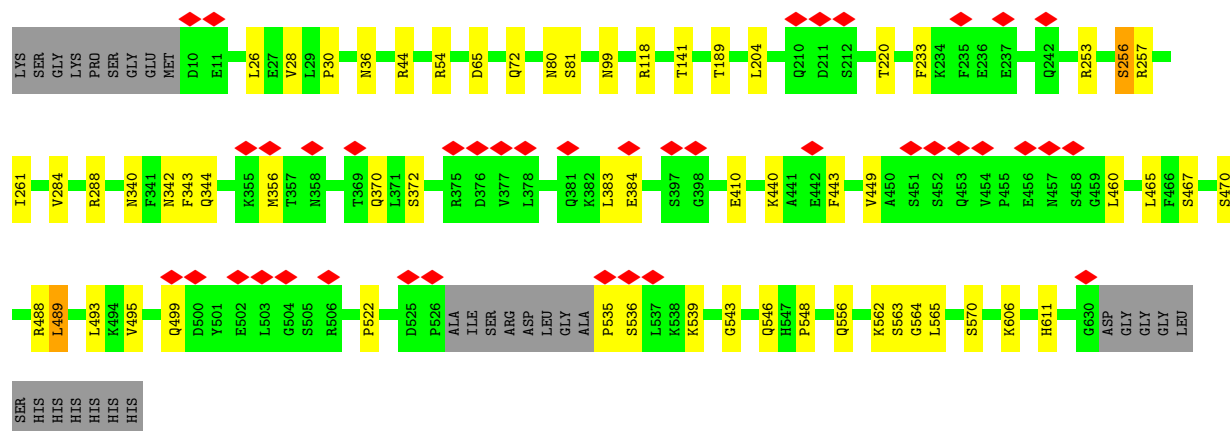
• Molecule 1: Macrophage-expressed gene 1 protein

Chain DD: 7% 86% 9% 5%



• Molecule 1: Macrophage-expressed gene 1 protein

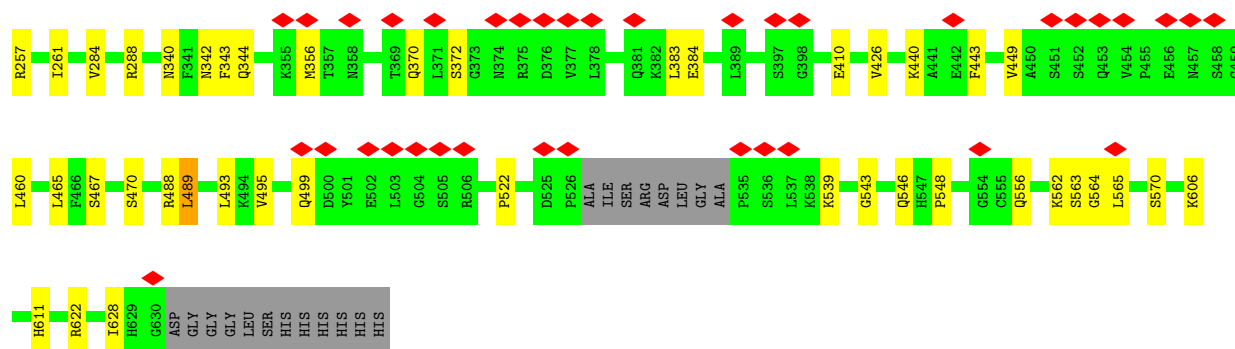
Chain EE: 6% 86% 9% 5%



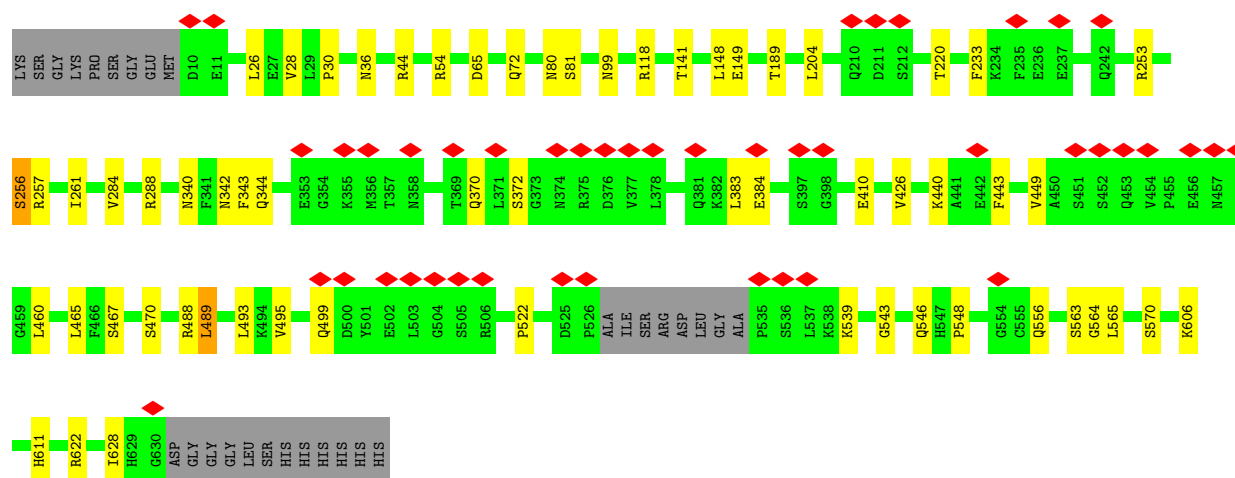
• Molecule 1: Macrophage-expressed gene 1 protein

Chain FF: 7% 86% 9% 5%

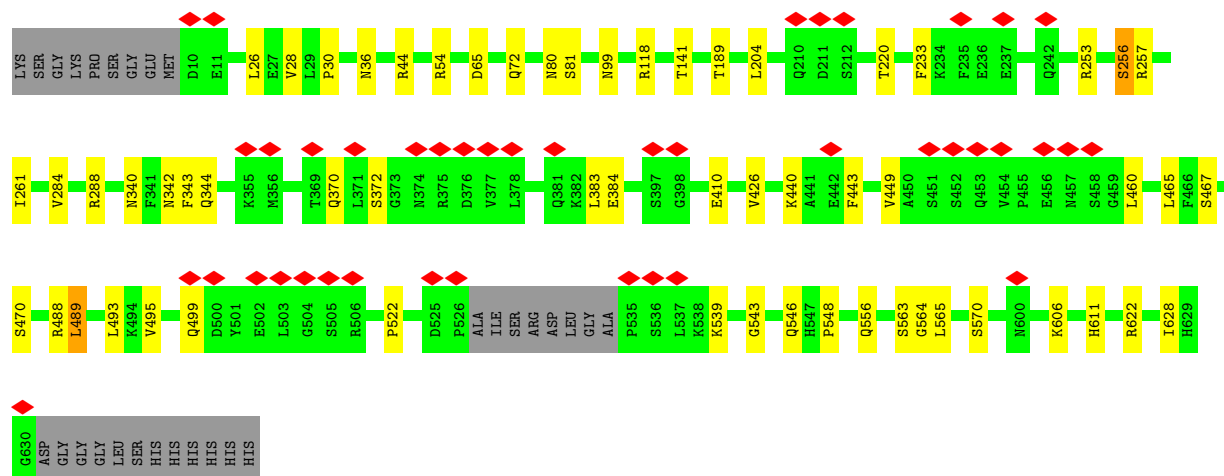
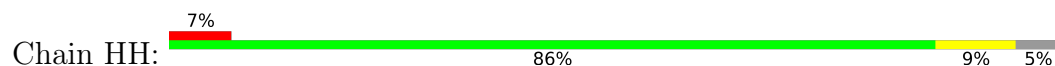




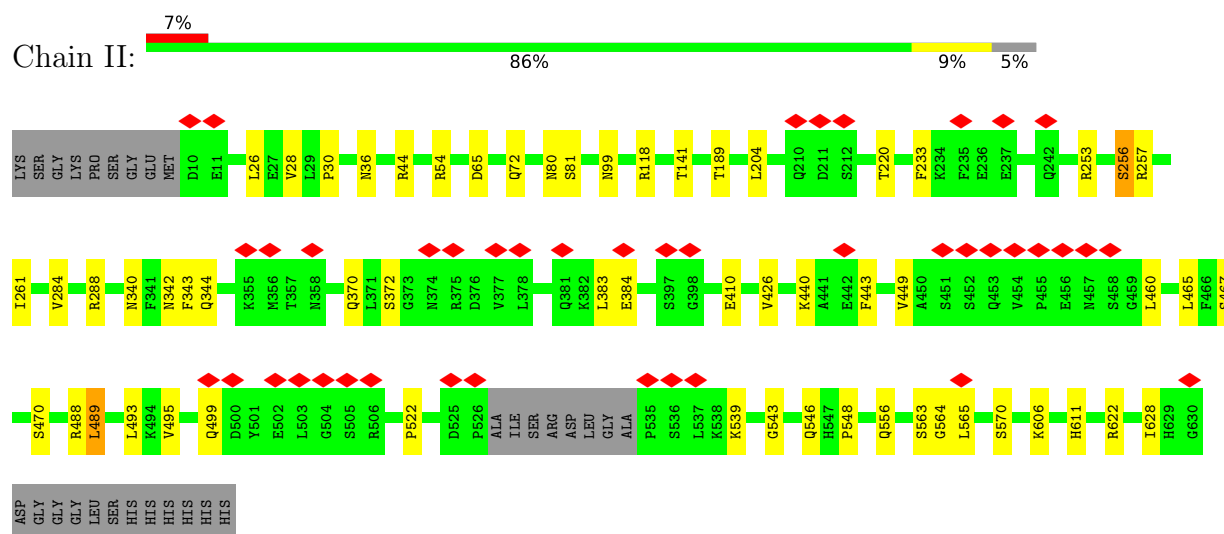
- Molecule 1: Macrophage-expressed gene 1 protein



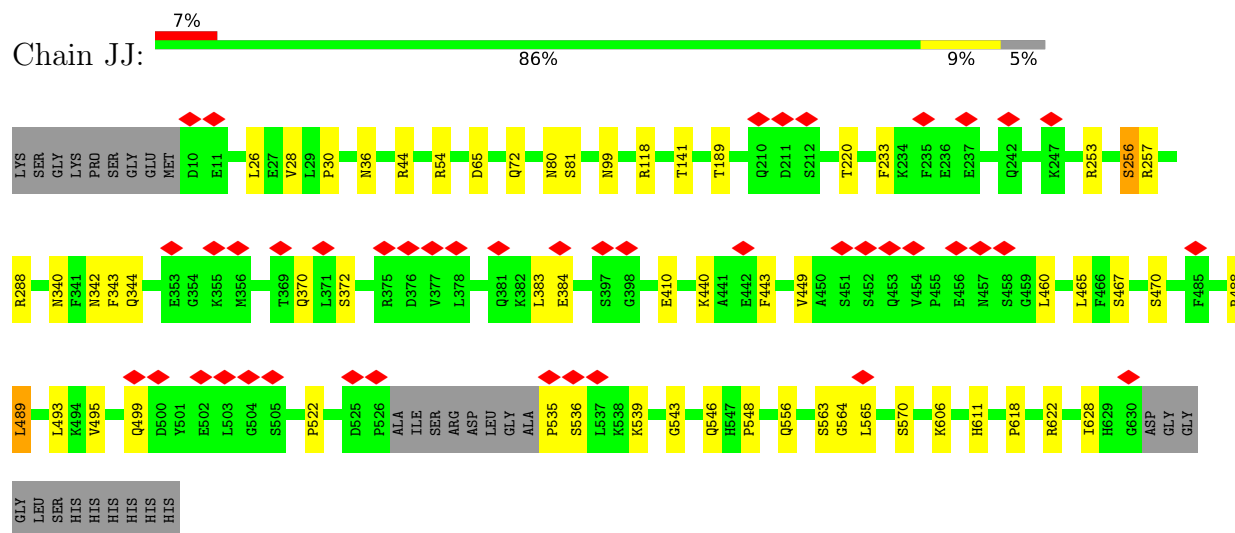
- Molecule 1: Macrophage-expressed gene 1 protein



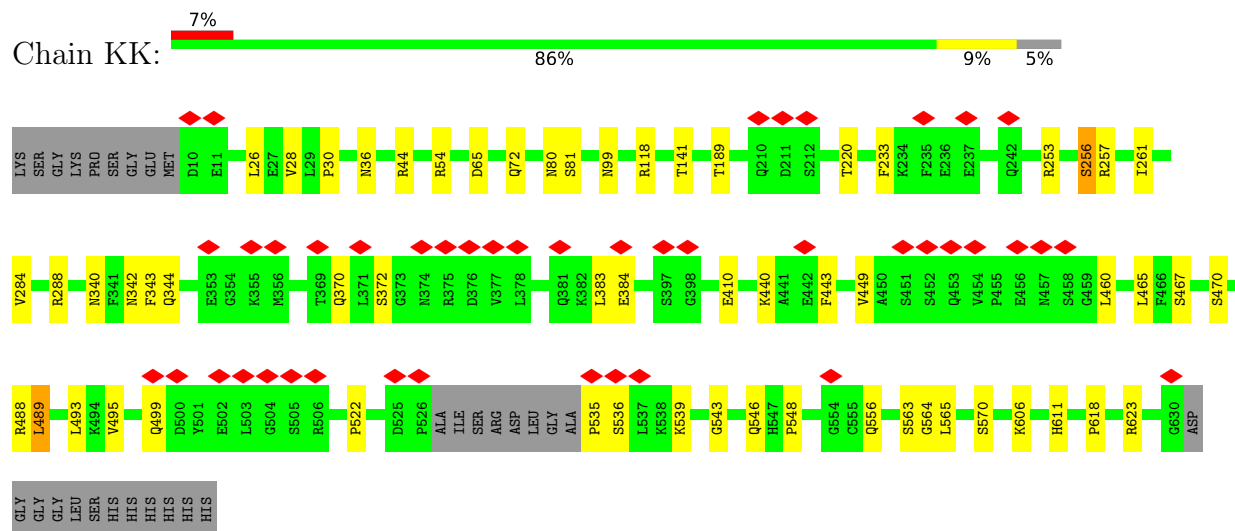
- Molecule 1: Macrophage-expressed gene 1 protein



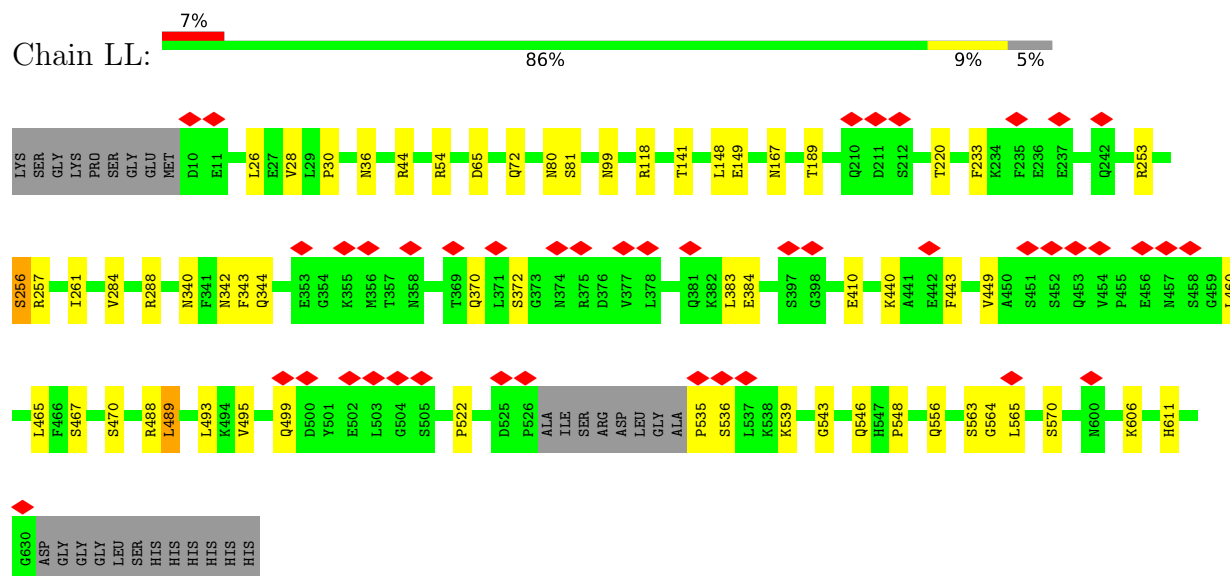
- Molecule 1: Macrophage-expressed gene 1 protein



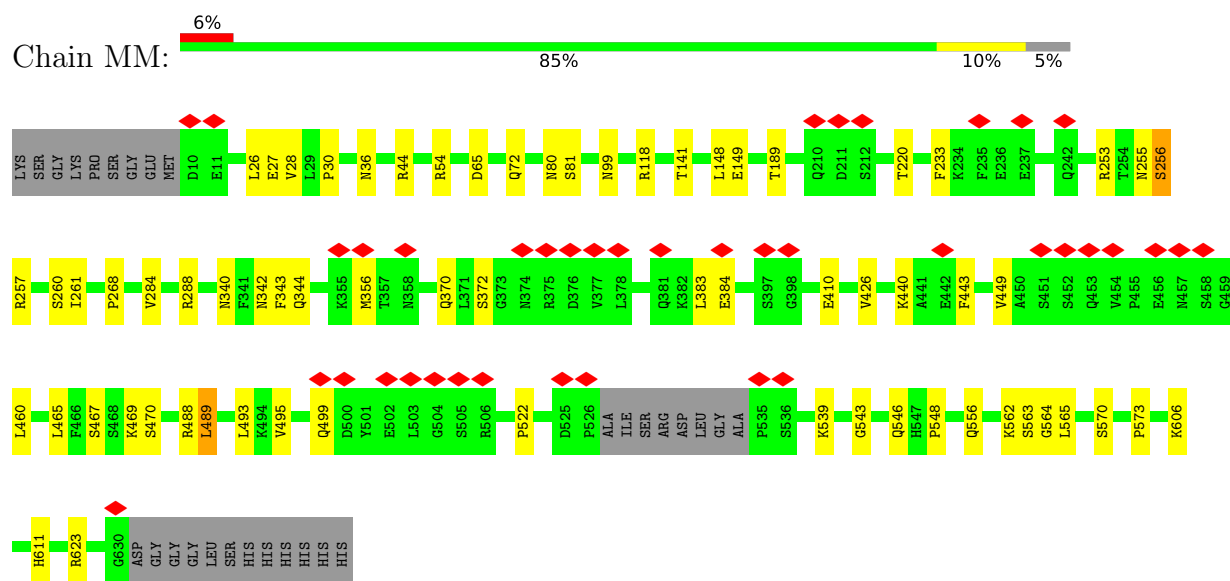
- Molecule 1: Macrophage-expressed gene 1 protein



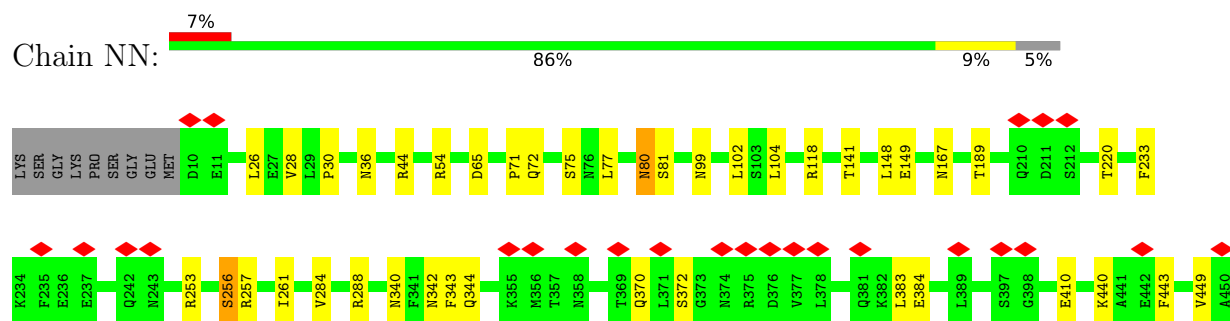
- Molecule 1: Macrophage-expressed gene 1 protein

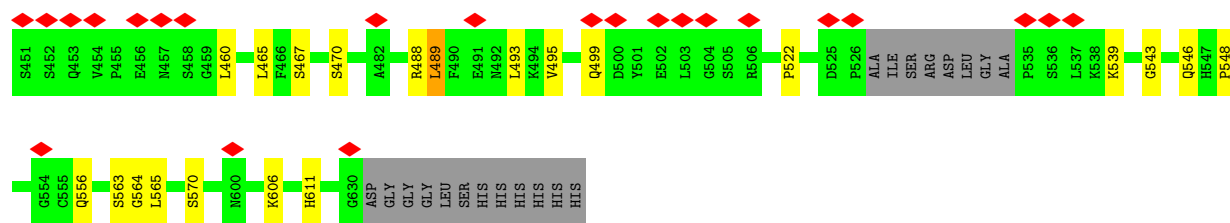


- Molecule 1: Macrophage-expressed gene 1 protein

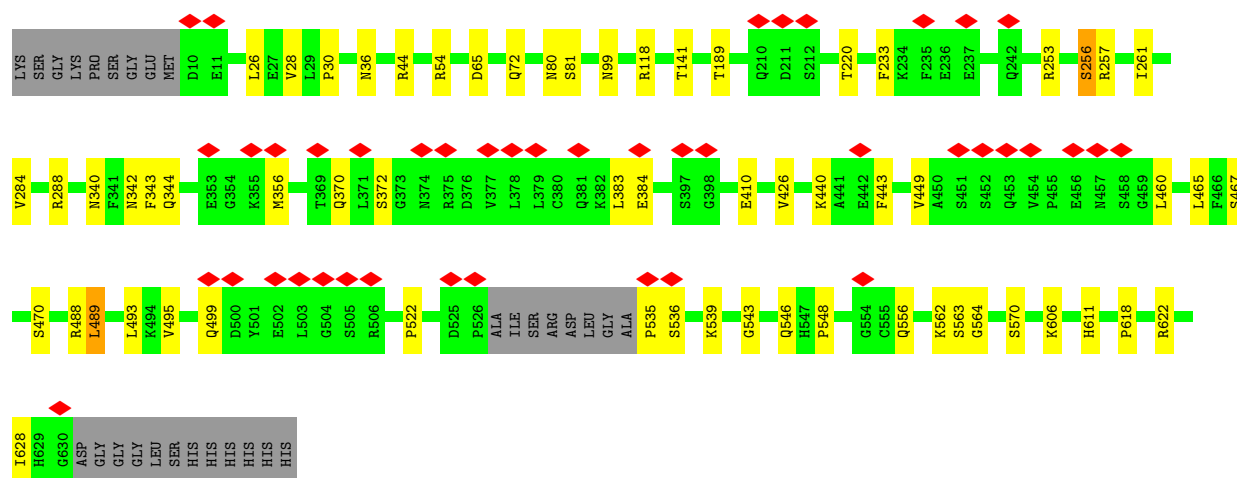
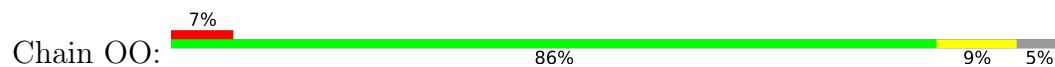


- Molecule 1: Macrophage-expressed gene 1 protein

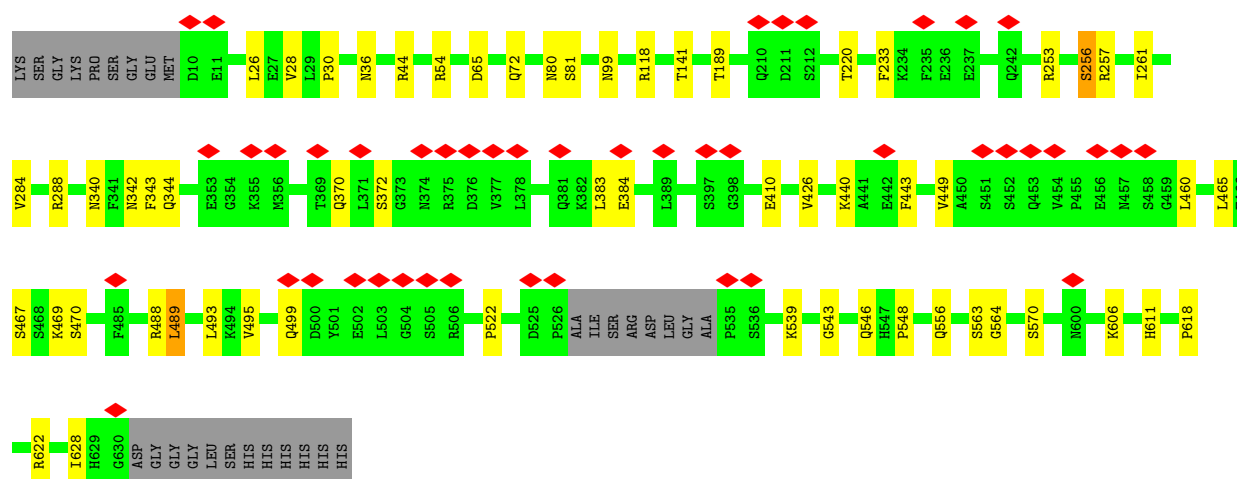
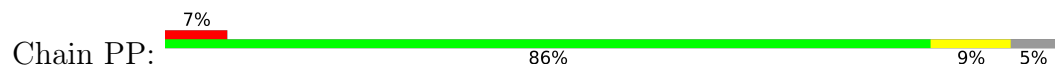




• Molecule 1: Macrophage-expressed gene 1 protein



• Molecule 1: Macrophage-expressed gene 1 protein



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





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



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



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



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



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



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



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



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



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



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



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



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

Chain c: 



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

Chain d: 



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

Chain e: 



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

Chain f: 



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

Chain g: 



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

Chain h: 



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



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



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



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



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



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





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



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



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



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6265	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.286	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0328	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/4870	0.57	1/6613 (0.0%)
1	AA	0.37	0/4870	0.57	1/6613 (0.0%)
1	B	0.79	18/4870 (0.4%)	0.57	1/6613 (0.0%)
1	BB	0.37	0/4870	0.57	1/6613 (0.0%)
1	C	0.37	0/4870	0.56	1/6613 (0.0%)
1	CC	0.37	0/4870	0.56	1/6613 (0.0%)
1	D	0.37	0/4869	0.57	1/6611 (0.0%)
1	DD	0.37	0/4869	0.57	1/6611 (0.0%)
1	E	0.37	0/4870	0.57	1/6613 (0.0%)
1	EE	0.37	0/4870	0.56	1/6613 (0.0%)
1	F	0.37	0/4870	0.57	1/6613 (0.0%)
1	FF	0.37	0/4870	0.57	1/6613 (0.0%)
1	G	0.37	0/4870	0.57	1/6613 (0.0%)
1	GG	0.37	0/4870	0.57	1/6613 (0.0%)
1	H	0.37	0/4870	0.56	1/6613 (0.0%)
1	HH	0.37	0/4870	0.57	1/6613 (0.0%)
1	I	0.37	0/4870	0.57	1/6613 (0.0%)
1	II	0.37	0/4870	0.56	1/6613 (0.0%)
1	J	0.37	0/4870	0.57	1/6613 (0.0%)
1	JJ	0.37	0/4870	0.56	1/6613 (0.0%)
1	K	0.37	0/4870	0.57	1/6613 (0.0%)
1	KK	0.37	0/4870	0.57	1/6613 (0.0%)
1	L	0.37	0/4869	0.56	1/6611 (0.0%)
1	LL	0.37	0/4869	0.57	1/6611 (0.0%)
1	M	0.37	0/4870	0.57	1/6613 (0.0%)
1	MM	0.37	0/4870	0.56	1/6613 (0.0%)
1	N	0.37	0/4870	0.57	1/6613 (0.0%)
1	NN	0.37	0/4870	0.57	1/6613 (0.0%)
1	O	0.37	0/4870	0.56	1/6613 (0.0%)
1	OO	0.37	0/4870	0.57	1/6613 (0.0%)
1	P	0.37	0/4870	0.57	1/6613 (0.0%)
1	PP	0.37	0/4870	0.56	1/6613 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	18/155836 (0.0%)	0.57	32/211608 (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	2
1	AA	0	2
1	B	0	2
1	BB	0	2
1	C	0	2
1	CC	0	2
1	D	0	2
1	DD	0	2
1	E	0	2
1	EE	0	2
1	F	0	2
1	FF	0	2
1	G	0	2
1	GG	0	2
1	H	0	2
1	HH	0	2
1	I	0	2
1	II	0	2
1	J	0	2
1	JJ	0	2
1	K	0	2
1	KK	0	2
1	L	0	2
1	LL	0	2
1	M	0	2
1	MM	0	2
1	N	0	2
1	NN	0	2
1	O	0	2
1	OO	0	2
1	P	0	2
1	PP	0	2
All	All	0	64

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	CYS	CB-SG	-12.13	1.79	2.03
1	B	480	CYS	CB-SG	-11.88	1.79	2.03
1	B	17	CYS	CB-SG	-11.83	1.79	2.03
1	B	395	CYS	CB-SG	-11.76	1.80	2.03
1	B	418	CYS	CB-SG	-11.69	1.80	2.03
1	B	448	CYS	CB-SG	-11.62	1.80	2.03
1	B	428	CYS	CB-SG	-11.62	1.80	2.03
1	B	540	CYS	CB-SG	-11.61	1.80	2.03
1	B	333	CYS	CB-SG	-11.49	1.80	2.03
1	B	560	CYS	CB-SG	-11.41	1.80	2.03
1	B	496	CYS	CB-SG	-11.32	1.80	2.03
1	B	555	CYS	CB-SG	-11.29	1.80	2.03
1	B	352	CYS	CB-SG	-11.28	1.80	2.03
1	B	432	CYS	CB-SG	-11.28	1.80	2.03
1	B	53	CYS	CB-SG	-11.05	1.81	2.03
1	B	517	CYS	CB-SG	-10.95	1.81	2.03
1	B	368	CYS	CB-SG	-10.63	1.82	2.03
1	B	380	CYS	CB-SG	-10.15	1.83	2.03

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	SER	N-CA-C	6.76	118.81	110.91
1	II	256	SER	N-CA-C	6.76	118.82	110.91
1	C	256	SER	N-CA-C	6.75	118.81	110.91
1	J	256	SER	N-CA-C	6.75	118.81	110.91
1	P	256	SER	N-CA-C	6.74	118.80	110.91
1	L	256	SER	N-CA-C	6.74	118.80	110.91
1	M	256	SER	N-CA-C	6.74	118.80	110.91
1	HH	256	SER	N-CA-C	6.73	118.79	110.91
1	BB	256	SER	N-CA-C	6.73	118.78	110.91
1	A	256	SER	N-CA-C	6.73	118.78	110.91
1	B	256	SER	N-CA-C	6.73	118.78	110.91
1	CC	256	SER	N-CA-C	6.73	118.78	110.91
1	OO	256	SER	N-CA-C	6.73	118.78	110.91
1	O	256	SER	N-CA-C	6.73	118.78	110.91
1	JJ	256	SER	N-CA-C	6.73	118.78	110.91
1	E	256	SER	N-CA-C	6.72	118.78	110.91
1	H	256	SER	N-CA-C	6.72	118.77	110.91
1	DD	256	SER	N-CA-C	6.72	118.77	110.91
1	K	256	SER	N-CA-C	6.71	118.77	110.91
1	LL	256	SER	N-CA-C	6.71	118.76	110.91
1	G	256	SER	N-CA-C	6.71	118.76	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	MM	256	SER	N-CA-C	6.71	118.76	110.91
1	KK	256	SER	N-CA-C	6.70	118.75	110.91
1	N	256	SER	N-CA-C	6.70	118.75	110.91
1	GG	256	SER	N-CA-C	6.70	118.75	110.91
1	PP	256	SER	N-CA-C	6.70	118.75	110.91
1	EE	256	SER	N-CA-C	6.70	118.74	110.91
1	F	256	SER	N-CA-C	6.69	118.74	110.91
1	I	256	SER	N-CA-C	6.69	118.74	110.91
1	AA	256	SER	N-CA-C	6.69	118.73	110.91
1	NN	256	SER	N-CA-C	6.68	118.73	110.91
1	FF	256	SER	N-CA-C	6.66	118.71	110.91

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	PHE	Peptide
1	A	489	LEU	Peptide
1	AA	233	PHE	Peptide
1	AA	489	LEU	Peptide
1	B	233	PHE	Peptide
1	B	489	LEU	Peptide
1	BB	233	PHE	Peptide
1	BB	489	LEU	Peptide
1	C	233	PHE	Peptide
1	C	489	LEU	Peptide
1	CC	233	PHE	Peptide
1	CC	489	LEU	Peptide
1	D	233	PHE	Peptide
1	D	489	LEU	Peptide
1	DD	233	PHE	Peptide
1	DD	489	LEU	Peptide
1	E	233	PHE	Peptide
1	E	489	LEU	Peptide
1	EE	233	PHE	Peptide
1	EE	489	LEU	Peptide
1	F	233	PHE	Peptide
1	F	489	LEU	Peptide
1	FF	233	PHE	Peptide
1	FF	489	LEU	Peptide
1	G	233	PHE	Peptide
1	G	489	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	GG	233	PHE	Peptide
1	GG	489	LEU	Peptide
1	H	233	PHE	Peptide
1	H	489	LEU	Peptide
1	HH	233	PHE	Peptide
1	HH	489	LEU	Peptide
1	I	233	PHE	Peptide
1	I	489	LEU	Peptide
1	II	233	PHE	Peptide
1	II	489	LEU	Peptide
1	J	233	PHE	Peptide
1	J	489	LEU	Peptide
1	JJ	233	PHE	Peptide
1	JJ	489	LEU	Peptide
1	K	233	PHE	Peptide
1	K	489	LEU	Peptide
1	KK	233	PHE	Peptide
1	KK	489	LEU	Peptide
1	L	233	PHE	Peptide
1	L	489	LEU	Peptide
1	LL	233	PHE	Peptide
1	LL	489	LEU	Peptide
1	M	233	PHE	Peptide
1	M	489	LEU	Peptide
1	MM	233	PHE	Peptide
1	MM	489	LEU	Peptide
1	N	233	PHE	Peptide
1	N	489	LEU	Peptide
1	NN	233	PHE	Peptide
1	NN	489	LEU	Peptide
1	O	233	PHE	Peptide
1	O	489	LEU	Peptide
1	OO	233	PHE	Peptide
1	OO	489	LEU	Peptide
1	P	233	PHE	Peptide
1	P	489	LEU	Peptide
1	PP	233	PHE	Peptide
1	PP	489	LEU	Peptide

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	4763	0	4654	32	0
1	AA	4763	0	4654	31	0
1	B	4763	0	4654	31	0
1	BB	4763	0	4654	31	0
1	C	4763	0	4654	30	0
1	CC	4763	0	4654	30	0
1	D	4762	0	4654	32	0
1	DD	4762	0	4654	30	0
1	E	4763	0	4654	30	0
1	EE	4763	0	4654	31	0
1	F	4763	0	4654	34	0
1	FF	4763	0	4654	33	0
1	G	4763	0	4654	31	0
1	GG	4763	0	4654	33	0
1	H	4763	0	4654	29	0
1	HH	4763	0	4654	32	0
1	I	4763	0	4654	30	0
1	II	4763	0	4654	32	0
1	J	4763	0	4654	31	0
1	JJ	4763	0	4654	31	0
1	K	4763	0	4654	29	0
1	KK	4763	0	4654	31	0
1	L	4762	0	4654	31	0
1	LL	4762	0	4654	31	0
1	M	4763	0	4654	31	0
1	MM	4763	0	4654	38	0
1	N	4763	0	4654	32	0
1	NN	4763	0	4654	36	0
1	O	4763	0	4654	34	0
1	OO	4763	0	4654	33	0
1	P	4763	0	4654	33	0
1	PP	4763	0	4654	32	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	0	0
2	h	28	0	25	0	0
2	i	28	0	25	0	0
2	j	28	0	25	0	0
2	k	28	0	25	0	0
2	l	28	0	25	0	0
2	m	28	0	25	0	0
2	n	28	0	25	0	0
2	o	28	0	25	0	0
2	p	28	0	25	0	0
2	q	28	0	25	0	0
2	r	28	0	25	0	0
2	s	28	0	25	0	0
2	t	28	0	25	0	0
2	u	28	0	25	0	0
2	v	28	0	25	0	0
3	A	14	0	13	0	0
3	AA	14	0	13	0	0
3	B	14	0	13	0	0
3	BB	14	0	13	0	0
3	C	14	0	13	0	0
3	CC	14	0	13	0	0
3	D	14	0	13	0	0
3	DD	14	0	13	0	0
3	E	14	0	13	0	0
3	EE	14	0	13	0	0
3	F	14	0	13	0	0
3	FF	14	0	13	0	0
3	G	14	0	13	0	0
3	GG	14	0	13	0	0
3	H	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HH	14	0	13	0	0
3	I	14	0	13	0	0
3	II	14	0	13	0	0
3	J	14	0	13	0	0
3	JJ	14	0	13	0	0
3	K	14	0	13	0	0
3	KK	14	0	13	0	0
3	L	14	0	13	0	0
3	LL	14	0	13	0	0
3	M	14	0	13	0	0
3	MM	14	0	13	0	0
3	N	14	0	13	0	0
3	NN	14	0	13	0	0
3	O	14	0	13	0	0
3	OO	14	0	13	0	0
3	P	14	0	13	0	0
3	PP	14	0	13	0	0
All	All	153756	0	150144	977	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 3.

All (977) 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:MM:72:GLN:NE2	1:MM:141:THR:OG1	2.35	0.60
1:J:72:GLN:NE2	1:J:141:THR:OG1	2.35	0.60
1:PP:72:GLN:NE2	1:PP:141:THR:OG1	2.35	0.60
1:F:36:ASN:ND2	1:F:99:ASN:OD1	2.35	0.60
1:M:72:GLN:NE2	1:M:141:THR:OG1	2.35	0.60
1:JJ:36:ASN:ND2	1:JJ:99:ASN:OD1	2.35	0.60
1:B:36:ASN:ND2	1:B:99:ASN:OD1	2.35	0.60
1:G:36:ASN:ND2	1:G:99:ASN:OD1	2.35	0.60
1:EE:36:ASN:ND2	1:EE:99:ASN:OD1	2.35	0.60
1:II:36:ASN:ND2	1:II:99:ASN:OD1	2.35	0.60
1:A:36:ASN:ND2	1:A:99:ASN:OD1	2.35	0.59
1:L:72:GLN:NE2	1:L:141:THR:OG1	2.35	0.59
1:JJ:72:GLN:NE2	1:JJ:141:THR:OG1	2.35	0.59
1:G:72:GLN:NE2	1:G:141:THR:OG1	2.35	0.59
1:DD:36:ASN:ND2	1:DD:99:ASN:OD1	2.35	0.59
1:OO:72:GLN:NE2	1:OO:141:THR:OG1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:GLN:NE2	1:O:141:THR:OG1	2.35	0.59
1:KK:72:GLN:NE2	1:KK:141:THR:OG1	2.35	0.59
1:E:36:ASN:ND2	1:E:99:ASN:OD1	2.35	0.59
1:P:72:GLN:NE2	1:P:141:THR:OG1	2.35	0.59
1:BB:72:GLN:NE2	1:BB:141:THR:OG1	2.35	0.59
1:CC:72:GLN:NE2	1:CC:141:THR:OG1	2.35	0.59
1:FF:36:ASN:ND2	1:FF:99:ASN:OD1	2.35	0.59
1:H:36:ASN:ND2	1:H:99:ASN:OD1	2.35	0.59
1:H:72:GLN:NE2	1:H:141:THR:OG1	2.35	0.59
1:I:72:GLN:NE2	1:I:141:THR:OG1	2.35	0.59
1:KK:36:ASN:ND2	1:KK:99:ASN:OD1	2.35	0.59
1:NN:72:GLN:NE2	1:NN:141:THR:OG1	2.35	0.59
1:C:36:ASN:ND2	1:C:99:ASN:OD1	2.35	0.59
1:HH:36:ASN:ND2	1:HH:99:ASN:OD1	2.35	0.59
1:K:72:GLN:NE2	1:K:141:THR:OG1	2.35	0.59
1:LL:72:GLN:NE2	1:LL:141:THR:OG1	2.35	0.59
1:J:36:ASN:ND2	1:J:99:ASN:OD1	2.35	0.59
1:MM:36:ASN:ND2	1:MM:99:ASN:OD1	2.35	0.59
1:F:72:GLN:NE2	1:F:141:THR:OG1	2.35	0.59
1:N:36:ASN:ND2	1:N:99:ASN:OD1	2.35	0.59
1:AA:36:ASN:ND2	1:AA:99:ASN:OD1	2.35	0.59
1:AA:72:GLN:NE2	1:AA:141:THR:OG1	2.35	0.59
1:II:72:GLN:NE2	1:II:141:THR:OG1	2.35	0.59
1:D:72:GLN:NE2	1:D:141:THR:OG1	2.35	0.58
1:K:36:ASN:ND2	1:K:99:ASN:OD1	2.35	0.58
1:GG:72:GLN:NE2	1:GG:141:THR:OG1	2.35	0.58
1:NN:36:ASN:ND2	1:NN:99:ASN:OD1	2.35	0.58
1:C:72:GLN:NE2	1:C:141:THR:OG1	2.35	0.58
1:D:36:ASN:ND2	1:D:99:ASN:OD1	2.35	0.58
1:N:72:GLN:NE2	1:N:141:THR:OG1	2.35	0.58
1:GG:36:ASN:ND2	1:GG:99:ASN:OD1	2.35	0.58
1:FF:72:GLN:NE2	1:FF:141:THR:OG1	2.35	0.58
1:DD:72:GLN:NE2	1:DD:141:THR:OG1	2.35	0.58
1:OO:36:ASN:ND2	1:OO:99:ASN:OD1	2.35	0.58
1:PP:36:ASN:ND2	1:PP:99:ASN:OD1	2.35	0.58
1:L:36:ASN:ND2	1:L:99:ASN:OD1	2.35	0.58
1:M:36:ASN:ND2	1:M:99:ASN:OD1	2.35	0.58
1:O:36:ASN:ND2	1:O:99:ASN:OD1	2.35	0.58
1:BB:36:ASN:ND2	1:BB:99:ASN:OD1	2.35	0.58
1:A:72:GLN:NE2	1:A:141:THR:OG1	2.35	0.58
1:B:72:GLN:NE2	1:B:141:THR:OG1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLN:NE2	1:E:141:THR:OG1	2.35	0.58
1:O:344:GLN:NE2	1:O:570:SER:O	2.37	0.58
1:BB:344:GLN:NE2	1:BB:570:SER:O	2.37	0.58
1:HH:72:GLN:NE2	1:HH:141:THR:OG1	2.35	0.58
1:N:344:GLN:NE2	1:N:570:SER:O	2.37	0.58
1:P:344:GLN:NE2	1:P:570:SER:O	2.37	0.58
1:AA:344:GLN:NE2	1:AA:570:SER:O	2.37	0.58
1:CC:344:GLN:NE2	1:CC:570:SER:O	2.37	0.58
1:EE:72:GLN:NE2	1:EE:141:THR:OG1	2.35	0.58
1:LL:36:ASN:ND2	1:LL:99:ASN:OD1	2.35	0.58
1:PP:344:GLN:NE2	1:PP:570:SER:O	2.37	0.58
1:M:344:GLN:NE2	1:M:570:SER:O	2.37	0.57
1:I:36:ASN:ND2	1:I:99:ASN:OD1	2.35	0.57
1:O:30:PRO:O	1:O:44:ARG:NH2	2.38	0.57
1:CC:30:PRO:O	1:CC:44:ARG:NH2	2.38	0.57
1:CC:36:ASN:ND2	1:CC:99:ASN:OD1	2.35	0.57
1:A:30:PRO:O	1:A:44:ARG:NH2	2.38	0.57
1:B:30:PRO:O	1:B:44:ARG:NH2	2.38	0.57
1:P:30:PRO:O	1:P:44:ARG:NH2	2.38	0.57
1:P:36:ASN:ND2	1:P:99:ASN:OD1	2.35	0.57
1:BB:30:PRO:O	1:BB:44:ARG:NH2	2.38	0.57
1:DD:30:PRO:O	1:DD:44:ARG:NH2	2.38	0.57
1:EE:30:PRO:O	1:EE:44:ARG:NH2	2.38	0.57
1:II:30:PRO:O	1:II:44:ARG:NH2	2.38	0.57
1:OO:344:GLN:NE2	1:OO:570:SER:O	2.37	0.57
1:F:30:PRO:O	1:F:44:ARG:NH2	2.38	0.57
1:L:344:GLN:NE2	1:L:570:SER:O	2.37	0.57
1:C:30:PRO:O	1:C:44:ARG:NH2	2.38	0.57
1:N:30:PRO:O	1:N:44:ARG:NH2	2.38	0.57
1:AA:30:PRO:O	1:AA:44:ARG:NH2	2.38	0.57
1:FF:30:PRO:O	1:FF:44:ARG:NH2	2.38	0.57
1:G:30:PRO:O	1:G:44:ARG:NH2	2.38	0.57
1:D:30:PRO:O	1:D:44:ARG:NH2	2.38	0.57
1:HH:30:PRO:O	1:HH:44:ARG:NH2	2.38	0.57
1:JJ:30:PRO:O	1:JJ:44:ARG:NH2	2.38	0.57
1:GG:30:PRO:O	1:GG:44:ARG:NH2	2.38	0.56
1:E:30:PRO:O	1:E:44:ARG:NH2	2.38	0.56
1:NN:344:GLN:NE2	1:NN:570:SER:O	2.37	0.56
1:G:344:GLN:NE2	1:G:570:SER:O	2.37	0.56
1:J:30:PRO:O	1:J:44:ARG:NH2	2.38	0.56
1:K:30:PRO:O	1:K:44:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:PRO:O	1:M:44:ARG:NH2	2.38	0.56
1:II:344:GLN:NE2	1:II:570:SER:O	2.37	0.56
1:JJ:344:GLN:NE2	1:JJ:570:SER:O	2.37	0.56
1:MM:30:PRO:O	1:MM:44:ARG:NH2	2.38	0.56
1:NN:30:PRO:O	1:NN:44:ARG:NH2	2.38	0.56
1:F:344:GLN:NE2	1:F:570:SER:O	2.37	0.56
1:K:344:GLN:NE2	1:K:570:SER:O	2.37	0.56
1:PP:30:PRO:O	1:PP:44:ARG:NH2	2.38	0.56
1:H:344:GLN:NE2	1:H:570:SER:O	2.37	0.56
1:L:30:PRO:O	1:L:44:ARG:NH2	2.38	0.56
1:HH:344:GLN:NE2	1:HH:570:SER:O	2.37	0.56
1:E:344:GLN:NE2	1:E:570:SER:O	2.37	0.56
1:EE:344:GLN:NE2	1:EE:570:SER:O	2.37	0.56
1:KK:344:GLN:NE2	1:KK:570:SER:O	2.37	0.56
1:OO:30:PRO:O	1:OO:44:ARG:NH2	2.38	0.56
1:I:30:PRO:O	1:I:44:ARG:NH2	2.38	0.56
1:LL:30:PRO:O	1:LL:44:ARG:NH2	2.38	0.56
1:B:344:GLN:NE2	1:B:570:SER:O	2.37	0.56
1:H:30:PRO:O	1:H:44:ARG:NH2	2.38	0.56
1:MM:344:GLN:NE2	1:MM:570:SER:O	2.37	0.55
1:O:426:VAL:HG21	1:GG:628:ILE:HD12	1.87	0.55
1:O:628:ILE:HD12	1:GG:426:VAL:HG21	1.88	0.55
1:KK:30:PRO:O	1:KK:44:ARG:NH2	2.38	0.55
1:J:344:GLN:NE2	1:J:570:SER:O	2.37	0.55
1:I:344:GLN:NE2	1:I:570:SER:O	2.37	0.55
1:LL:344:GLN:NE2	1:LL:570:SER:O	2.37	0.55
1:GG:344:GLN:NE2	1:GG:570:SER:O	2.37	0.55
1:D:344:GLN:NE2	1:D:570:SER:O	2.37	0.55
1:DD:344:GLN:NE2	1:DD:570:SER:O	2.37	0.55
1:A:344:GLN:NE2	1:A:570:SER:O	2.37	0.55
1:O:622:ARG:HH11	1:GG:622:ARG:HH11	1.55	0.54
1:MM:539:LYS:O	1:MM:546:GLN:NE2	2.40	0.54
1:P:628:ILE:HD12	1:FF:426:VAL:HG21	1.88	0.54
1:LL:539:LYS:O	1:LL:546:GLN:NE2	2.40	0.54
1:I:539:LYS:O	1:I:546:GLN:NE2	2.40	0.54
1:H:539:LYS:O	1:H:546:GLN:NE2	2.40	0.54
1:KK:539:LYS:O	1:KK:546:GLN:NE2	2.40	0.54
1:P:426:VAL:HG21	1:FF:628:ILE:HD12	1.89	0.54
1:FF:539:LYS:O	1:FF:546:GLN:NE2	2.40	0.54
1:GG:539:LYS:O	1:GG:546:GLN:NE2	2.40	0.54
1:C:539:LYS:O	1:C:546:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:LYS:O	1:D:546:GLN:NE2	2.40	0.54
1:G:539:LYS:O	1:G:546:GLN:NE2	2.40	0.54
1:N:426:VAL:HG21	1:HH:628:ILE:HD12	1.88	0.54
1:FF:344:GLN:NE2	1:FF:570:SER:O	2.37	0.54
1:HH:539:LYS:O	1:HH:546:GLN:NE2	2.40	0.54
1:C:344:GLN:NE2	1:C:570:SER:O	2.37	0.54
1:F:539:LYS:O	1:F:546:GLN:NE2	2.40	0.54
1:II:539:LYS:O	1:II:546:GLN:NE2	2.40	0.54
1:JJ:539:LYS:O	1:JJ:546:GLN:NE2	2.41	0.54
1:E:539:LYS:O	1:E:546:GLN:NE2	2.40	0.54
1:O:356:MET:SD	1:O:562:LYS:NZ	2.77	0.53
1:C:370:GLN:NE2	1:C:372:SER:O	2.42	0.53
1:P:622:ARG:HH11	1:FF:622:ARG:HH11	1.57	0.53
1:B:370:GLN:NE2	1:B:372:SER:O	2.42	0.53
1:EE:370:GLN:NE2	1:EE:372:SER:O	2.42	0.53
1:FF:370:GLN:NE2	1:FF:372:SER:O	2.42	0.53
1:A:370:GLN:NE2	1:A:372:SER:O	2.42	0.53
1:DD:370:GLN:NE2	1:DD:372:SER:O	2.42	0.53
1:K:410:GLU:HG2	1:K:440:LYS:HG2	1.91	0.53
1:L:410:GLU:HG2	1:L:440:LYS:HG2	1.91	0.52
1:CC:370:GLN:NE2	1:CC:372:SER:O	2.42	0.52
1:C:410:GLU:HG2	1:C:440:LYS:HG2	1.91	0.52
1:M:410:GLU:HG2	1:M:440:LYS:HG2	1.92	0.52
1:P:370:GLN:NE2	1:P:372:SER:O	2.42	0.52
1:DD:410:GLU:HG2	1:DD:440:LYS:HG2	1.91	0.52
1:FF:410:GLU:HG2	1:FF:440:LYS:HG2	1.91	0.52
1:NN:410:GLU:HG2	1:NN:440:LYS:HG2	1.91	0.52
1:A:410:GLU:HG2	1:A:440:LYS:HG2	1.91	0.52
1:J:410:GLU:HG2	1:J:440:LYS:HG2	1.92	0.52
1:EE:410:GLU:HG2	1:EE:440:LYS:HG2	1.92	0.52
1:GG:410:GLU:HG2	1:GG:440:LYS:HG2	1.91	0.52
1:OO:410:GLU:HG2	1:OO:440:LYS:HG2	1.92	0.52
1:B:410:GLU:HG2	1:B:440:LYS:HG2	1.92	0.52
1:D:410:GLU:HG2	1:D:440:LYS:HG2	1.91	0.52
1:J:606:LYS:NZ	1:J:611:HIS:O	2.43	0.52
1:N:410:GLU:HG2	1:N:440:LYS:HG2	1.91	0.52
1:O:410:GLU:HG2	1:O:440:LYS:HG2	1.92	0.52
1:BB:410:GLU:HG2	1:BB:440:LYS:HG2	1.91	0.52
1:MM:410:GLU:HG2	1:MM:440:LYS:HG2	1.92	0.52
1:PP:410:GLU:HG2	1:PP:440:LYS:HG2	1.92	0.52
1:I:410:GLU:HG2	1:I:440:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:410:GLU:HG2	1:CC:440:LYS:HG2	1.92	0.52
1:LL:410:GLU:HG2	1:LL:440:LYS:HG2	1.92	0.52
1:M:606:LYS:NZ	1:M:611:HIS:O	2.43	0.52
1:P:410:GLU:HG2	1:P:440:LYS:HG2	1.91	0.52
1:AA:410:GLU:HG2	1:AA:440:LYS:HG2	1.92	0.52
1:E:410:GLU:HG2	1:E:440:LYS:HG2	1.92	0.52
1:N:628:ILE:HD12	1:HH:426:VAL:HG21	1.92	0.52
1:P:606:LYS:NZ	1:P:611:HIS:O	2.43	0.52
1:CC:606:LYS:NZ	1:CC:611:HIS:O	2.43	0.52
1:HH:410:GLU:HG2	1:HH:440:LYS:HG2	1.91	0.52
1:KK:410:GLU:HG2	1:KK:440:LYS:HG2	1.91	0.52
1:H:410:GLU:HG2	1:H:440:LYS:HG2	1.91	0.52
1:K:370:GLN:NE2	1:K:372:SER:O	2.42	0.52
1:K:606:LYS:NZ	1:K:611:HIS:O	2.43	0.52
1:BB:606:LYS:NZ	1:BB:611:HIS:O	2.43	0.52
1:NN:370:GLN:NE2	1:NN:372:SER:O	2.42	0.52
1:PP:606:LYS:NZ	1:PP:611:HIS:O	2.43	0.52
1:O:606:LYS:NZ	1:O:611:HIS:O	2.43	0.52
1:BB:370:GLN:NE2	1:BB:372:SER:O	2.42	0.52
1:MM:370:GLN:NE2	1:MM:372:SER:O	2.42	0.52
1:F:410:GLU:HG2	1:F:440:LYS:HG2	1.92	0.52
1:O:370:GLN:NE2	1:O:372:SER:O	2.42	0.52
1:II:410:GLU:HG2	1:II:440:LYS:HG2	1.91	0.52
1:MM:260:SER:HB3	1:NN:75:SER:HB3	1.92	0.52
1:NN:606:LYS:NZ	1:NN:611:HIS:O	2.43	0.52
1:J:370:GLN:NE2	1:J:372:SER:O	2.42	0.51
1:OO:606:LYS:NZ	1:OO:611:HIS:O	2.43	0.51
1:I:606:LYS:NZ	1:I:611:HIS:O	2.43	0.51
1:JJ:410:GLU:HG2	1:JJ:440:LYS:HG2	1.92	0.51
1:G:410:GLU:HG2	1:G:440:LYS:HG2	1.91	0.51
1:L:606:LYS:NZ	1:L:611:HIS:O	2.43	0.51
1:DD:606:LYS:NZ	1:DD:611:HIS:O	2.43	0.51
1:LL:606:LYS:NZ	1:LL:611:HIS:O	2.43	0.51
1:A:606:LYS:NZ	1:A:611:HIS:O	2.43	0.51
1:C:606:LYS:NZ	1:C:611:HIS:O	2.43	0.51
1:L:356:MET:SD	1:L:562:LYS:NZ	2.78	0.51
1:OO:356:MET:SD	1:OO:562:LYS:NZ	2.77	0.51
1:I:370:GLN:NE2	1:I:372:SER:O	2.42	0.51
1:LL:370:GLN:NE2	1:LL:372:SER:O	2.42	0.51
1:FF:606:LYS:NZ	1:FF:611:HIS:O	2.43	0.51
1:M:356:MET:SD	1:M:562:LYS:NZ	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:622:ARG:HH11	1:HH:622:ARG:HH11	1.59	0.51
1:N:606:LYS:NZ	1:N:611:HIS:O	2.43	0.51
1:AA:606:LYS:NZ	1:AA:611:HIS:O	2.43	0.51
1:KK:370:GLN:NE2	1:KK:372:SER:O	2.42	0.51
1:OO:370:GLN:NE2	1:OO:372:SER:O	2.42	0.51
1:AA:370:GLN:NE2	1:AA:372:SER:O	2.42	0.51
1:L:370:GLN:NE2	1:L:372:SER:O	2.42	0.50
1:N:370:GLN:NE2	1:N:372:SER:O	2.42	0.50
1:H:370:GLN:NE2	1:H:372:SER:O	2.42	0.50
1:MM:340:ASN:HD22	1:MM:543:GLY:HA2	1.77	0.50
1:I:628:ILE:HD12	1:MM:426:VAL:HG21	1.93	0.50
1:A:340:ASN:HD22	1:A:543:GLY:HA2	1.77	0.50
1:J:340:ASN:HD22	1:J:543:GLY:HA2	1.77	0.50
1:N:539:LYS:O	1:N:546:GLN:NE2	2.40	0.50
1:AA:539:LYS:O	1:AA:546:GLN:NE2	2.40	0.50
1:BB:539:LYS:O	1:BB:546:GLN:NE2	2.41	0.50
1:EE:340:ASN:HD22	1:EE:543:GLY:HA2	1.77	0.50
1:LL:340:ASN:HD22	1:LL:543:GLY:HA2	1.77	0.50
1:MM:255:ASN:O	1:NN:80:ASN:HB2	2.11	0.50
1:B:340:ASN:HD22	1:B:543:GLY:HA2	1.77	0.50
1:I:340:ASN:HD22	1:I:543:GLY:HA2	1.77	0.50
1:O:539:LYS:O	1:O:546:GLN:NE2	2.40	0.50
1:DD:340:ASN:HD22	1:DD:543:GLY:HA2	1.77	0.50
1:JJ:370:GLN:NE2	1:JJ:372:SER:O	2.42	0.50
1:NN:340:ASN:HD22	1:NN:543:GLY:HA2	1.77	0.50
1:K:340:ASN:HD22	1:K:543:GLY:HA2	1.77	0.50
1:M:340:ASN:HD22	1:M:543:GLY:HA2	1.77	0.50
1:M:539:LYS:O	1:M:546:GLN:NE2	2.40	0.50
1:O:340:ASN:HD22	1:O:543:GLY:HA2	1.77	0.50
1:P:340:ASN:HD22	1:P:543:GLY:HA2	1.77	0.50
1:CC:340:ASN:HD22	1:CC:543:GLY:HA2	1.77	0.50
1:OO:340:ASN:HD22	1:OO:543:GLY:HA2	1.77	0.50
1:PP:539:LYS:O	1:PP:546:GLN:NE2	2.40	0.50
1:C:340:ASN:HD22	1:C:543:GLY:HA2	1.77	0.50
1:G:370:GLN:NE2	1:G:372:SER:O	2.42	0.50
1:L:340:ASN:HD22	1:L:543:GLY:HA2	1.77	0.50
1:BB:340:ASN:HD22	1:BB:543:GLY:HA2	1.77	0.50
1:KK:340:ASN:HD22	1:KK:543:GLY:HA2	1.77	0.50
1:PP:340:ASN:HD22	1:PP:543:GLY:HA2	1.77	0.50
1:H:253:ARG:HD3	1:H:256:SER:HB2	1.94	0.50
1:H:340:ASN:HD22	1:H:543:GLY:HA2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:340:ASN:HD22	1:N:543:GLY:HA2	1.77	0.50
1:AA:340:ASN:HD22	1:AA:543:GLY:HA2	1.77	0.50
1:CC:539:LYS:O	1:CC:546:GLN:NE2	2.40	0.50
1:FF:340:ASN:HD22	1:FF:543:GLY:HA2	1.77	0.50
1:D:340:ASN:HD22	1:D:543:GLY:HA2	1.77	0.50
1:O:253:ARG:HD3	1:O:256:SER:HB2	1.94	0.50
1:BB:253:ARG:HD3	1:BB:256:SER:HB2	1.94	0.50
1:KK:253:ARG:HD3	1:KK:256:SER:HB2	1.94	0.50
1:E:253:ARG:HD3	1:E:256:SER:HB2	1.94	0.49
1:P:539:LYS:O	1:P:546:GLN:NE2	2.40	0.49
1:C:618:PRO:HB2	1:BB:618:PRO:HB2	1.94	0.49
1:G:340:ASN:HD22	1:G:543:GLY:HA2	1.77	0.49
1:J:253:ARG:HD3	1:J:256:SER:HB2	1.94	0.49
1:J:618:PRO:HB2	1:KK:618:PRO:HB2	1.95	0.49
1:GG:340:ASN:HD22	1:GG:543:GLY:HA2	1.77	0.49
1:II:370:GLN:NE2	1:II:372:SER:O	2.42	0.49
1:JJ:340:ASN:HD22	1:JJ:543:GLY:HA2	1.77	0.49
1:PP:370:GLN:NE2	1:PP:372:SER:O	2.42	0.49
1:B:253:ARG:HD3	1:B:256:SER:HB2	1.94	0.49
1:H:449:VAL:HG21	1:H:522:PRO:HG2	1.95	0.49
1:L:539:LYS:O	1:L:546:GLN:NE2	2.40	0.49
1:EE:253:ARG:HD3	1:EE:256:SER:HB2	1.94	0.49
1:HH:253:ARG:HD3	1:HH:256:SER:HB2	1.94	0.49
1:HH:340:ASN:HD22	1:HH:543:GLY:HA2	1.77	0.49
1:MM:253:ARG:HD3	1:MM:256:SER:HB2	1.94	0.49
1:A:253:ARG:HD3	1:A:256:SER:HB2	1.94	0.49
1:F:340:ASN:HD22	1:F:543:GLY:HA2	1.77	0.49
1:M:370:GLN:NE2	1:M:372:SER:O	2.42	0.49
1:N:253:ARG:HD3	1:N:256:SER:HB2	1.94	0.49
1:JJ:449:VAL:HG21	1:JJ:522:PRO:HG2	1.95	0.49
1:KK:449:VAL:HG21	1:KK:522:PRO:HG2	1.95	0.49
1:OO:253:ARG:HD3	1:OO:256:SER:HB2	1.94	0.49
1:F:370:GLN:NE2	1:F:372:SER:O	2.42	0.49
1:G:449:VAL:HG21	1:G:522:PRO:HG2	1.95	0.49
1:I:449:VAL:HG21	1:I:522:PRO:HG2	1.95	0.49
1:L:253:ARG:HD3	1:L:256:SER:HB2	1.94	0.49
1:N:449:VAL:HG21	1:N:522:PRO:HG2	1.95	0.49
1:BB:449:VAL:HG21	1:BB:522:PRO:HG2	1.95	0.49
1:DD:253:ARG:HD3	1:DD:256:SER:HB2	1.94	0.49
1:II:340:ASN:HD22	1:II:543:GLY:HA2	1.77	0.49
1:II:449:VAL:HG21	1:II:522:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJ:253:ARG:HD3	1:JJ:256:SER:HB2	1.94	0.49
1:OO:539:LYS:O	1:OO:546:GLN:NE2	2.41	0.49
1:E:340:ASN:HD22	1:E:543:GLY:HA2	1.77	0.49
1:G:253:ARG:HD3	1:G:256:SER:HB2	1.94	0.49
1:J:539:LYS:O	1:J:546:GLN:NE2	2.40	0.49
1:M:253:ARG:HD3	1:M:256:SER:HB2	1.94	0.49
1:M:449:VAL:HG21	1:M:522:PRO:HG2	1.95	0.49
1:O:449:VAL:HG21	1:O:522:PRO:HG2	1.95	0.49
1:AA:253:ARG:HD3	1:AA:256:SER:HB2	1.95	0.49
1:AA:449:VAL:HG21	1:AA:522:PRO:HG2	1.95	0.49
1:DD:539:LYS:O	1:DD:546:GLN:NE2	2.40	0.49
1:HH:370:GLN:NE2	1:HH:372:SER:O	2.42	0.49
1:LL:449:VAL:HG21	1:LL:522:PRO:HG2	1.95	0.49
1:PP:253:ARG:HD3	1:PP:256:SER:HB2	1.94	0.49
1:PP:449:VAL:HG21	1:PP:522:PRO:HG2	1.95	0.49
1:F:449:VAL:HG21	1:F:522:PRO:HG2	1.95	0.49
1:J:449:VAL:HG21	1:J:522:PRO:HG2	1.95	0.49
1:L:449:VAL:HG21	1:L:522:PRO:HG2	1.95	0.49
1:DD:449:VAL:HG21	1:DD:522:PRO:HG2	1.95	0.49
1:HH:449:VAL:HG21	1:HH:522:PRO:HG2	1.95	0.49
1:OO:449:VAL:HG21	1:OO:522:PRO:HG2	1.95	0.49
1:A:118:ARG:HH12	1:A:257:ARG:HB2	1.78	0.49
1:A:449:VAL:HG21	1:A:522:PRO:HG2	1.95	0.49
1:E:449:VAL:HG21	1:E:522:PRO:HG2	1.95	0.49
1:P:449:VAL:HG21	1:P:522:PRO:HG2	1.95	0.49
1:FF:449:VAL:HG21	1:FF:522:PRO:HG2	1.95	0.49
1:GG:253:ARG:HD3	1:GG:256:SER:HB2	1.94	0.49
1:GG:449:VAL:HG21	1:GG:522:PRO:HG2	1.95	0.49
1:MM:449:VAL:HG21	1:MM:522:PRO:HG2	1.95	0.49
1:A:539:LYS:O	1:A:546:GLN:NE2	2.40	0.49
1:C:449:VAL:HG21	1:C:522:PRO:HG2	1.95	0.49
1:D:449:VAL:HG21	1:D:522:PRO:HG2	1.95	0.49
1:K:118:ARG:HH12	1:K:257:ARG:HB2	1.78	0.49
1:N:118:ARG:HH12	1:N:257:ARG:HB2	1.78	0.49
1:AA:118:ARG:HH12	1:AA:257:ARG:HB2	1.78	0.49
1:CC:118:ARG:HH12	1:CC:257:ARG:HB2	1.78	0.49
1:CC:449:VAL:HG21	1:CC:522:PRO:HG2	1.95	0.49
1:DD:118:ARG:HH12	1:DD:257:ARG:HB2	1.78	0.49
1:EE:449:VAL:HG21	1:EE:522:PRO:HG2	1.95	0.49
1:NN:118:ARG:HH12	1:NN:257:ARG:HB2	1.78	0.49
1:NN:449:VAL:HG21	1:NN:522:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ARG:HD3	1:D:256:SER:HB2	1.95	0.49
1:E:370:GLN:NE2	1:E:372:SER:O	2.42	0.49
1:I:118:ARG:HH12	1:I:257:ARG:HB2	1.78	0.49
1:K:253:ARG:HD3	1:K:256:SER:HB2	1.94	0.49
1:P:118:ARG:HH12	1:P:257:ARG:HB2	1.78	0.49
1:GG:370:GLN:NE2	1:GG:372:SER:O	2.42	0.49
1:LL:118:ARG:HH12	1:LL:257:ARG:HB2	1.78	0.49
1:B:118:ARG:HH12	1:B:257:ARG:HB2	1.78	0.48
1:B:449:VAL:HG21	1:B:522:PRO:HG2	1.95	0.48
1:L:118:ARG:HH12	1:L:257:ARG:HB2	1.78	0.48
1:EE:118:ARG:HH12	1:EE:257:ARG:HB2	1.78	0.48
1:OO:118:ARG:HH12	1:OO:257:ARG:HB2	1.78	0.48
1:F:118:ARG:HH12	1:F:257:ARG:HB2	1.78	0.48
1:F:253:ARG:HD3	1:F:256:SER:HB2	1.95	0.48
1:G:118:ARG:HH12	1:G:257:ARG:HB2	1.78	0.48
1:K:449:VAL:HG21	1:K:522:PRO:HG2	1.95	0.48
1:K:539:LYS:O	1:K:546:GLN:NE2	2.40	0.48
1:II:118:ARG:HH12	1:II:257:ARG:HB2	1.78	0.48
1:II:253:ARG:HD3	1:II:256:SER:HB2	1.94	0.48
1:NN:253:ARG:HD3	1:NN:256:SER:HB2	1.94	0.48
1:D:370:GLN:NE2	1:D:372:SER:O	2.42	0.48
1:J:118:ARG:HH12	1:J:257:ARG:HB2	1.78	0.48
1:M:426:VAL:HG21	1:II:628:ILE:HD12	1.93	0.48
1:JJ:118:ARG:HH12	1:JJ:257:ARG:HB2	1.78	0.48
1:NN:539:LYS:O	1:NN:546:GLN:NE2	2.41	0.48
1:G:606:LYS:NZ	1:G:611:HIS:O	2.43	0.48
1:H:384:GLU:O	1:H:488:ARG:NH2	2.46	0.48
1:O:489:LEU:HB3	1:O:493:LEU:HB2	1.96	0.48
1:P:253:ARG:HD3	1:P:256:SER:HB2	1.94	0.48
1:HH:118:ARG:HH12	1:HH:257:ARG:HB2	1.78	0.48
1:JJ:606:LYS:NZ	1:JJ:611:HIS:O	2.43	0.48
1:PP:489:LEU:HB3	1:PP:493:LEU:HB2	1.96	0.48
1:C:118:ARG:HH12	1:C:257:ARG:HB2	1.78	0.48
1:E:118:ARG:HH12	1:E:257:ARG:HB2	1.78	0.48
1:I:253:ARG:HD3	1:I:256:SER:HB2	1.94	0.48
1:M:489:LEU:HB3	1:M:493:LEU:HB2	1.96	0.48
1:M:622:ARG:HH11	1:II:622:ARG:HH11	1.61	0.48
1:P:384:GLU:O	1:P:488:ARG:NH2	2.47	0.48
1:P:489:LEU:HB3	1:P:493:LEU:HB2	1.96	0.48
1:AA:489:LEU:HB3	1:AA:493:LEU:HB2	1.96	0.48
1:BB:489:LEU:HB3	1:BB:493:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:384:GLU:O	1:CC:488:ARG:NH2	2.47	0.48
1:CC:489:LEU:HB3	1:CC:493:LEU:HB2	1.96	0.48
1:FF:118:ARG:HH12	1:FF:257:ARG:HB2	1.78	0.48
1:KK:384:GLU:O	1:KK:488:ARG:NH2	2.47	0.48
1:MM:118:ARG:HH12	1:MM:257:ARG:HB2	1.78	0.48
1:C:253:ARG:HD3	1:C:256:SER:HB2	1.94	0.48
1:I:384:GLU:O	1:I:488:ARG:NH2	2.47	0.48
1:M:118:ARG:HH12	1:M:257:ARG:HB2	1.78	0.48
1:N:489:LEU:HB3	1:N:493:LEU:HB2	1.96	0.48
1:O:384:GLU:O	1:O:488:ARG:NH2	2.46	0.48
1:BB:384:GLU:O	1:BB:488:ARG:NH2	2.47	0.48
1:DD:384:GLU:O	1:DD:488:ARG:NH2	2.46	0.48
1:JJ:384:GLU:O	1:JJ:488:ARG:NH2	2.46	0.48
1:LL:253:ARG:HD3	1:LL:256:SER:HB2	1.94	0.48
1:LL:384:GLU:O	1:LL:488:ARG:NH2	2.47	0.48
1:A:384:GLU:O	1:A:488:ARG:NH2	2.47	0.48
1:H:606:LYS:NZ	1:H:611:HIS:O	2.43	0.48
1:EE:384:GLU:O	1:EE:488:ARG:NH2	2.46	0.48
1:II:606:LYS:NZ	1:II:611:HIS:O	2.43	0.48
1:MM:606:LYS:NZ	1:MM:611:HIS:O	2.43	0.48
1:D:118:ARG:HH12	1:D:257:ARG:HB2	1.78	0.48
1:G:384:GLU:O	1:G:488:ARG:NH2	2.47	0.48
1:L:489:LEU:HB3	1:L:493:LEU:HB2	1.96	0.48
1:CC:253:ARG:HD3	1:CC:256:SER:HB2	1.94	0.48
1:FF:253:ARG:HD3	1:FF:256:SER:HB2	1.94	0.48
1:KK:606:LYS:NZ	1:KK:611:HIS:O	2.43	0.48
1:OO:489:LEU:HB3	1:OO:493:LEU:HB2	1.95	0.48
1:PP:118:ARG:HH12	1:PP:257:ARG:HB2	1.78	0.48
1:B:384:GLU:O	1:B:488:ARG:NH2	2.47	0.48
1:B:618:PRO:HB2	1:CC:618:PRO:HB2	1.95	0.48
1:D:606:LYS:NZ	1:D:611:HIS:O	2.43	0.48
1:F:606:LYS:NZ	1:F:611:HIS:O	2.43	0.48
1:J:384:GLU:O	1:J:488:ARG:NH2	2.47	0.48
1:EE:489:LEU:HB3	1:EE:493:LEU:HB2	1.96	0.48
1:EE:539:LYS:O	1:EE:546:GLN:NE2	2.40	0.48
1:MM:384:GLU:O	1:MM:488:ARG:NH2	2.46	0.48
1:NN:489:LEU:HB3	1:NN:493:LEU:HB2	1.96	0.48
1:B:539:LYS:O	1:B:546:GLN:NE2	2.40	0.48
1:F:54:ARG:HD3	1:F:65:ASP:HA	1.96	0.48
1:GG:118:ARG:HH12	1:GG:257:ARG:HB2	1.78	0.48
1:GG:606:LYS:NZ	1:GG:611:HIS:O	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:II:54:ARG:HD3	1:II:65:ASP:HA	1.96	0.48
1:A:489:LEU:HB3	1:A:493:LEU:HB2	1.96	0.47
1:B:54:ARG:HD3	1:B:65:ASP:HA	1.96	0.47
1:B:489:LEU:HB3	1:B:493:LEU:HB2	1.96	0.47
1:C:384:GLU:O	1:C:488:ARG:NH2	2.47	0.47
1:K:489:LEU:HB3	1:K:493:LEU:HB2	1.96	0.47
1:O:118:ARG:HH12	1:O:257:ARG:HB2	1.78	0.47
1:AA:384:GLU:O	1:AA:488:ARG:NH2	2.47	0.47
1:BB:118:ARG:HH12	1:BB:257:ARG:HB2	1.78	0.47
1:DD:489:LEU:HB3	1:DD:493:LEU:HB2	1.96	0.47
1:EE:54:ARG:HD3	1:EE:65:ASP:HA	1.96	0.47
1:FF:384:GLU:O	1:FF:488:ARG:NH2	2.47	0.47
1:II:384:GLU:O	1:II:488:ARG:NH2	2.47	0.47
1:KK:118:ARG:HH12	1:KK:257:ARG:HB2	1.78	0.47
1:E:54:ARG:HD3	1:E:65:ASP:HA	1.96	0.47
1:E:606:LYS:NZ	1:E:611:HIS:O	2.43	0.47
1:N:384:GLU:O	1:N:488:ARG:NH2	2.46	0.47
1:F:384:GLU:O	1:F:488:ARG:NH2	2.47	0.47
1:H:118:ARG:HH12	1:H:257:ARG:HB2	1.78	0.47
1:HH:54:ARG:HD3	1:HH:65:ASP:HA	1.96	0.47
1:HH:606:LYS:NZ	1:HH:611:HIS:O	2.43	0.47
1:A:54:ARG:HD3	1:A:65:ASP:HA	1.96	0.47
1:J:489:LEU:HB3	1:J:493:LEU:HB2	1.96	0.47
1:FF:489:LEU:HB3	1:FF:493:LEU:HB2	1.96	0.47
1:MM:489:LEU:HB3	1:MM:493:LEU:HB2	1.96	0.47
1:C:489:LEU:HB3	1:C:493:LEU:HB2	1.96	0.47
1:G:54:ARG:HD3	1:G:65:ASP:HA	1.96	0.47
1:G:460:LEU:HD23	1:G:499:GLN:HB3	1.97	0.47
1:G:489:LEU:HB3	1:G:493:LEU:HB2	1.96	0.47
1:K:384:GLU:O	1:K:488:ARG:NH2	2.46	0.47
1:M:384:GLU:O	1:M:488:ARG:NH2	2.46	0.47
1:FF:54:ARG:HD3	1:FF:65:ASP:HA	1.96	0.47
1:II:460:LEU:HD23	1:II:499:GLN:HB3	1.97	0.47
1:JJ:54:ARG:HD3	1:JJ:65:ASP:HA	1.96	0.47
1:JJ:460:LEU:HD23	1:JJ:499:GLN:HB3	1.97	0.47
1:KK:460:LEU:HD23	1:KK:499:GLN:HB3	1.97	0.47
1:C:54:ARG:HD3	1:C:65:ASP:HA	1.96	0.47
1:E:460:LEU:HD23	1:E:499:GLN:HB3	1.97	0.47
1:F:460:LEU:HD23	1:F:499:GLN:HB3	1.97	0.47
1:M:460:LEU:HD23	1:M:499:GLN:HB3	1.97	0.47
1:BB:81:SER:H	1:BB:220:THR:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:54:ARG:HD3	1:DD:65:ASP:HA	1.96	0.47
1:HH:460:LEU:HD23	1:HH:499:GLN:HB3	1.97	0.47
1:JJ:489:LEU:HB3	1:JJ:493:LEU:HB2	1.96	0.47
1:NN:384:GLU:O	1:NN:488:ARG:NH2	2.46	0.47
1:PP:384:GLU:O	1:PP:488:ARG:NH2	2.47	0.47
1:D:81:SER:H	1:D:220:THR:HG22	1.80	0.47
1:E:81:SER:H	1:E:220:THR:HG22	1.80	0.47
1:E:489:LEU:HB3	1:E:493:LEU:HB2	1.96	0.47
1:G:81:SER:H	1:G:220:THR:HG22	1.80	0.47
1:H:460:LEU:HD23	1:H:499:GLN:HB3	1.97	0.47
1:I:460:LEU:HD23	1:I:499:GLN:HB3	1.97	0.47
1:K:618:PRO:HB2	1:JJ:618:PRO:HB2	1.97	0.47
1:L:384:GLU:O	1:L:488:ARG:NH2	2.47	0.47
1:L:460:LEU:HD23	1:L:499:GLN:HB3	1.97	0.47
1:N:81:SER:H	1:N:220:THR:HG22	1.80	0.47
1:N:460:LEU:HD23	1:N:499:GLN:HB3	1.97	0.47
1:O:81:SER:H	1:O:220:THR:HG22	1.80	0.47
1:CC:460:LEU:HD23	1:CC:499:GLN:HB3	1.97	0.47
1:GG:81:SER:H	1:GG:220:THR:HG22	1.80	0.47
1:HH:81:SER:H	1:HH:220:THR:HG22	1.80	0.47
1:HH:489:LEU:HB3	1:HH:493:LEU:HB2	1.96	0.47
1:II:489:LEU:HB3	1:II:493:LEU:HB2	1.96	0.47
1:JJ:81:SER:H	1:JJ:220:THR:HG22	1.80	0.47
1:KK:489:LEU:HB3	1:KK:493:LEU:HB2	1.96	0.47
1:LL:460:LEU:HD23	1:LL:499:GLN:HB3	1.97	0.47
1:NN:460:LEU:HD23	1:NN:499:GLN:HB3	1.97	0.47
1:OO:384:GLU:O	1:OO:488:ARG:NH2	2.47	0.47
1:OO:460:LEU:HD23	1:OO:499:GLN:HB3	1.97	0.47
1:PP:460:LEU:HD23	1:PP:499:GLN:HB3	1.97	0.47
1:B:606:LYS:NZ	1:B:611:HIS:O	2.43	0.47
1:D:489:LEU:HB3	1:D:493:LEU:HB2	1.96	0.47
1:F:81:SER:H	1:F:220:THR:HG22	1.80	0.47
1:F:489:LEU:HB3	1:F:493:LEU:HB2	1.96	0.47
1:H:81:SER:H	1:H:220:THR:HG22	1.80	0.47
1:H:489:LEU:HB3	1:H:493:LEU:HB2	1.96	0.47
1:I:81:SER:H	1:I:220:THR:HG22	1.80	0.47
1:K:460:LEU:HD23	1:K:499:GLN:HB3	1.97	0.47
1:P:81:SER:H	1:P:220:THR:HG22	1.80	0.47
1:AA:81:SER:H	1:AA:220:THR:HG22	1.80	0.47
1:AA:460:LEU:HD23	1:AA:499:GLN:HB3	1.97	0.47
1:BB:460:LEU:HD23	1:BB:499:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:460:LEU:HD23	1:DD:499:GLN:HB3	1.97	0.47
1:GG:460:LEU:HD23	1:GG:499:GLN:HB3	1.97	0.47
1:HH:384:GLU:O	1:HH:488:ARG:NH2	2.46	0.47
1:II:81:SER:H	1:II:220:THR:HG22	1.80	0.47
1:KK:81:SER:H	1:KK:220:THR:HG22	1.80	0.47
1:LL:81:SER:H	1:LL:220:THR:HG22	1.80	0.47
1:A:460:LEU:HD23	1:A:499:GLN:HB3	1.97	0.47
1:I:489:LEU:HB3	1:I:493:LEU:HB2	1.96	0.47
1:O:460:LEU:HD23	1:O:499:GLN:HB3	1.97	0.47
1:P:460:LEU:HD23	1:P:499:GLN:HB3	1.97	0.47
1:EE:460:LEU:HD23	1:EE:499:GLN:HB3	1.97	0.47
1:FF:81:SER:H	1:FF:220:THR:HG22	1.80	0.47
1:FF:460:LEU:HD23	1:FF:499:GLN:HB3	1.97	0.47
1:MM:54:ARG:HD3	1:MM:65:ASP:HA	1.96	0.47
1:PP:81:SER:H	1:PP:220:THR:HG22	1.80	0.47
1:B:460:LEU:HD23	1:B:499:GLN:HB3	1.97	0.47
1:C:81:SER:H	1:C:220:THR:HG22	1.80	0.47
1:D:460:LEU:HD23	1:D:499:GLN:HB3	1.97	0.47
1:E:384:GLU:O	1:E:488:ARG:NH2	2.47	0.47
1:I:54:ARG:HD3	1:I:65:ASP:HA	1.96	0.47
1:J:54:ARG:HD3	1:J:65:ASP:HA	1.96	0.47
1:J:460:LEU:HD23	1:J:499:GLN:HB3	1.97	0.47
1:M:81:SER:H	1:M:220:THR:HG22	1.80	0.47
1:CC:81:SER:H	1:CC:220:THR:HG22	1.80	0.47
1:GG:489:LEU:HB3	1:GG:493:LEU:HB2	1.96	0.47
1:LL:489:LEU:HB3	1:LL:493:LEU:HB2	1.96	0.47
1:MM:81:SER:H	1:MM:220:THR:HG22	1.80	0.47
1:C:460:LEU:HD23	1:C:499:GLN:HB3	1.97	0.46
1:D:54:ARG:HD3	1:D:65:ASP:HA	1.96	0.46
1:J:81:SER:H	1:J:220:THR:HG22	1.80	0.46
1:K:81:SER:H	1:K:220:THR:HG22	1.80	0.46
1:EE:606:LYS:NZ	1:EE:611:HIS:O	2.43	0.46
1:LL:54:ARG:HD3	1:LL:65:ASP:HA	1.96	0.46
1:MM:460:LEU:HD23	1:MM:499:GLN:HB3	1.97	0.46
1:M:628:ILE:HD12	1:II:426:VAL:HG21	1.97	0.46
1:A:81:SER:H	1:A:220:THR:HG22	1.80	0.46
1:B:81:SER:H	1:B:220:THR:HG22	1.80	0.46
1:N:54:ARG:HD3	1:N:65:ASP:HA	1.96	0.46
1:AA:54:ARG:HD3	1:AA:65:ASP:HA	1.96	0.46
1:NN:81:SER:H	1:NN:220:THR:HG22	1.80	0.46
1:D:384:GLU:O	1:D:488:ARG:NH2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:SER:H	1:L:220:THR:HG22	1.80	0.46
1:DD:81:SER:H	1:DD:220:THR:HG22	1.80	0.46
1:EE:81:SER:H	1:EE:220:THR:HG22	1.80	0.46
1:GG:54:ARG:HD3	1:GG:65:ASP:HA	1.96	0.46
1:OO:81:SER:H	1:OO:220:THR:HG22	1.80	0.46
1:P:54:ARG:HD3	1:P:65:ASP:HA	1.96	0.46
1:BB:54:ARG:HD3	1:BB:65:ASP:HA	1.96	0.46
1:GG:384:GLU:O	1:GG:488:ARG:NH2	2.47	0.46
1:PP:54:ARG:HD3	1:PP:65:ASP:HA	1.96	0.46
1:K:54:ARG:HD3	1:K:65:ASP:HA	1.96	0.46
1:M:54:ARG:HD3	1:M:65:ASP:HA	1.96	0.46
1:O:54:ARG:HD3	1:O:65:ASP:HA	1.96	0.46
1:CC:54:ARG:HD3	1:CC:65:ASP:HA	1.96	0.46
1:KK:54:ARG:HD3	1:KK:65:ASP:HA	1.96	0.46
1:NN:54:ARG:HD3	1:NN:65:ASP:HA	1.96	0.46
1:L:54:ARG:HD3	1:L:65:ASP:HA	1.96	0.46
1:OO:54:ARG:HD3	1:OO:65:ASP:HA	1.96	0.46
1:H:54:ARG:HD3	1:H:65:ASP:HA	1.96	0.46
1:FF:356:MET:SD	1:FF:562:LYS:NZ	2.78	0.45
1:MM:356:MET:SD	1:MM:562:LYS:NZ	2.78	0.45
1:J:356:MET:SD	1:J:562:LYS:NZ	2.78	0.45
1:LL:465:LEU:HD23	1:LL:493:LEU:HD22	1.99	0.45
1:E:465:LEU:HG	1:E:495:VAL:HG22	1.99	0.45
1:F:465:LEU:HG	1:F:495:VAL:HG22	1.99	0.45
1:EE:465:LEU:HG	1:EE:495:VAL:HG22	1.99	0.45
1:II:465:LEU:HG	1:II:495:VAL:HG22	1.99	0.45
1:F:465:LEU:HD23	1:F:493:LEU:HD22	1.99	0.45
1:I:465:LEU:HD23	1:I:493:LEU:HD22	1.99	0.45
1:HH:465:LEU:HG	1:HH:495:VAL:HG22	1.99	0.45
1:MM:573:PRO:HG2	1:NN:102:LEU:HG	1.99	0.45
1:A:465:LEU:HG	1:A:495:VAL:HG22	1.99	0.45
1:B:465:LEU:HG	1:B:495:VAL:HG22	1.99	0.45
1:E:618:PRO:HB2	1:PP:618:PRO:HB2	1.99	0.45
1:I:465:LEU:HG	1:I:495:VAL:HG22	1.99	0.45
1:J:465:LEU:HG	1:J:495:VAL:HG22	1.99	0.45
1:DD:465:LEU:HG	1:DD:495:VAL:HG22	1.99	0.45
1:II:465:LEU:HD23	1:II:493:LEU:HD22	1.99	0.45
1:MM:465:LEU:HG	1:MM:495:VAL:HG22	1.99	0.45
1:OO:465:LEU:HD23	1:OO:493:LEU:HD22	1.99	0.45
1:L:465:LEU:HD23	1:L:493:LEU:HD22	1.99	0.45
1:LL:465:LEU:HG	1:LL:495:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MM:27:GLU:HB2	1:NN:71:PRO:HG3	1.99	0.45
1:F:383:LEU:HD21	1:F:443:PHE:HB3	1.99	0.45
1:G:465:LEU:HG	1:G:495:VAL:HG22	1.99	0.45
1:J:383:LEU:HD21	1:J:443:PHE:HB3	1.99	0.45
1:II:383:LEU:HD21	1:II:443:PHE:HB3	1.99	0.45
1:JJ:465:LEU:HG	1:JJ:495:VAL:HG22	1.99	0.45
1:G:548:PRO:HB3	1:G:556:GLN:HE21	1.82	0.44
1:J:465:LEU:HD23	1:J:493:LEU:HD22	1.99	0.44
1:K:548:PRO:HB3	1:K:556:GLN:HE21	1.82	0.44
1:M:383:LEU:HD21	1:M:443:PHE:HB3	2.00	0.44
1:N:342:ASN:ND2	1:N:343:PHE:O	2.50	0.44
1:AA:342:ASN:ND2	1:AA:343:PHE:O	2.50	0.44
1:FF:548:PRO:HB3	1:FF:556:GLN:HE21	1.82	0.44
1:II:548:PRO:HB3	1:II:556:GLN:HE21	1.82	0.44
1:JJ:548:PRO:HB3	1:JJ:556:GLN:HE21	1.82	0.44
1:PP:383:LEU:HD21	1:PP:443:PHE:HB3	1.99	0.44
1:B:548:PRO:HB3	1:B:556:GLN:HE21	1.82	0.44
1:F:548:PRO:HB3	1:F:556:GLN:HE21	1.82	0.44
1:O:342:ASN:ND2	1:O:343:PHE:O	2.50	0.44
1:AA:383:LEU:HD21	1:AA:443:PHE:HB3	1.99	0.44
1:DD:548:PRO:HB3	1:DD:556:GLN:HE21	1.82	0.44
1:EE:548:PRO:HB3	1:EE:556:GLN:HE21	1.82	0.44
1:HH:548:PRO:HB3	1:HH:556:GLN:HE21	1.82	0.44
1:KK:465:LEU:HD23	1:KK:493:LEU:HD22	1.99	0.44
1:MM:383:LEU:HD21	1:MM:443:PHE:HB3	2.00	0.44
1:NN:548:PRO:HB3	1:NN:556:GLN:HE21	1.82	0.44
1:C:548:PRO:HB3	1:C:556:GLN:HE21	1.82	0.44
1:G:465:LEU:HD23	1:G:493:LEU:HD22	1.99	0.44
1:H:465:LEU:HD23	1:H:493:LEU:HD22	1.99	0.44
1:J:548:PRO:HB3	1:J:556:GLN:HE21	1.82	0.44
1:N:383:LEU:HD21	1:N:443:PHE:HB3	2.00	0.44
1:BB:342:ASN:ND2	1:BB:343:PHE:O	2.50	0.44
1:CC:548:PRO:HB3	1:CC:556:GLN:HE21	1.82	0.44
1:DD:342:ASN:ND2	1:DD:343:PHE:O	2.50	0.44
1:FF:465:LEU:HG	1:FF:495:VAL:HG22	1.99	0.44
1:GG:548:PRO:HB3	1:GG:556:GLN:HE21	1.82	0.44
1:KK:548:PRO:HB3	1:KK:556:GLN:HE21	1.82	0.44
1:MM:465:LEU:HD23	1:MM:493:LEU:HD22	1.99	0.44
1:NN:465:LEU:HD23	1:NN:493:LEU:HD22	1.99	0.44
1:A:548:PRO:HB3	1:A:556:GLN:HE21	1.82	0.44
1:D:548:PRO:HB3	1:D:556:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ASN:ND2	1:E:343:PHE:O	2.50	0.44
1:E:548:PRO:HB3	1:E:556:GLN:HE21	1.82	0.44
1:G:622:ARG:HH11	1:OO:622:ARG:HH11	1.65	0.44
1:H:548:PRO:HB3	1:H:556:GLN:HE21	1.82	0.44
1:I:383:LEU:HD21	1:I:443:PHE:HB3	2.00	0.44
1:N:465:LEU:HG	1:N:495:VAL:HG22	1.99	0.44
1:JJ:383:LEU:HD21	1:JJ:443:PHE:HB3	2.00	0.44
1:MM:548:PRO:HB3	1:MM:556:GLN:HE21	1.82	0.44
1:NN:465:LEU:HG	1:NN:495:VAL:HG22	1.99	0.44
1:A:342:ASN:ND2	1:A:343:PHE:O	2.50	0.44
1:C:465:LEU:HG	1:C:495:VAL:HG22	1.99	0.44
1:D:618:PRO:HB2	1:AA:618:PRO:HB2	1.99	0.44
1:G:383:LEU:HD21	1:G:443:PHE:HB3	2.00	0.44
1:K:465:LEU:HD23	1:K:493:LEU:HD22	1.99	0.44
1:M:342:ASN:ND2	1:M:343:PHE:O	2.50	0.44
1:M:465:LEU:HG	1:M:495:VAL:HG22	1.99	0.44
1:AA:465:LEU:HG	1:AA:495:VAL:HG22	1.99	0.44
1:LL:383:LEU:HD21	1:LL:443:PHE:HB3	2.00	0.44
1:LL:548:PRO:HB3	1:LL:556:GLN:HE21	1.82	0.44
1:B:342:ASN:ND2	1:B:343:PHE:O	2.50	0.44
1:D:342:ASN:ND2	1:D:343:PHE:O	2.50	0.44
1:D:465:LEU:HG	1:D:495:VAL:HG22	1.99	0.44
1:E:383:LEU:HD21	1:E:443:PHE:HB3	2.00	0.44
1:E:465:LEU:HD23	1:E:493:LEU:HD22	1.99	0.44
1:F:622:ARG:HH11	1:PP:622:ARG:HH11	1.66	0.44
1:I:342:ASN:ND2	1:I:343:PHE:O	2.50	0.44
1:I:548:PRO:HB3	1:I:556:GLN:HE21	1.82	0.44
1:K:465:LEU:HG	1:K:495:VAL:HG22	1.99	0.44
1:L:342:ASN:ND2	1:L:343:PHE:O	2.50	0.44
1:L:548:PRO:HB3	1:L:556:GLN:HE21	1.82	0.44
1:P:548:PRO:HB3	1:P:556:GLN:HE21	1.82	0.44
1:EE:383:LEU:HD21	1:EE:443:PHE:HB3	1.99	0.44
1:FF:465:LEU:HD23	1:FF:493:LEU:HD22	1.99	0.44
1:GG:342:ASN:ND2	1:GG:343:PHE:O	2.50	0.44
1:GG:465:LEU:HG	1:GG:495:VAL:HG22	1.99	0.44
1:HH:342:ASN:ND2	1:HH:343:PHE:O	2.50	0.44
1:HH:465:LEU:HD23	1:HH:493:LEU:HD22	1.99	0.44
1:JJ:465:LEU:HD23	1:JJ:493:LEU:HD22	1.99	0.44
1:LL:342:ASN:ND2	1:LL:343:PHE:O	2.50	0.44
1:MM:342:ASN:ND2	1:MM:343:PHE:O	2.50	0.44
1:OO:342:ASN:ND2	1:OO:343:PHE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OO:548:PRO:HB3	1:OO:556:GLN:HE21	1.82	0.44
1:PP:342:ASN:ND2	1:PP:343:PHE:O	2.50	0.44
1:D:356:MET:SD	1:D:562:LYS:NZ	2.78	0.44
1:F:342:ASN:ND2	1:F:343:PHE:O	2.50	0.44
1:J:342:ASN:ND2	1:J:343:PHE:O	2.50	0.44
1:AA:563:SER:OG	1:AA:564:GLY:N	2.51	0.44
1:BB:548:PRO:HB3	1:BB:556:GLN:HE21	1.82	0.44
1:EE:342:ASN:ND2	1:EE:343:PHE:O	2.50	0.44
1:NN:383:LEU:HD21	1:NN:443:PHE:HB3	2.00	0.44
1:PP:465:LEU:HG	1:PP:495:VAL:HG22	1.99	0.44
1:B:383:LEU:HD21	1:B:443:PHE:HB3	2.00	0.44
1:C:465:LEU:HD23	1:C:493:LEU:HD22	1.99	0.44
1:H:563:SER:OG	1:H:564:GLY:N	2.51	0.44
1:N:563:SER:OG	1:N:564:GLY:N	2.51	0.44
1:HH:383:LEU:HD21	1:HH:443:PHE:HB3	2.00	0.44
1:II:342:ASN:ND2	1:II:343:PHE:O	2.50	0.44
1:KK:342:ASN:ND2	1:KK:343:PHE:O	2.50	0.44
1:A:383:LEU:HD21	1:A:443:PHE:HB3	2.00	0.44
1:D:465:LEU:HD23	1:D:493:LEU:HD22	1.99	0.44
1:H:465:LEU:HG	1:H:495:VAL:HG22	1.99	0.44
1:K:383:LEU:HD21	1:K:443:PHE:HB3	2.00	0.44
1:N:465:LEU:HD23	1:N:493:LEU:HD22	1.99	0.44
1:P:465:LEU:HG	1:P:495:VAL:HG22	1.99	0.44
1:AA:465:LEU:HD23	1:AA:493:LEU:HD22	1.99	0.44
1:EE:535:PRO:HB2	1:EE:536:SER:H	1.66	0.44
1:FF:383:LEU:HD21	1:FF:443:PHE:HB3	2.00	0.44
1:KK:563:SER:OG	1:KK:564:GLY:N	2.51	0.44
1:C:342:ASN:ND2	1:C:343:PHE:O	2.50	0.43
1:C:383:LEU:HD21	1:C:443:PHE:HB3	2.00	0.43
1:E:563:SER:OG	1:E:564:GLY:N	2.51	0.43
1:H:342:ASN:ND2	1:H:343:PHE:O	2.50	0.43
1:L:383:LEU:HD21	1:L:443:PHE:HB3	2.00	0.43
1:M:465:LEU:HD23	1:M:493:LEU:HD22	1.99	0.43
1:O:548:PRO:HB3	1:O:556:GLN:HE21	1.82	0.43
1:BB:383:LEU:HD21	1:BB:443:PHE:HB3	1.99	0.43
1:CC:342:ASN:ND2	1:CC:343:PHE:O	2.50	0.43
1:CC:465:LEU:HG	1:CC:495:VAL:HG22	1.99	0.43
1:DD:383:LEU:HD21	1:DD:443:PHE:HB3	2.00	0.43
1:FF:342:ASN:ND2	1:FF:343:PHE:O	2.50	0.43
1:GG:465:LEU:HD23	1:GG:493:LEU:HD22	1.99	0.43
1:NN:342:ASN:ND2	1:NN:343:PHE:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NN:563:SER:OG	1:NN:564:GLY:N	2.51	0.43
1:OO:535:PRO:HB2	1:OO:536:SER:H	1.67	0.43
1:A:563:SER:OG	1:A:564:GLY:N	2.51	0.43
1:K:342:ASN:ND2	1:K:343:PHE:O	2.50	0.43
1:K:563:SER:OG	1:K:564:GLY:N	2.51	0.43
1:O:465:LEU:HD23	1:O:493:LEU:HD22	1.99	0.43
1:O:465:LEU:HG	1:O:495:VAL:HG22	1.99	0.43
1:P:342:ASN:ND2	1:P:343:PHE:O	2.50	0.43
1:BB:465:LEU:HG	1:BB:495:VAL:HG22	1.99	0.43
1:DD:563:SER:OG	1:DD:564:GLY:N	2.51	0.43
1:HH:563:SER:OG	1:HH:564:GLY:N	2.51	0.43
1:LL:563:SER:OG	1:LL:564:GLY:N	2.51	0.43
1:I:563:SER:OG	1:I:564:GLY:N	2.51	0.43
1:O:383:LEU:HD21	1:O:443:PHE:HB3	1.99	0.43
1:BB:465:LEU:HD23	1:BB:493:LEU:HD22	1.99	0.43
1:DD:465:LEU:HD23	1:DD:493:LEU:HD22	1.99	0.43
1:KK:465:LEU:HG	1:KK:495:VAL:HG22	1.99	0.43
1:OO:383:LEU:HD21	1:OO:443:PHE:HB3	2.00	0.43
1:PP:465:LEU:HD23	1:PP:493:LEU:HD22	1.99	0.43
1:A:356:MET:SD	1:A:562:LYS:NZ	2.77	0.43
1:A:465:LEU:HD23	1:A:493:LEU:HD22	1.99	0.43
1:F:563:SER:OG	1:F:564:GLY:N	2.51	0.43
1:G:342:ASN:ND2	1:G:343:PHE:O	2.50	0.43
1:M:563:SER:OG	1:M:564:GLY:N	2.51	0.43
1:P:26:LEU:HD23	1:P:28:VAL:H	1.84	0.43
1:P:465:LEU:HD23	1:P:493:LEU:HD22	1.99	0.43
1:P:563:SER:OG	1:P:564:GLY:N	2.51	0.43
1:AA:548:PRO:HB3	1:AA:556:GLN:HE21	1.82	0.43
1:CC:465:LEU:HD23	1:CC:493:LEU:HD22	1.99	0.43
1:II:563:SER:OG	1:II:564:GLY:N	2.51	0.43
1:G:26:LEU:HD23	1:G:28:VAL:H	1.84	0.43
1:J:563:SER:OG	1:J:564:GLY:N	2.51	0.43
1:CC:563:SER:OG	1:CC:564:GLY:N	2.51	0.43
1:JJ:26:LEU:HD23	1:JJ:28:VAL:H	1.84	0.43
1:JJ:342:ASN:ND2	1:JJ:343:PHE:O	2.50	0.43
1:PP:563:SER:OG	1:PP:564:GLY:N	2.51	0.43
1:H:26:LEU:HD23	1:H:28:VAL:H	1.84	0.43
1:H:383:LEU:HD21	1:H:443:PHE:HB3	1.99	0.43
1:L:465:LEU:HG	1:L:495:VAL:HG22	1.99	0.43
1:L:622:ARG:HH11	1:JJ:622:ARG:HH11	1.67	0.43
1:CC:26:LEU:HD23	1:CC:28:VAL:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EE:563:SER:OG	1:EE:564:GLY:N	2.51	0.43
1:LL:26:LEU:HD23	1:LL:28:VAL:H	1.84	0.43
1:MM:563:SER:OG	1:MM:564:GLY:N	2.51	0.43
1:OO:563:SER:OG	1:OO:564:GLY:N	2.51	0.43
1:B:535:PRO:HB2	1:B:536:SER:H	1.67	0.43
1:B:563:SER:OG	1:B:564:GLY:N	2.51	0.43
1:F:356:MET:SD	1:F:562:LYS:NZ	2.78	0.43
1:L:535:PRO:HB2	1:L:536:SER:H	1.66	0.43
1:L:563:SER:OG	1:L:564:GLY:N	2.51	0.43
1:N:548:PRO:HB3	1:N:556:GLN:HE21	1.82	0.43
1:BB:563:SER:OG	1:BB:564:GLY:N	2.51	0.43
1:HH:26:LEU:HD23	1:HH:28:VAL:H	1.84	0.43
1:KK:26:LEU:HD23	1:KK:28:VAL:H	1.84	0.43
1:KK:383:LEU:HD21	1:KK:443:PHE:HB3	1.99	0.43
1:B:26:LEU:HD23	1:B:28:VAL:H	1.84	0.43
1:C:26:LEU:HD23	1:C:28:VAL:H	1.84	0.43
1:E:26:LEU:HD23	1:E:28:VAL:H	1.84	0.43
1:F:618:PRO:HB2	1:OO:618:PRO:HB2	2.01	0.43
1:I:26:LEU:HD23	1:I:28:VAL:H	1.84	0.43
1:N:26:LEU:HD23	1:N:28:VAL:H	1.84	0.43
1:O:563:SER:OG	1:O:564:GLY:N	2.51	0.43
1:P:383:LEU:HD21	1:P:443:PHE:HB3	2.00	0.43
1:AA:26:LEU:HD23	1:AA:28:VAL:H	1.84	0.43
1:CC:383:LEU:HD21	1:CC:443:PHE:HB3	2.00	0.43
1:EE:26:LEU:HD23	1:EE:28:VAL:H	1.84	0.43
1:FF:26:LEU:HD23	1:FF:28:VAL:H	1.84	0.43
1:GG:383:LEU:HD21	1:GG:443:PHE:HB3	2.00	0.43
1:PP:548:PRO:HB3	1:PP:556:GLN:HE21	1.82	0.43
1:D:26:LEU:HD23	1:D:28:VAL:H	1.84	0.43
1:O:26:LEU:HD23	1:O:28:VAL:H	1.84	0.43
1:BB:26:LEU:HD23	1:BB:28:VAL:H	1.84	0.43
1:EE:465:LEU:HD23	1:EE:493:LEU:HD22	1.99	0.43
1:GG:26:LEU:HD23	1:GG:28:VAL:H	1.84	0.43
1:LL:535:PRO:HB2	1:LL:536:SER:H	1.67	0.43
1:OO:465:LEU:HG	1:OO:495:VAL:HG22	1.99	0.43
1:B:465:LEU:HD23	1:B:493:LEU:HD22	1.99	0.43
1:M:26:LEU:HD23	1:M:28:VAL:H	1.84	0.43
1:KK:623:ARG:HH22	1:LL:167:ASN:ND2	2.17	0.43
1:MM:623:ARG:HH22	1:NN:167:ASN:ND2	2.17	0.43
1:B:189:THR:HG21	1:B:288:ARG:HH11	1.84	0.42
1:D:383:LEU:HD21	1:D:443:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:548:PRO:HB3	1:M:556:GLN:HE21	1.82	0.42
1:EE:189:THR:HG21	1:EE:288:ARG:HH11	1.84	0.42
1:MM:26:LEU:HD23	1:MM:28:VAL:H	1.84	0.42
1:OO:189:THR:HG21	1:OO:288:ARG:HH11	1.84	0.42
1:PP:26:LEU:HD23	1:PP:28:VAL:H	1.84	0.42
1:E:189:THR:HG21	1:E:288:ARG:HH11	1.84	0.42
1:L:189:THR:HG21	1:L:288:ARG:HH11	1.84	0.42
1:G:189:THR:HG21	1:G:288:ARG:HH11	1.84	0.42
1:I:189:THR:HG21	1:I:288:ARG:HH11	1.84	0.42
1:J:26:LEU:HD23	1:J:28:VAL:H	1.84	0.42
1:K:26:LEU:HD23	1:K:28:VAL:H	1.84	0.42
1:O:189:THR:HG21	1:O:288:ARG:HH11	1.84	0.42
1:JJ:189:THR:HG21	1:JJ:288:ARG:HH11	1.84	0.42
1:LL:189:THR:HG21	1:LL:288:ARG:HH11	1.84	0.42
1:J:189:THR:HG21	1:J:288:ARG:HH11	1.84	0.42
1:L:26:LEU:HD23	1:L:28:VAL:H	1.84	0.42
1:BB:189:THR:HG21	1:BB:288:ARG:HH11	1.84	0.42
1:BB:535:PRO:HB2	1:BB:536:SER:H	1.67	0.42
1:HH:189:THR:HG21	1:HH:288:ARG:HH11	1.84	0.42
1:NN:467:SER:H	1:NN:470:SER:HB3	1.85	0.42
1:OO:26:LEU:HD23	1:OO:28:VAL:H	1.84	0.42
1:B:261:ILE:HG22	1:B:284:VAL:HG21	2.02	0.42
1:I:535:PRO:HB2	1:I:536:SER:H	1.67	0.42
1:K:467:SER:H	1:K:470:SER:HB3	1.85	0.42
1:L:261:ILE:HG22	1:L:284:VAL:HG21	2.02	0.42
1:M:261:ILE:HG22	1:M:284:VAL:HG21	2.02	0.42
1:EE:261:ILE:HG22	1:EE:284:VAL:HG21	2.02	0.42
1:GG:189:THR:HG21	1:GG:288:ARG:HH11	1.84	0.42
1:MM:189:THR:HG21	1:MM:288:ARG:HH11	1.84	0.42
1:NN:26:LEU:HD23	1:NN:28:VAL:H	1.84	0.42
1:PP:261:ILE:HG22	1:PP:284:VAL:HG21	2.02	0.42
1:D:189:THR:HG21	1:D:288:ARG:HH11	1.84	0.42
1:D:563:SER:OG	1:D:564:GLY:N	2.51	0.42
1:G:563:SER:OG	1:G:564:GLY:N	2.51	0.42
1:I:467:SER:H	1:I:470:SER:HB3	1.85	0.42
1:L:467:SER:H	1:L:470:SER:HB3	1.85	0.42
1:FF:563:SER:OG	1:FF:564:GLY:N	2.51	0.42
1:JJ:563:SER:OG	1:JJ:564:GLY:N	2.51	0.42
1:LL:467:SER:H	1:LL:470:SER:HB3	1.85	0.42
1:OO:261:ILE:HG22	1:OO:284:VAL:HG21	2.02	0.42
1:OO:467:SER:H	1:OO:470:SER:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HG22	1:A:284:VAL:HG21	2.02	0.42
1:C:189:THR:HG21	1:C:288:ARG:HH11	1.84	0.42
1:C:563:SER:OG	1:C:564:GLY:N	2.51	0.42
1:M:467:SER:H	1:M:470:SER:HB3	1.85	0.42
1:PP:467:SER:H	1:PP:470:SER:HB3	1.85	0.42
1:A:26:LEU:HD23	1:A:28:VAL:H	1.84	0.42
1:L:426:VAL:HG21	1:JJ:628:ILE:HD12	2.01	0.42
1:AA:261:ILE:HG22	1:AA:284:VAL:HG21	2.02	0.42
1:DD:467:SER:H	1:DD:470:SER:HB3	1.85	0.42
1:EE:467:SER:H	1:EE:470:SER:HB3	1.85	0.42
1:GG:563:SER:OG	1:GG:564:GLY:N	2.51	0.42
1:LL:261:ILE:HG22	1:LL:284:VAL:HG21	2.02	0.42
1:A:467:SER:H	1:A:470:SER:HB3	1.85	0.42
1:B:467:SER:H	1:B:470:SER:HB3	1.85	0.42
1:F:26:LEU:HD23	1:F:28:VAL:H	1.84	0.42
1:I:261:ILE:HG22	1:I:284:VAL:HG21	2.02	0.42
1:N:189:THR:HG21	1:N:288:ARG:HH11	1.84	0.42
1:N:261:ILE:HG22	1:N:284:VAL:HG21	2.02	0.42
1:O:467:SER:H	1:O:470:SER:HB3	1.85	0.42
1:P:189:THR:HG21	1:P:288:ARG:HH11	1.84	0.42
1:P:467:SER:H	1:P:470:SER:HB3	1.85	0.42
1:AA:189:THR:HG21	1:AA:288:ARG:HH11	1.84	0.42
1:CC:467:SER:H	1:CC:470:SER:HB3	1.85	0.42
1:DD:26:LEU:HD23	1:DD:28:VAL:H	1.84	0.42
1:DD:261:ILE:HG22	1:DD:284:VAL:HG21	2.02	0.42
1:FF:189:THR:HG21	1:FF:288:ARG:HH11	1.84	0.42
1:II:26:LEU:HD23	1:II:28:VAL:H	1.84	0.42
1:M:189:THR:HG21	1:M:288:ARG:HH11	1.84	0.42
1:O:535:PRO:HB2	1:O:536:SER:H	1.67	0.42
1:BB:467:SER:H	1:BB:470:SER:HB3	1.85	0.42
1:GG:467:SER:H	1:GG:470:SER:HB3	1.85	0.42
1:JJ:467:SER:H	1:JJ:470:SER:HB3	1.85	0.42
1:E:261:ILE:HG22	1:E:284:VAL:HG21	2.02	0.41
1:F:467:SER:H	1:F:470:SER:HB3	1.85	0.41
1:G:467:SER:H	1:G:470:SER:HB3	1.85	0.41
1:H:261:ILE:HG22	1:H:284:VAL:HG21	2.02	0.41
1:EE:356:MET:SD	1:EE:562:LYS:NZ	2.78	0.41
1:FF:261:ILE:HG22	1:FF:284:VAL:HG21	2.02	0.41
1:HH:261:ILE:HG22	1:HH:284:VAL:HG21	2.02	0.41
1:KK:261:ILE:HG22	1:KK:284:VAL:HG21	2.02	0.41
1:NN:189:THR:HG21	1:NN:288:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:SER:H	1:D:470:SER:HB3	1.85	0.41
1:G:628:ILE:HD12	1:OO:426:VAL:HG21	2.01	0.41
1:CC:189:THR:HG21	1:CC:288:ARG:HH11	1.84	0.41
1:DD:189:THR:HG21	1:DD:288:ARG:HH11	1.84	0.41
1:KK:467:SER:H	1:KK:470:SER:HB3	1.85	0.41
1:PP:189:THR:HG21	1:PP:288:ARG:HH11	1.84	0.41
1:C:261:ILE:HG22	1:C:284:VAL:HG21	2.02	0.41
1:K:189:THR:HG21	1:K:288:ARG:HH11	1.84	0.41
1:K:261:ILE:HG22	1:K:284:VAL:HG21	2.02	0.41
1:BB:261:ILE:HG22	1:BB:284:VAL:HG21	2.02	0.41
1:II:261:ILE:HG22	1:II:284:VAL:HG21	2.02	0.41
1:II:467:SER:H	1:II:470:SER:HB3	1.85	0.41
1:KK:189:THR:HG21	1:KK:288:ARG:HH11	1.84	0.41
1:F:261:ILE:HG22	1:F:284:VAL:HG21	2.02	0.41
1:H:189:THR:HG21	1:H:288:ARG:HH11	1.84	0.41
1:N:467:SER:H	1:N:470:SER:HB3	1.85	0.41
1:P:261:ILE:HG22	1:P:284:VAL:HG21	2.02	0.41
1:AA:467:SER:H	1:AA:470:SER:HB3	1.85	0.41
1:MM:261:ILE:HG22	1:MM:284:VAL:HG21	2.02	0.41
1:A:189:THR:HG21	1:A:288:ARG:HH11	1.85	0.41
1:NN:261:ILE:HG22	1:NN:284:VAL:HG21	2.02	0.41
1:H:467:SER:H	1:H:470:SER:HB3	1.85	0.41
1:J:261:ILE:HG22	1:J:284:VAL:HG21	2.02	0.41
1:J:467:SER:H	1:J:470:SER:HB3	1.85	0.41
1:O:261:ILE:HG22	1:O:284:VAL:HG21	2.02	0.41
1:II:189:THR:HG21	1:II:288:ARG:HH11	1.84	0.41
1:CC:261:ILE:HG22	1:CC:284:VAL:HG21	2.02	0.41
1:HH:467:SER:H	1:HH:470:SER:HB3	1.85	0.41
1:F:189:THR:HG21	1:F:288:ARG:HH11	1.84	0.41
1:G:426:VAL:HG21	1:OO:628:ILE:HD12	2.03	0.41
1:MM:268:PRO:HD3	1:NN:77:LEU:HD11	2.03	0.41
1:MM:467:SER:H	1:MM:470:SER:HB3	1.85	0.41
1:C:204:LEU:HD23	1:C:253:ARG:HA	2.03	0.41
1:D:261:ILE:HG22	1:D:284:VAL:HG21	2.02	0.41
1:E:467:SER:H	1:E:470:SER:HB3	1.85	0.41
1:AA:148:LEU:HD12	1:AA:149:GLU:H	1.86	0.41
1:A:148:LEU:HD12	1:A:149:GLU:H	1.86	0.41
1:F:628:ILE:HD12	1:PP:426:VAL:HG21	2.01	0.41
1:H:535:PRO:HB2	1:H:536:SER:H	1.67	0.41
1:P:204:LEU:HD23	1:P:253:ARG:HA	2.03	0.41
1:CC:204:LEU:HD23	1:CC:253:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DD:204:LEU:HD23	1:DD:253:ARG:HA	2.03	0.41
1:FF:204:LEU:HD23	1:FF:253:ARG:HA	2.03	0.41
1:A:104:LEU:HD11	1:P:469:LYS:HA	2.04	0.40
1:A:204:LEU:HD23	1:A:253:ARG:HA	2.03	0.40
1:E:204:LEU:HD23	1:E:253:ARG:HA	2.03	0.40
1:F:426:VAL:HG21	1:PP:628:ILE:HD12	2.02	0.40
1:K:148:LEU:HD12	1:K:149:GLU:H	1.86	0.40
1:N:148:LEU:HD12	1:N:149:GLU:H	1.87	0.40
1:FF:563:SER:OG	1:FF:565:LEU:N	2.55	0.40
1:GG:204:LEU:HD23	1:GG:253:ARG:HA	2.03	0.40
1:GG:261:ILE:HG22	1:GG:284:VAL:HG21	2.02	0.40
1:HH:204:LEU:HD23	1:HH:253:ARG:HA	2.03	0.40
1:KK:535:PRO:HB2	1:KK:536:SER:H	1.67	0.40
1:B:204:LEU:HD23	1:B:253:ARG:HA	2.03	0.40
1:B:563:SER:OG	1:B:565:LEU:N	2.55	0.40
1:C:563:SER:OG	1:C:565:LEU:N	2.55	0.40
1:D:204:LEU:HD23	1:D:253:ARG:HA	2.03	0.40
1:D:563:SER:OG	1:D:565:LEU:N	2.55	0.40
1:AA:204:LEU:HD23	1:AA:253:ARG:HA	2.03	0.40
1:DD:148:LEU:HD12	1:DD:149:GLU:H	1.87	0.40
1:EE:204:LEU:HD23	1:EE:253:ARG:HA	2.03	0.40
1:JJ:535:PRO:HB2	1:JJ:536:SER:H	1.66	0.40
1:MM:469:LYS:HA	1:NN:104:LEU:HD11	2.02	0.40
1:D:148:LEU:HD12	1:D:149:GLU:H	1.86	0.40
1:G:535:PRO:HB2	1:G:536:SER:H	1.67	0.40
1:N:204:LEU:HD23	1:N:253:ARG:HA	2.03	0.40
1:O:563:SER:OG	1:O:565:LEU:N	2.55	0.40
1:BB:204:LEU:HD23	1:BB:253:ARG:HA	2.03	0.40
1:BB:563:SER:OG	1:BB:565:LEU:N	2.55	0.40
1:EE:563:SER:OG	1:EE:565:LEU:N	2.55	0.40
1:FF:467:SER:H	1:FF:470:SER:HB3	1.85	0.40
1:GG:563:SER:OG	1:GG:565:LEU:N	2.55	0.40
1:MM:148:LEU:HD12	1:MM:149:GLU:H	1.86	0.40
1:A:563:SER:OG	1:A:565:LEU:N	2.55	0.40
1:C:467:SER:H	1:C:470:SER:HB3	1.85	0.40
1:E:563:SER:OG	1:E:565:LEU:N	2.55	0.40
1:F:204:LEU:HD23	1:F:253:ARG:HA	2.03	0.40
1:J:148:LEU:HD12	1:J:149:GLU:H	1.86	0.40
1:O:204:LEU:HD23	1:O:253:ARG:HA	2.03	0.40
1:DD:563:SER:OG	1:DD:565:LEU:N	2.55	0.40
1:GG:148:LEU:HD12	1:GG:149:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HH:563:SER:OG	1:HH:565:LEU:N	2.55	0.40
1:II:204:LEU:HD23	1:II:253:ARG:HA	2.03	0.40
1:KK:563:SER:OG	1:KK:565:LEU:N	2.55	0.40
1:MM:563:SER:OG	1:MM:565:LEU:N	2.55	0.40
1:NN:148:LEU:HD12	1:NN:149:GLU:H	1.87	0.40
1:F:563:SER:OG	1:F:565:LEU:N	2.55	0.40
1:G:563:SER:OG	1:G:565:LEU:N	2.55	0.40
1:H:563:SER:OG	1:H:565:LEU:N	2.55	0.40
1:I:563:SER:OG	1:I:565:LEU:N	2.55	0.40
1:J:563:SER:OG	1:J:565:LEU:N	2.55	0.40
1:P:563:SER:OG	1:P:565:LEU:N	2.55	0.40
1:AA:104:LEU:HD11	1:PP:469:LYS:HA	2.04	0.40
1:CC:563:SER:OG	1:CC:565:LEU:N	2.55	0.40
1:II:563:SER:OG	1:II:565:LEU:N	2.55	0.40
1:JJ:563:SER:OG	1:JJ:565:LEU:N	2.55	0.40
1:LL:148:LEU:HD12	1:LL:149:GLU:H	1.86	0.40
1:LL:563:SER:OG	1:LL:565:LEU:N	2.55	0.40
1:NN:563:SER:OG	1:NN:565:LEU:N	2.55	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	609/642 (95%)	565 (93%)	44 (7%)	0	100	100
1	AA	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	B	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	BB	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	C	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	CC	609/642 (95%)	566 (93%)	43 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	DD	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	E	609/642 (95%)	565 (93%)	44 (7%)	0	100	100
1	EE	609/642 (95%)	565 (93%)	44 (7%)	0	100	100
1	F	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	FF	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	G	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	GG	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	H	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	HH	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	I	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	II	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	J	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	JJ	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	K	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	KK	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	L	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	LL	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	M	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	MM	609/642 (95%)	565 (93%)	44 (7%)	0	100	100
1	N	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	NN	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	O	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	OO	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	P	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
1	PP	609/642 (95%)	566 (93%)	43 (7%)	0	100	100
All	All	19488/20544 (95%)	18108 (93%)	1380 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	AA	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	B	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	BB	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	C	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	CC	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	D	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	DD	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	E	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	EE	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	F	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	FF	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	G	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	GG	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	H	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	HH	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	I	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	II	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	J	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	JJ	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	K	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	KK	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	L	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	LL	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	M	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	MM	534/562 (95%)	533 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	NN	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	O	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	OO	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	P	534/562 (95%)	533 (100%)	1 (0%)	87	95
1	PP	534/562 (95%)	533 (100%)	1 (0%)	87	95
All	All	17088/17984 (95%)	17056 (100%)	32 (0%)	85	95

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	B	80	ASN
1	C	80	ASN
1	D	80	ASN
1	E	80	ASN
1	F	80	ASN
1	G	80	ASN
1	H	80	ASN
1	I	80	ASN
1	J	80	ASN
1	K	80	ASN
1	L	80	ASN
1	M	80	ASN
1	N	80	ASN
1	O	80	ASN
1	P	80	ASN
1	AA	80	ASN
1	BB	80	ASN
1	CC	80	ASN
1	DD	80	ASN
1	EE	80	ASN
1	FF	80	ASN
1	GG	80	ASN
1	HH	80	ASN
1	II	80	ASN
1	JJ	80	ASN
1	KK	80	ASN
1	LL	80	ASN
1	MM	80	ASN

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Mol	Chain	Res	Type
1	NN	80	ASN
1	OO	80	ASN
1	PP	80	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (391) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	39	ASN
1	A	72	GLN
1	A	74	GLN
1	A	76	ASN
1	A	80	ASN
1	A	137	ASN
1	A	167	ASN
1	A	281	ASN
1	A	342	ASN
1	A	499	GLN
1	A	556	GLN
1	A	600	ASN
1	B	36	ASN
1	B	39	ASN
1	B	72	GLN
1	B	76	ASN
1	B	80	ASN
1	B	137	ASN
1	B	167	ASN
1	B	229	ASN
1	B	340	ASN
1	B	342	ASN
1	B	499	GLN
1	B	556	GLN
1	B	600	ASN
1	C	36	ASN
1	C	39	ASN
1	C	72	GLN
1	C	76	ASN
1	C	80	ASN
1	C	137	ASN
1	C	167	ASN
1	C	342	ASN
1	C	499	GLN

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Mol	Chain	Res	Type
1	C	556	GLN
1	C	600	ASN
1	D	36	ASN
1	D	39	ASN
1	D	72	GLN
1	D	76	ASN
1	D	80	ASN
1	D	137	ASN
1	D	167	ASN
1	D	229	ASN
1	D	281	ASN
1	D	342	ASN
1	D	499	GLN
1	D	556	GLN
1	D	600	ASN
1	E	36	ASN
1	E	39	ASN
1	E	72	GLN
1	E	76	ASN
1	E	80	ASN
1	E	137	ASN
1	E	167	ASN
1	E	281	ASN
1	E	340	ASN
1	E	342	ASN
1	E	374	ASN
1	E	499	GLN
1	E	556	GLN
1	E	600	ASN
1	F	36	ASN
1	F	39	ASN
1	F	72	GLN
1	F	76	ASN
1	F	80	ASN
1	F	137	ASN
1	F	167	ASN
1	F	342	ASN
1	F	499	GLN
1	F	556	GLN
1	F	600	ASN
1	G	36	ASN
1	G	39	ASN

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Mol	Chain	Res	Type
1	G	72	GLN
1	G	76	ASN
1	G	80	ASN
1	G	137	ASN
1	G	167	ASN
1	G	342	ASN
1	G	374	ASN
1	G	499	GLN
1	G	556	GLN
1	G	600	ASN
1	H	36	ASN
1	H	39	ASN
1	H	72	GLN
1	H	76	ASN
1	H	80	ASN
1	H	123	GLN
1	H	137	ASN
1	H	167	ASN
1	H	342	ASN
1	H	499	GLN
1	H	556	GLN
1	H	626	ASN
1	I	36	ASN
1	I	39	ASN
1	I	72	GLN
1	I	76	ASN
1	I	80	ASN
1	I	137	ASN
1	I	167	ASN
1	I	229	ASN
1	I	281	ASN
1	I	342	ASN
1	I	499	GLN
1	I	556	GLN
1	I	600	ASN
1	J	36	ASN
1	J	39	ASN
1	J	72	GLN
1	J	76	ASN
1	J	80	ASN
1	J	137	ASN
1	J	167	ASN

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Mol	Chain	Res	Type
1	J	229	ASN
1	J	342	ASN
1	J	414	ASN
1	J	499	GLN
1	J	556	GLN
1	J	600	ASN
1	K	36	ASN
1	K	39	ASN
1	K	72	GLN
1	K	76	ASN
1	K	80	ASN
1	K	137	ASN
1	K	167	ASN
1	K	229	ASN
1	K	342	ASN
1	K	499	GLN
1	K	556	GLN
1	K	600	ASN
1	L	36	ASN
1	L	39	ASN
1	L	72	GLN
1	L	76	ASN
1	L	80	ASN
1	L	123	GLN
1	L	137	ASN
1	L	167	ASN
1	L	229	ASN
1	L	342	ASN
1	L	499	GLN
1	L	556	GLN
1	L	600	ASN
1	M	36	ASN
1	M	39	ASN
1	M	72	GLN
1	M	76	ASN
1	M	80	ASN
1	M	137	ASN
1	M	167	ASN
1	M	229	ASN
1	M	342	ASN
1	M	499	GLN
1	M	556	GLN

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Mol	Chain	Res	Type
1	N	36	ASN
1	N	39	ASN
1	N	72	GLN
1	N	76	ASN
1	N	80	ASN
1	N	137	ASN
1	N	167	ASN
1	N	229	ASN
1	N	281	ASN
1	N	342	ASN
1	N	374	ASN
1	N	414	ASN
1	N	499	GLN
1	N	556	GLN
1	O	36	ASN
1	O	39	ASN
1	O	72	GLN
1	O	76	ASN
1	O	80	ASN
1	O	137	ASN
1	O	167	ASN
1	O	281	ASN
1	O	342	ASN
1	O	499	GLN
1	O	556	GLN
1	P	36	ASN
1	P	39	ASN
1	P	72	GLN
1	P	76	ASN
1	P	80	ASN
1	P	137	ASN
1	P	167	ASN
1	P	229	ASN
1	P	281	ASN
1	P	342	ASN
1	P	499	GLN
1	P	556	GLN
1	AA	36	ASN
1	AA	39	ASN
1	AA	72	GLN
1	AA	74	GLN
1	AA	76	ASN

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Mol	Chain	Res	Type
1	AA	80	ASN
1	AA	137	ASN
1	AA	167	ASN
1	AA	229	ASN
1	AA	281	ASN
1	AA	342	ASN
1	AA	414	ASN
1	AA	499	GLN
1	AA	556	GLN
1	AA	600	ASN
1	BB	36	ASN
1	BB	39	ASN
1	BB	72	GLN
1	BB	76	ASN
1	BB	80	ASN
1	BB	137	ASN
1	BB	167	ASN
1	BB	281	ASN
1	BB	342	ASN
1	BB	499	GLN
1	BB	556	GLN
1	BB	600	ASN
1	CC	36	ASN
1	CC	39	ASN
1	CC	72	GLN
1	CC	76	ASN
1	CC	80	ASN
1	CC	137	ASN
1	CC	167	ASN
1	CC	229	ASN
1	CC	342	ASN
1	CC	499	GLN
1	CC	556	GLN
1	CC	600	ASN
1	DD	36	ASN
1	DD	39	ASN
1	DD	72	GLN
1	DD	76	ASN
1	DD	80	ASN
1	DD	137	ASN
1	DD	167	ASN
1	DD	232	ASN

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Mol	Chain	Res	Type
1	DD	281	ASN
1	DD	342	ASN
1	DD	414	ASN
1	DD	499	GLN
1	DD	556	GLN
1	DD	600	ASN
1	EE	36	ASN
1	EE	39	ASN
1	EE	72	GLN
1	EE	76	ASN
1	EE	80	ASN
1	EE	137	ASN
1	EE	167	ASN
1	EE	229	ASN
1	EE	281	ASN
1	EE	342	ASN
1	EE	499	GLN
1	EE	556	GLN
1	EE	600	ASN
1	FF	36	ASN
1	FF	39	ASN
1	FF	72	GLN
1	FF	76	ASN
1	FF	80	ASN
1	FF	137	ASN
1	FF	167	ASN
1	FF	342	ASN
1	FF	499	GLN
1	FF	556	GLN
1	GG	36	ASN
1	GG	39	ASN
1	GG	72	GLN
1	GG	76	ASN
1	GG	80	ASN
1	GG	137	ASN
1	GG	167	ASN
1	GG	229	ASN
1	GG	281	ASN
1	GG	342	ASN
1	GG	499	GLN
1	GG	556	GLN
1	HH	36	ASN

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Mol	Chain	Res	Type
1	HH	39	ASN
1	HH	72	GLN
1	HH	76	ASN
1	HH	80	ASN
1	HH	137	ASN
1	HH	167	ASN
1	HH	340	ASN
1	HH	342	ASN
1	HH	499	GLN
1	HH	556	GLN
1	II	36	ASN
1	II	39	ASN
1	II	72	GLN
1	II	76	ASN
1	II	80	ASN
1	II	137	ASN
1	II	167	ASN
1	II	229	ASN
1	II	342	ASN
1	II	499	GLN
1	II	556	GLN
1	JJ	36	ASN
1	JJ	39	ASN
1	JJ	72	GLN
1	JJ	76	ASN
1	JJ	80	ASN
1	JJ	137	ASN
1	JJ	167	ASN
1	JJ	342	ASN
1	JJ	499	GLN
1	JJ	556	GLN
1	JJ	600	ASN
1	KK	36	ASN
1	KK	39	ASN
1	KK	72	GLN
1	KK	76	ASN
1	KK	80	ASN
1	KK	123	GLN
1	KK	137	ASN
1	KK	167	ASN
1	KK	342	ASN
1	KK	499	GLN

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Mol	Chain	Res	Type
1	KK	556	GLN
1	KK	600	ASN
1	LL	36	ASN
1	LL	39	ASN
1	LL	72	GLN
1	LL	76	ASN
1	LL	80	ASN
1	LL	137	ASN
1	LL	167	ASN
1	LL	229	ASN
1	LL	342	ASN
1	LL	499	GLN
1	LL	556	GLN
1	LL	600	ASN
1	MM	36	ASN
1	MM	39	ASN
1	MM	72	GLN
1	MM	76	ASN
1	MM	80	ASN
1	MM	137	ASN
1	MM	167	ASN
1	MM	229	ASN
1	MM	342	ASN
1	MM	499	GLN
1	MM	556	GLN
1	NN	36	ASN
1	NN	39	ASN
1	NN	72	GLN
1	NN	74	GLN
1	NN	76	ASN
1	NN	80	ASN
1	NN	137	ASN
1	NN	167	ASN
1	NN	229	ASN
1	NN	342	ASN
1	NN	499	GLN
1	NN	556	GLN
1	NN	600	ASN
1	OO	36	ASN
1	OO	39	ASN
1	OO	72	GLN
1	OO	80	ASN

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Mol	Chain	Res	Type
1	OO	123	GLN
1	OO	137	ASN
1	OO	167	ASN
1	OO	229	ASN
1	OO	342	ASN
1	OO	374	ASN
1	OO	499	GLN
1	OO	556	GLN
1	OO	600	ASN
1	PP	36	ASN
1	PP	39	ASN
1	PP	72	GLN
1	PP	76	ASN
1	PP	80	ASN
1	PP	137	ASN
1	PP	167	ASN
1	PP	342	ASN
1	PP	499	GLN
1	PP	556	GLN
1	PP	600	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 ⓘ

64 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Q	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	Q	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	R	2	2	14,14,15	0.44	0	17,19,21	0.99	1 (5%)
2	NAG	S	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	S	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	T	1	1,2	14,14,15	0.42	0	17,19,21	0.66	0
2	NAG	T	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	U	1	1,2	14,14,15	0.42	0	17,19,21	0.65	0
2	NAG	U	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	V	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	V	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	W	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	X	1	1,2	14,14,15	0.41	0	17,19,21	0.64	0
2	NAG	X	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	Y	1	1,2	14,14,15	0.40	0	17,19,21	0.65	0
2	NAG	Y	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	Z	1	1,2	14,14,15	0.42	0	17,19,21	0.65	0
2	NAG	Z	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	a	1	1,2	14,14,15	0.41	0	17,19,21	0.64	0
2	NAG	a	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	b	1	1,2	14,14,15	0.41	0	17,19,21	0.66	0
2	NAG	b	2	2	14,14,15	0.44	0	17,19,21	0.99	1 (5%)
2	NAG	c	1	1,2	14,14,15	0.41	0	17,19,21	0.64	0
2	NAG	c	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	d	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	d	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	e	1	1,2	14,14,15	0.41	0	17,19,21	0.64	0
2	NAG	e	2	2	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
2	NAG	f	1	1,2	14,14,15	0.40	0	17,19,21	0.64	0
2	NAG	f	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	g	1	1,2	14,14,15	0.40	0	17,19,21	0.65	0
2	NAG	g	2	2	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
2	NAG	h	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	h	2	2	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
2	NAG	i	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	i	2	2	14,14,15	0.46	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	j	1	1,2	14,14,15	0.42	0	17,19,21	0.65	0
2	NAG	j	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	k	1	1,2	14,14,15	0.40	0	17,19,21	0.65	0
2	NAG	k	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	l	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	l	2	2	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
2	NAG	m	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	m	2	2	14,14,15	0.46	0	17,19,21	1.01	1 (5%)
2	NAG	n	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	n	2	2	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
2	NAG	o	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	o	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	p	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	p	2	2	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
2	NAG	q	1	1,2	14,14,15	0.42	0	17,19,21	0.65	0
2	NAG	q	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	r	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	r	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	s	1	1,2	14,14,15	0.40	0	17,19,21	0.65	0
2	NAG	s	2	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	t	1	1,2	14,14,15	0.42	0	17,19,21	0.65	0
2	NAG	t	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	u	1	1,2	14,14,15	0.41	0	17,19,21	0.65	0
2	NAG	u	2	2	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	v	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	v	2	2	14,14,15	0.46	0	17,19,21	1.00	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	4/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	S	2	2	-	4/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	4/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	4/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	4/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	4/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	4/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	4/6/23/26	0/1/1/1
2	NAG	b	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	4/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	4/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	e	2	2	-	4/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	f	2	2	-	4/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	4/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	4/6/23/26	0/1/1/1
2	NAG	i	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	i	2	2	-	4/6/23/26	0/1/1/1
2	NAG	j	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	j	2	2	-	4/6/23/26	0/1/1/1
2	NAG	k	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	k	2	2	-	4/6/23/26	0/1/1/1
2	NAG	l	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	l	2	2	-	4/6/23/26	0/1/1/1
2	NAG	m	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	4/6/23/26	0/1/1/1
2	NAG	n	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	n	2	2	-	4/6/23/26	0/1/1/1
2	NAG	o	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	o	2	2	-	4/6/23/26	0/1/1/1
2	NAG	p	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	p	2	2	-	4/6/23/26	0/1/1/1
2	NAG	q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	q	2	2	-	4/6/23/26	0/1/1/1
2	NAG	r	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	4/6/23/26	0/1/1/1
2	NAG	s	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	4/6/23/26	0/1/1/1
2	NAG	t	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	t	2	2	-	4/6/23/26	0/1/1/1
2	NAG	u	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	u	2	2	-	4/6/23/26	0/1/1/1
2	NAG	v	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	v	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p	2	NAG	C2-N2-C7	3.26	127.27	122.90
2	i	2	NAG	C2-N2-C7	3.25	127.26	122.90
2	n	2	NAG	C2-N2-C7	3.24	127.25	122.90
2	W	2	NAG	C2-N2-C7	3.23	127.23	122.90
2	Q	2	NAG	C2-N2-C7	3.23	127.22	122.90
2	j	2	NAG	C2-N2-C7	3.23	127.22	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	NAG	C2-N2-C7	3.22	127.22	122.90
2	k	2	NAG	C2-N2-C7	3.22	127.22	122.90
2	e	2	NAG	C2-N2-C7	3.22	127.22	122.90
2	X	2	NAG	C2-N2-C7	3.22	127.22	122.90
2	S	2	NAG	C2-N2-C7	3.22	127.21	122.90
2	m	2	NAG	C2-N2-C7	3.22	127.21	122.90
2	u	2	NAG	C2-N2-C7	3.21	127.21	122.90
2	c	2	NAG	C2-N2-C7	3.21	127.20	122.90
2	h	2	NAG	C2-N2-C7	3.21	127.20	122.90
2	f	2	NAG	C2-N2-C7	3.21	127.20	122.90
2	q	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	t	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	v	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	r	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	a	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	T	2	NAG	C2-N2-C7	3.20	127.18	122.90
2	V	2	NAG	C2-N2-C7	3.19	127.17	122.90
2	o	2	NAG	C2-N2-C7	3.19	127.17	122.90
2	d	2	NAG	C2-N2-C7	3.19	127.17	122.90
2	s	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	Y	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	g	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	R	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	l	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	Z	2	NAG	C2-N2-C7	3.18	127.16	122.90
2	b	2	NAG	C2-N2-C7	3.18	127.16	122.90

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	e	2	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
2	q	2	NAG	C4-C5-C6-O6
2	r	2	NAG	C4-C5-C6-O6
2	t	2	NAG	C4-C5-C6-O6
2	v	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	l	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	p	2	NAG	C4-C5-C6-O6
2	s	2	NAG	C4-C5-C6-O6
2	u	2	NAG	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	t	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	p	2	NAG	O5-C5-C6-O6
2	q	2	NAG	O5-C5-C6-O6
2	s	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	u	2	NAG	O5-C5-C6-O6
2	v	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	l	2	NAG	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	i	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
2	l	1	NAG	C4-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	n	1	NAG	C4-C5-C6-O6
2	o	1	NAG	C4-C5-C6-O6
2	p	1	NAG	C4-C5-C6-O6
2	q	1	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
2	s	1	NAG	C4-C5-C6-O6
2	t	1	NAG	C4-C5-C6-O6
2	u	1	NAG	C4-C5-C6-O6
2	j	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	v	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	t	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	j	1	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	o	1	NAG	O5-C5-C6-O6
2	q	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	s	1	NAG	O5-C5-C6-O6
2	u	1	NAG	O5-C5-C6-O6
2	v	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	p	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	l	1	NAG	O5-C5-C6-O6
2	Q	2	NAG	C1-C2-N2-C7
2	R	2	NAG	C1-C2-N2-C7
2	S	2	NAG	C1-C2-N2-C7
2	T	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C1-C2-N2-C7
2	V	2	NAG	C1-C2-N2-C7
2	W	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7
2	Y	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	Z	2	NAG	C1-C2-N2-C7
2	a	2	NAG	C1-C2-N2-C7
2	b	2	NAG	C1-C2-N2-C7
2	c	2	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
2	e	2	NAG	C1-C2-N2-C7
2	f	2	NAG	C1-C2-N2-C7
2	g	2	NAG	C1-C2-N2-C7
2	h	2	NAG	C1-C2-N2-C7
2	i	2	NAG	C1-C2-N2-C7
2	j	2	NAG	C1-C2-N2-C7
2	k	2	NAG	C1-C2-N2-C7
2	l	2	NAG	C1-C2-N2-C7
2	m	2	NAG	C1-C2-N2-C7
2	n	2	NAG	C1-C2-N2-C7
2	o	2	NAG	C1-C2-N2-C7
2	p	2	NAG	C1-C2-N2-C7
2	q	2	NAG	C1-C2-N2-C7
2	r	2	NAG	C1-C2-N2-C7
2	s	2	NAG	C1-C2-N2-C7
2	t	2	NAG	C1-C2-N2-C7
2	u	2	NAG	C1-C2-N2-C7
2	v	2	NAG	C1-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7
2	R	2	NAG	C3-C2-N2-C7
2	S	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C3-C2-N2-C7
2	U	2	NAG	C3-C2-N2-C7
2	V	2	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	Y	2	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
2	a	2	NAG	C3-C2-N2-C7
2	b	2	NAG	C3-C2-N2-C7
2	c	2	NAG	C3-C2-N2-C7
2	d	2	NAG	C3-C2-N2-C7
2	e	2	NAG	C3-C2-N2-C7
2	f	2	NAG	C3-C2-N2-C7
2	g	2	NAG	C3-C2-N2-C7
2	h	2	NAG	C3-C2-N2-C7
2	i	2	NAG	C3-C2-N2-C7

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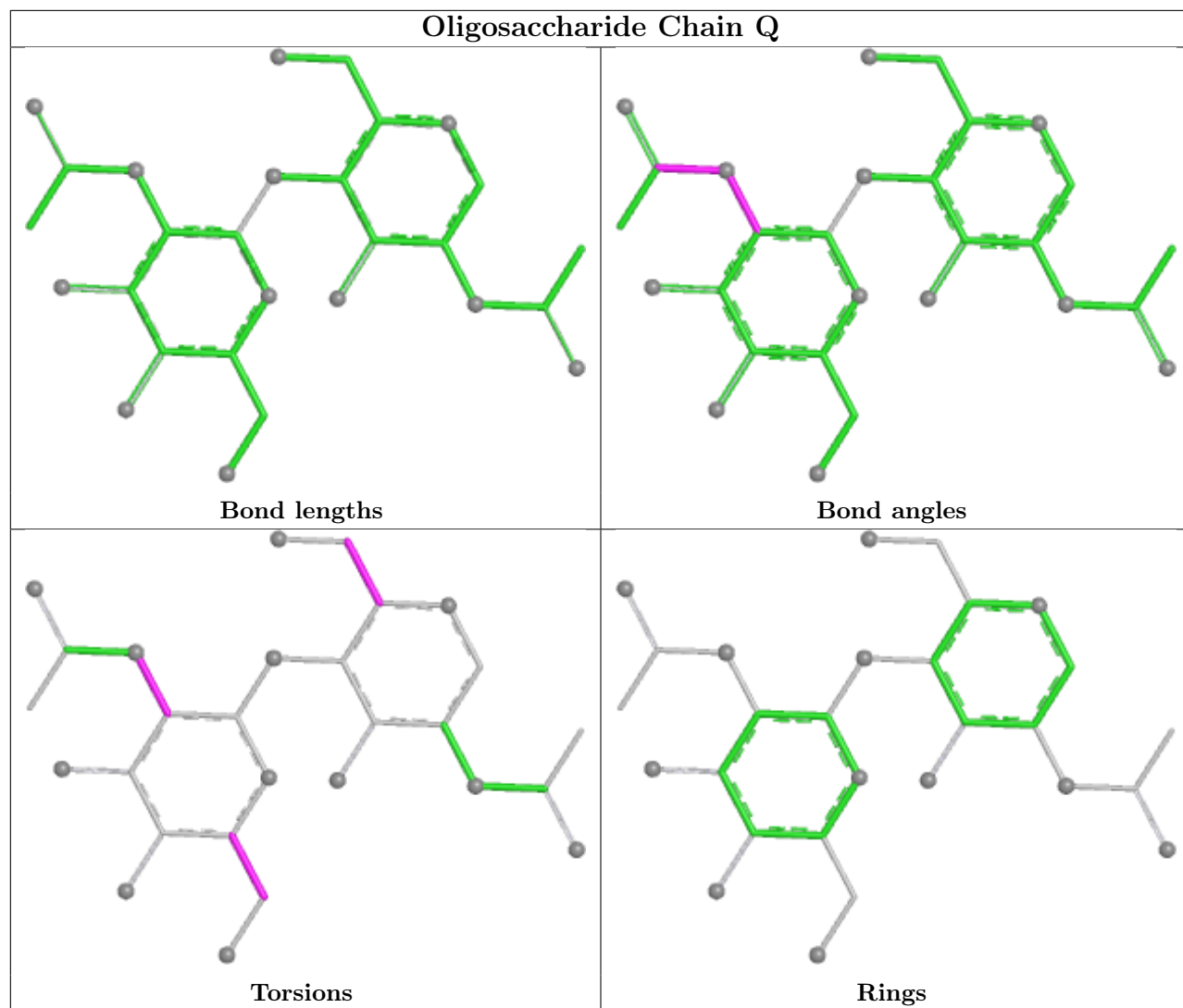
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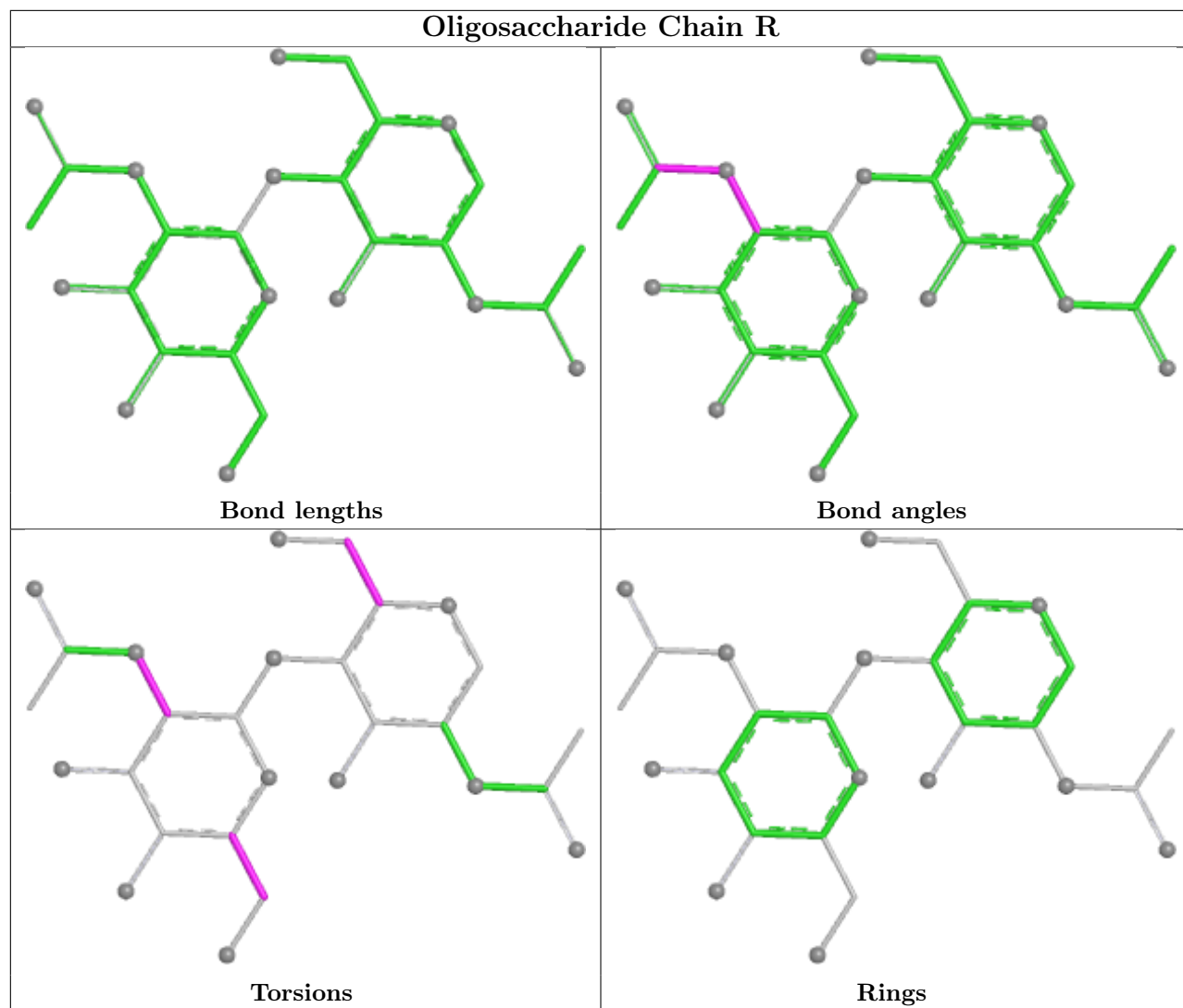
Mol	Chain	Res	Type	Atoms
2	j	2	NAG	C3-C2-N2-C7
2	k	2	NAG	C3-C2-N2-C7
2	l	2	NAG	C3-C2-N2-C7
2	m	2	NAG	C3-C2-N2-C7
2	n	2	NAG	C3-C2-N2-C7
2	o	2	NAG	C3-C2-N2-C7
2	p	2	NAG	C3-C2-N2-C7
2	q	2	NAG	C3-C2-N2-C7
2	r	2	NAG	C3-C2-N2-C7
2	s	2	NAG	C3-C2-N2-C7
2	t	2	NAG	C3-C2-N2-C7
2	u	2	NAG	C3-C2-N2-C7
2	v	2	NAG	C3-C2-N2-C7

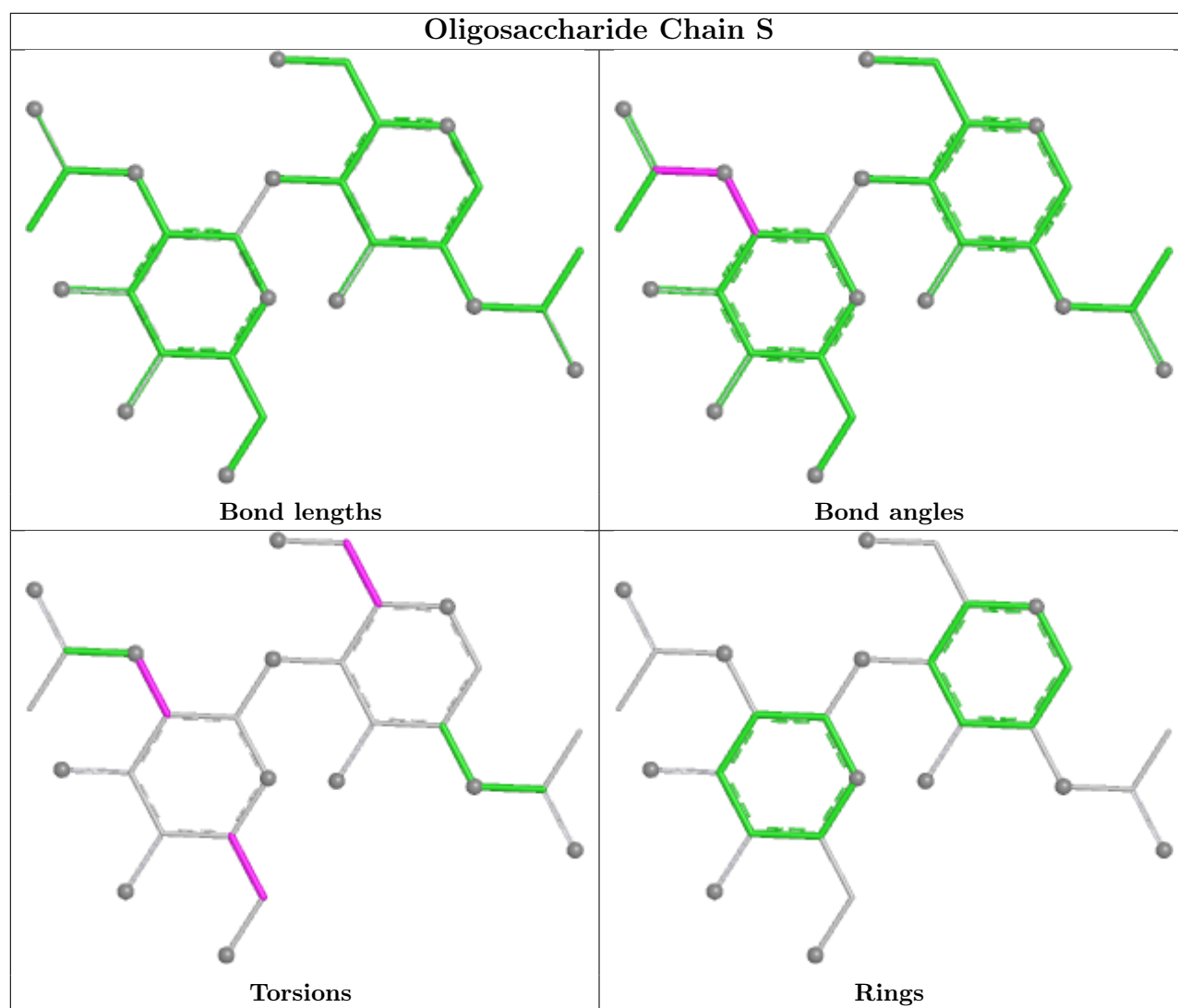
There are no ring outliers.

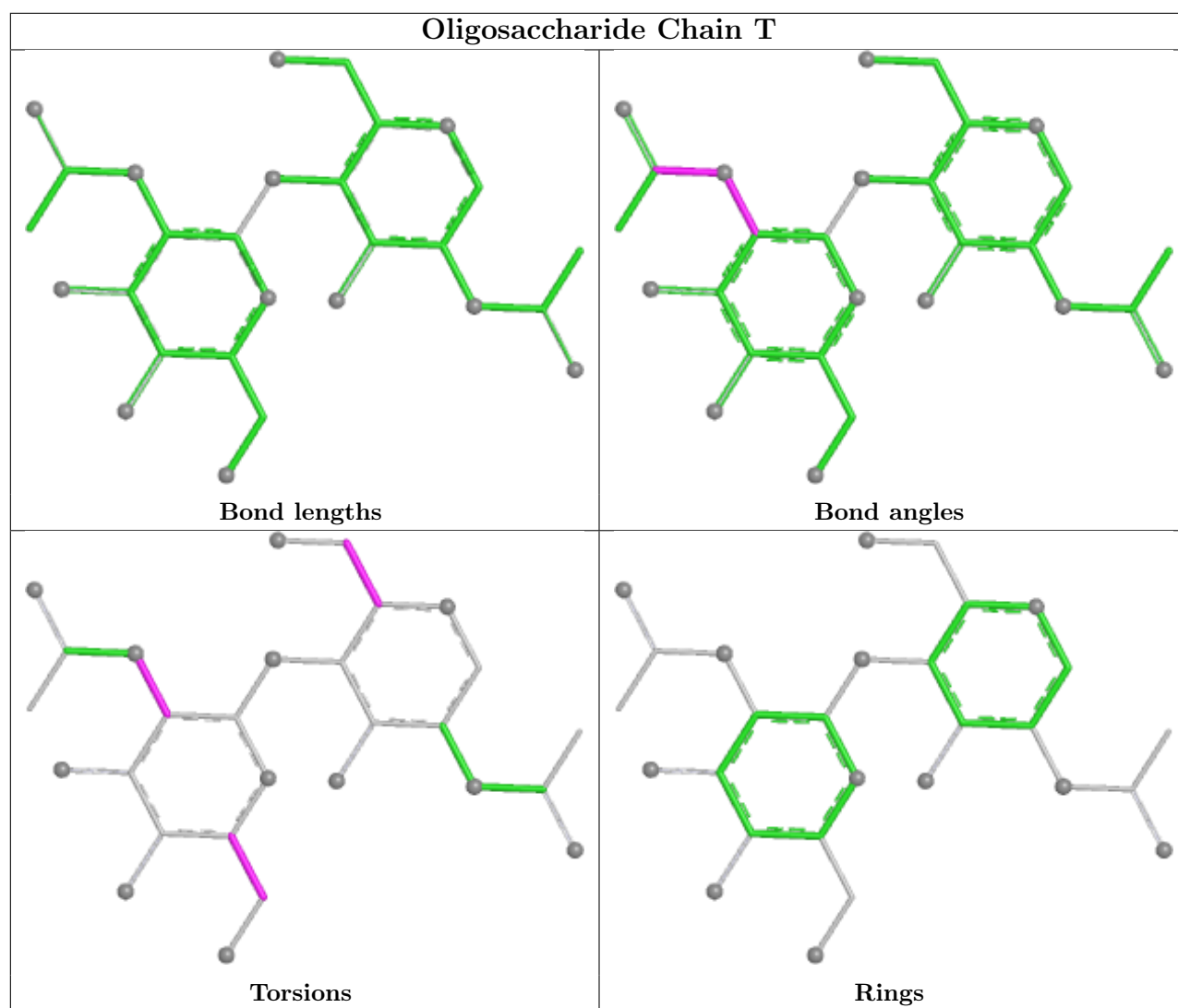
No monomer is involved in short contacts.

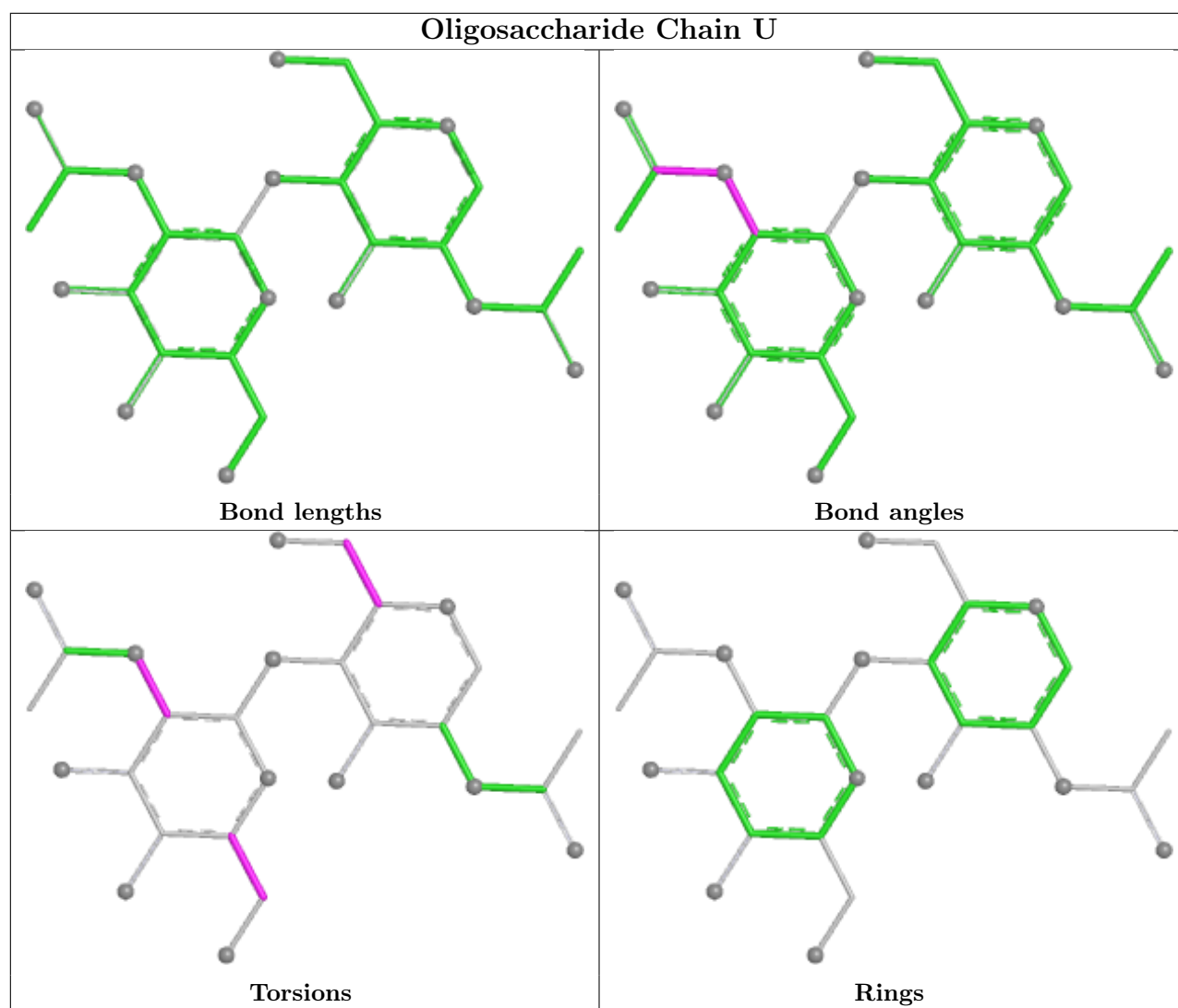
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

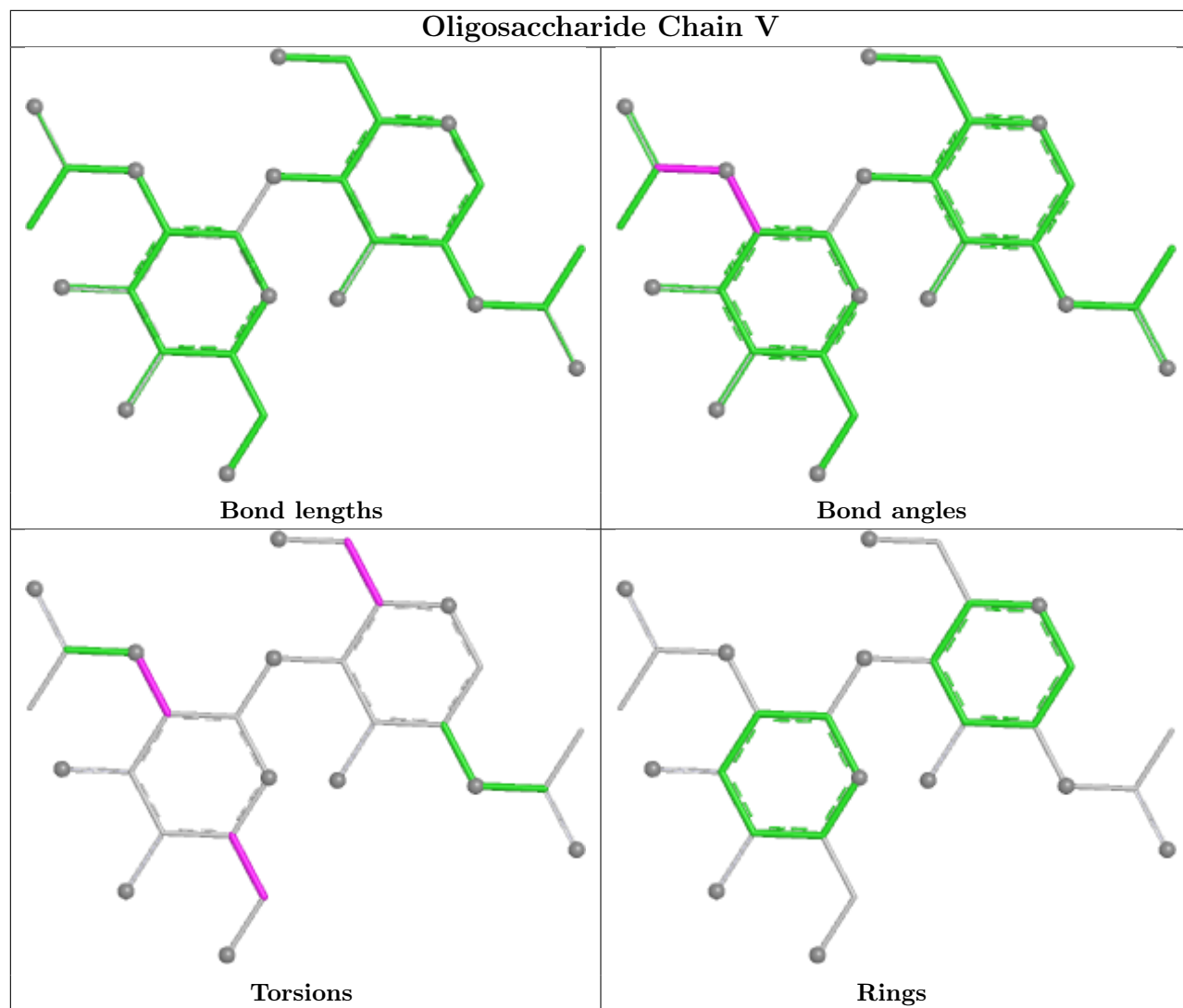


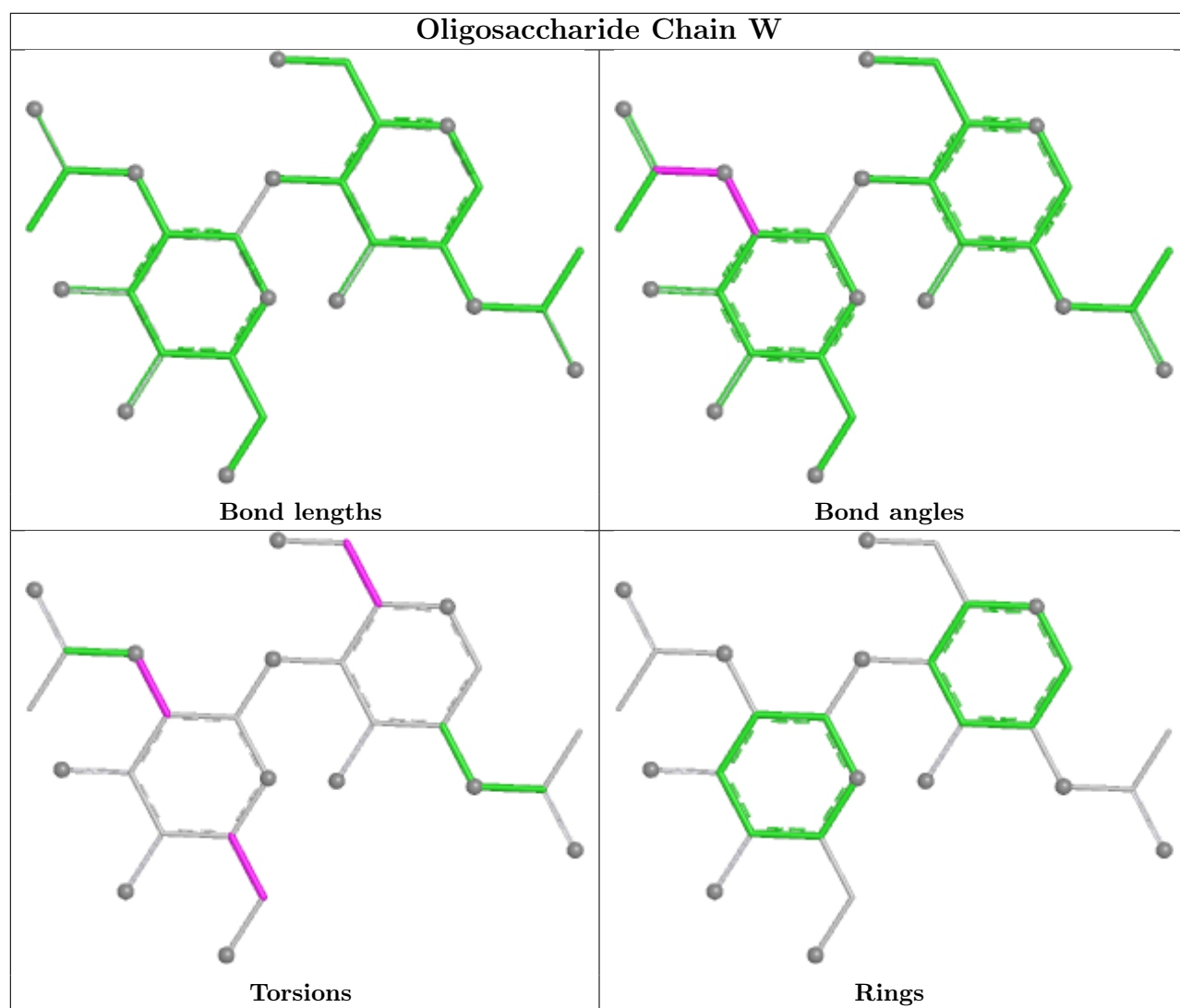


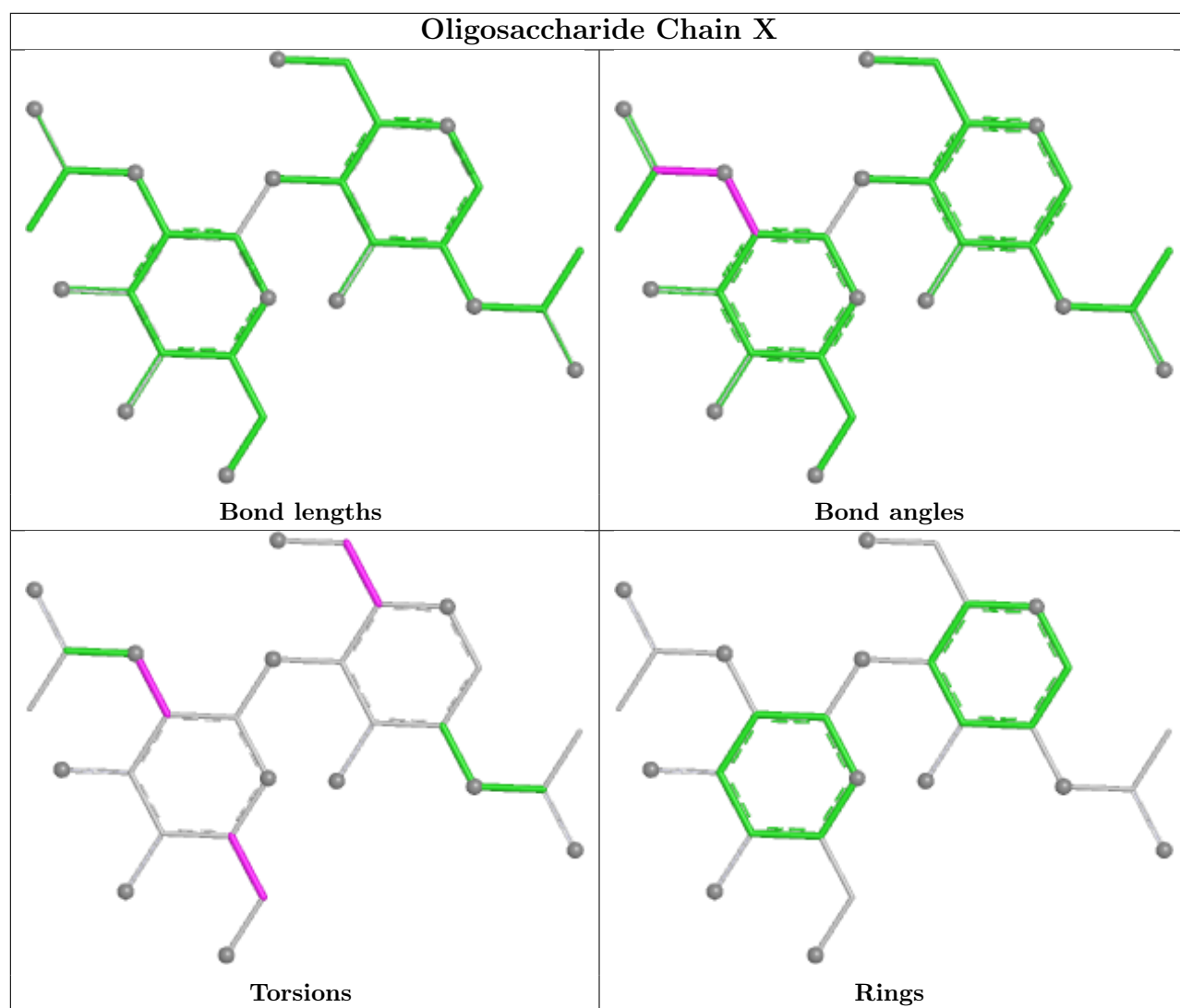


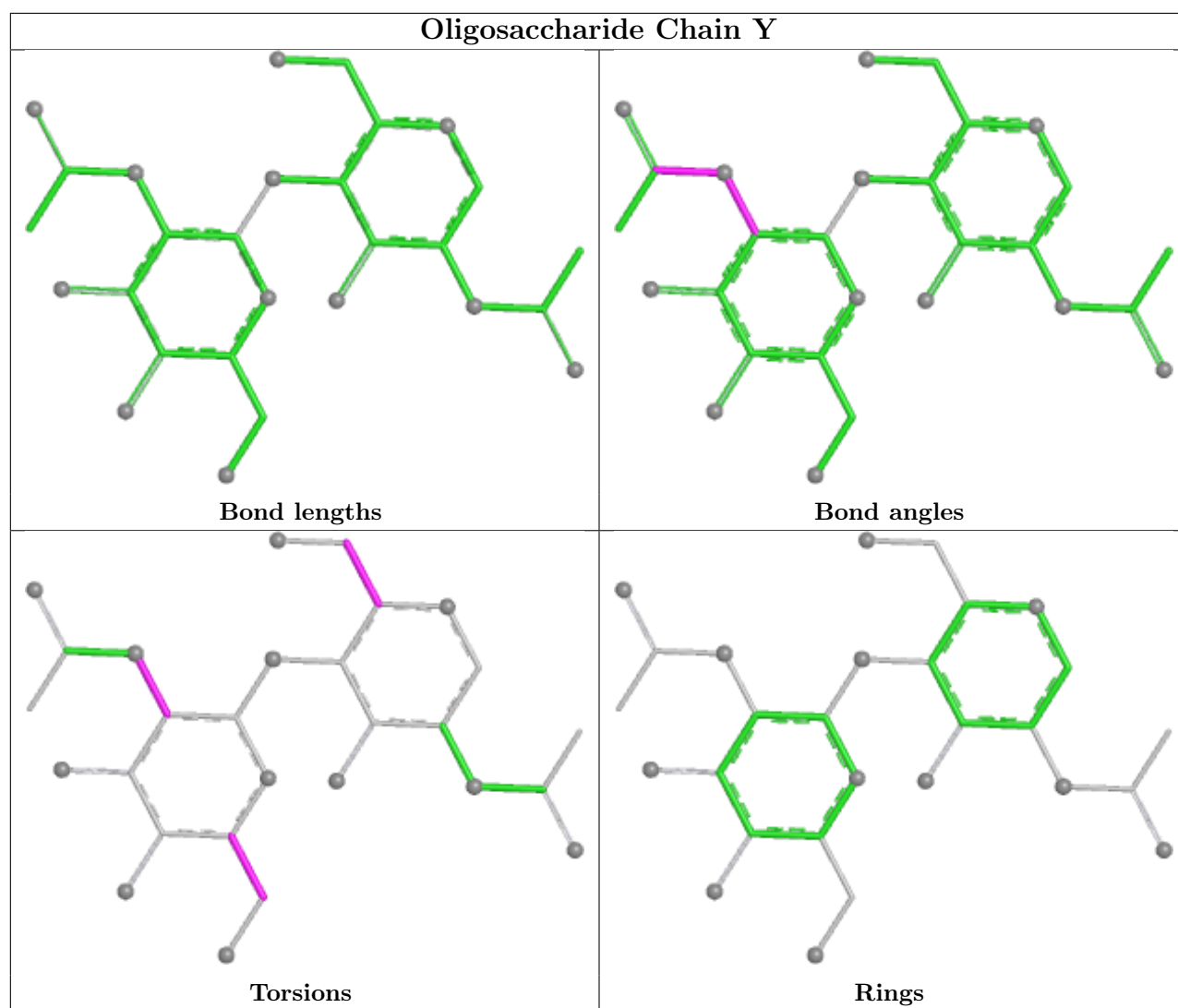


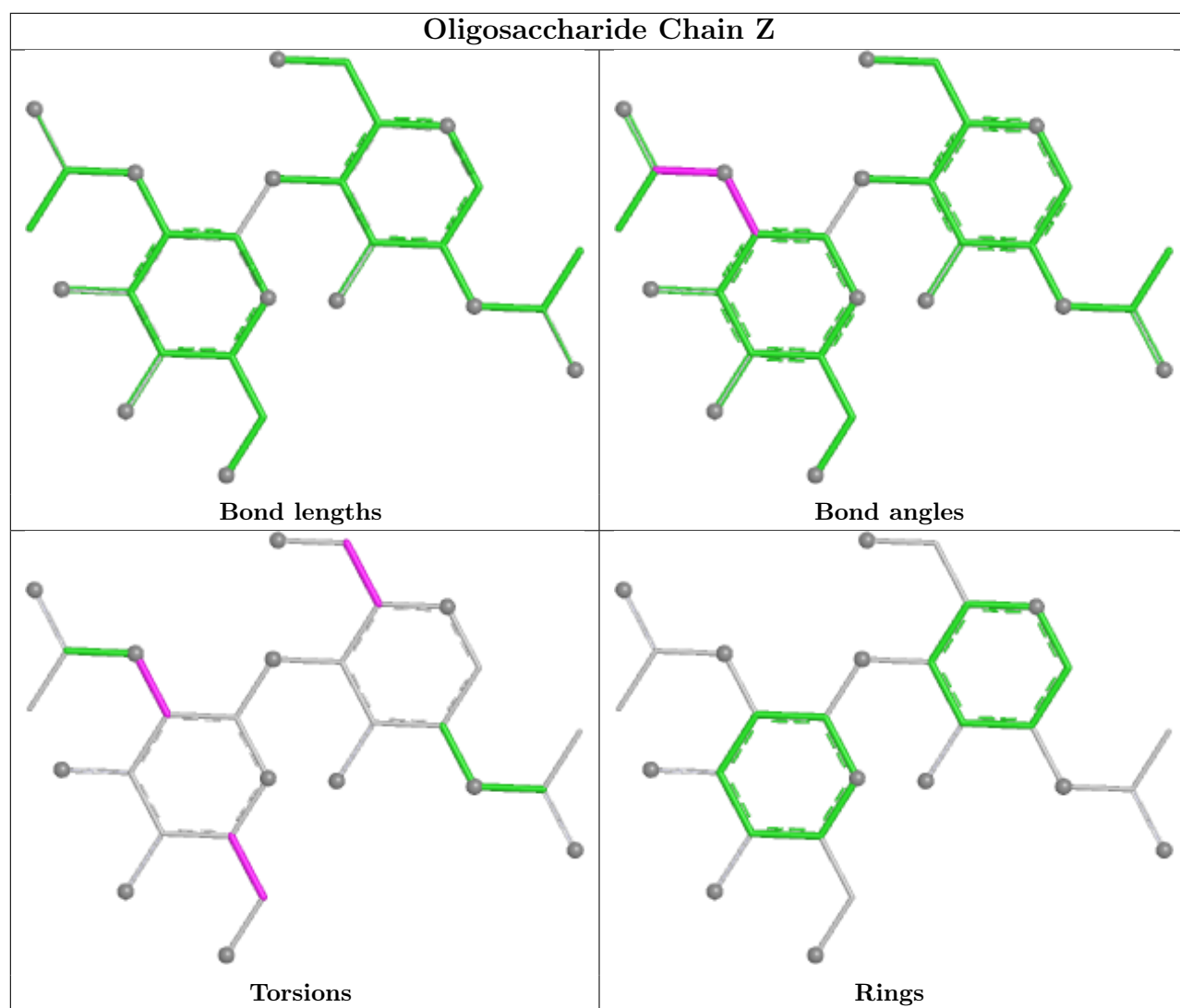


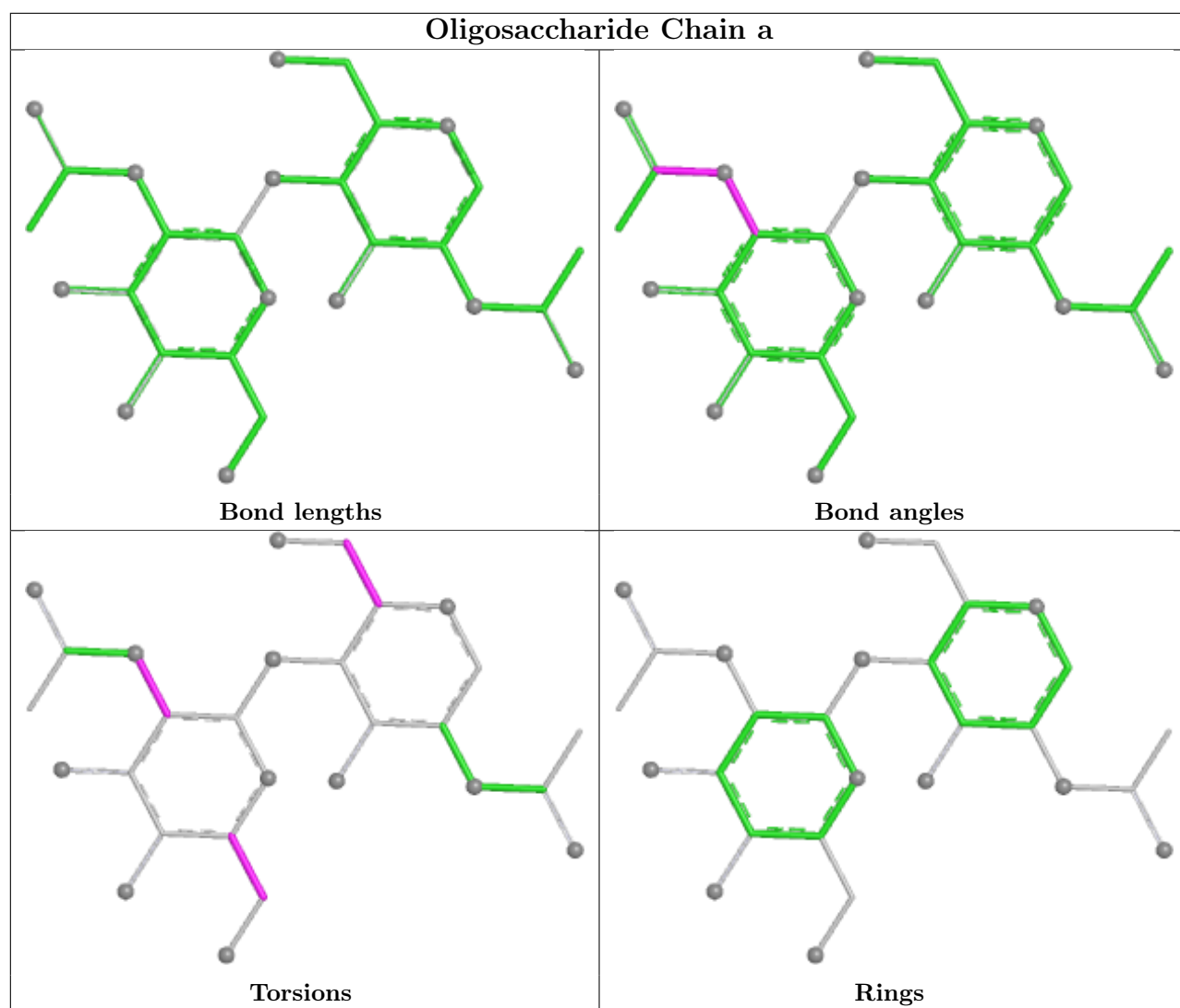


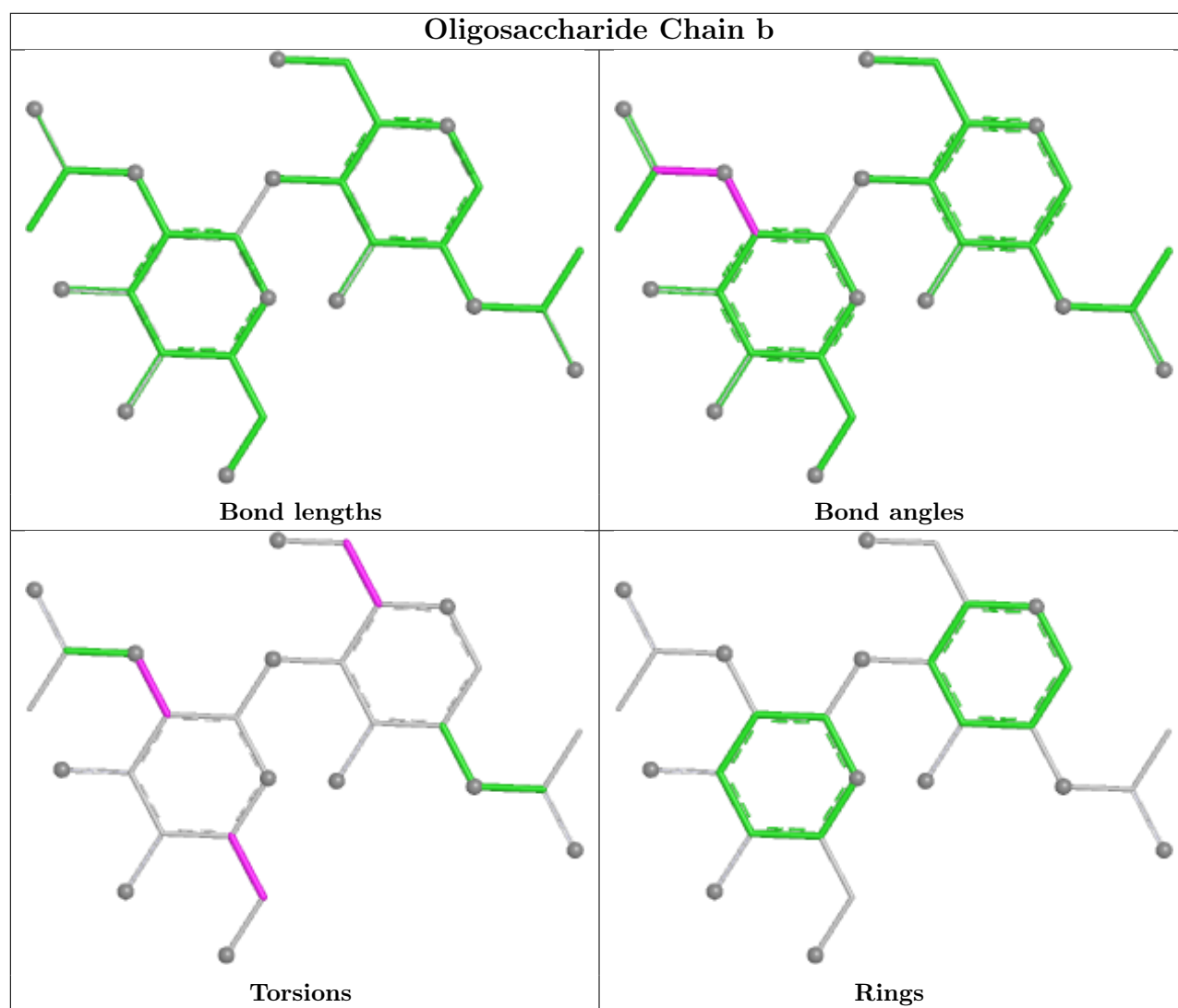


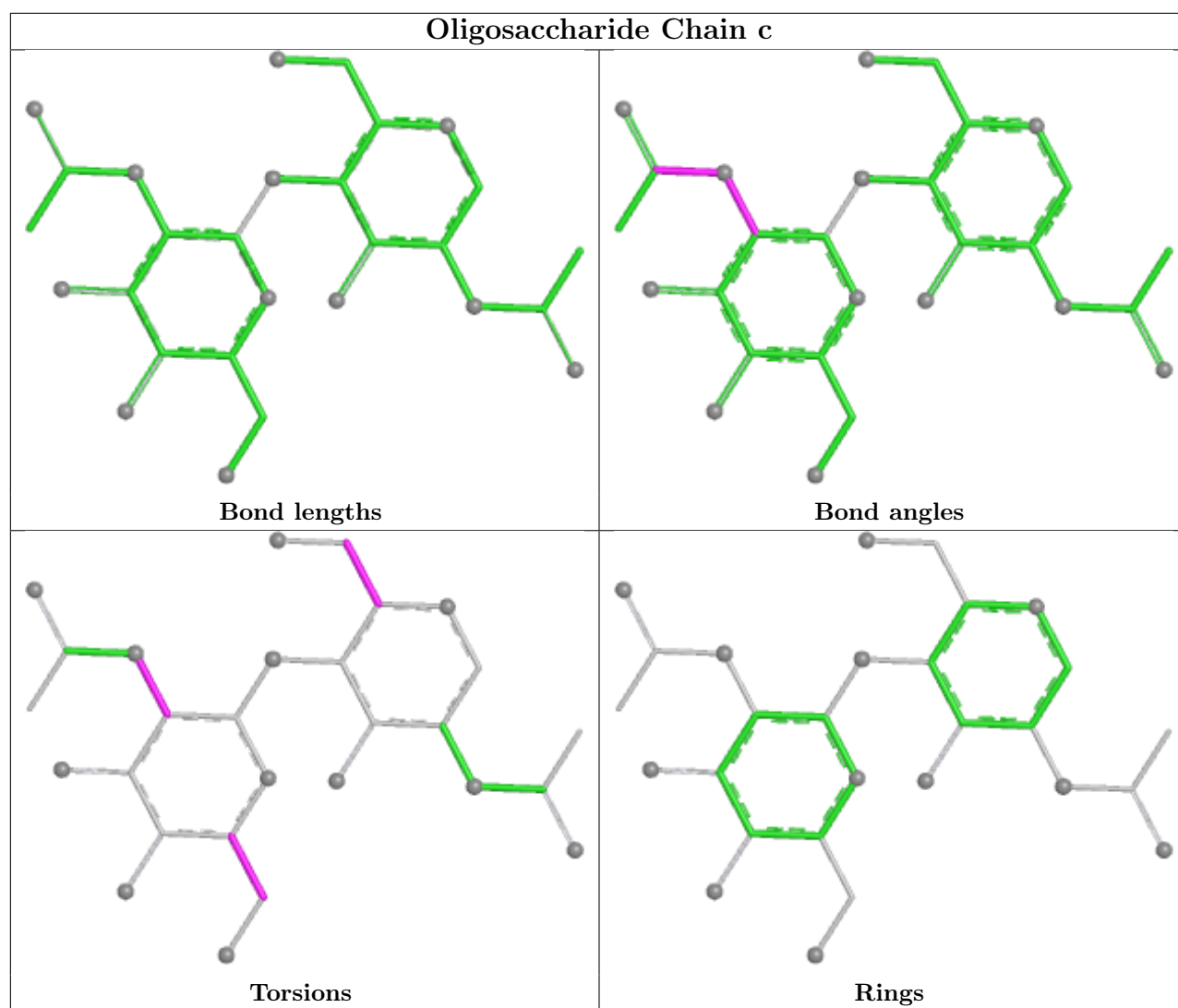


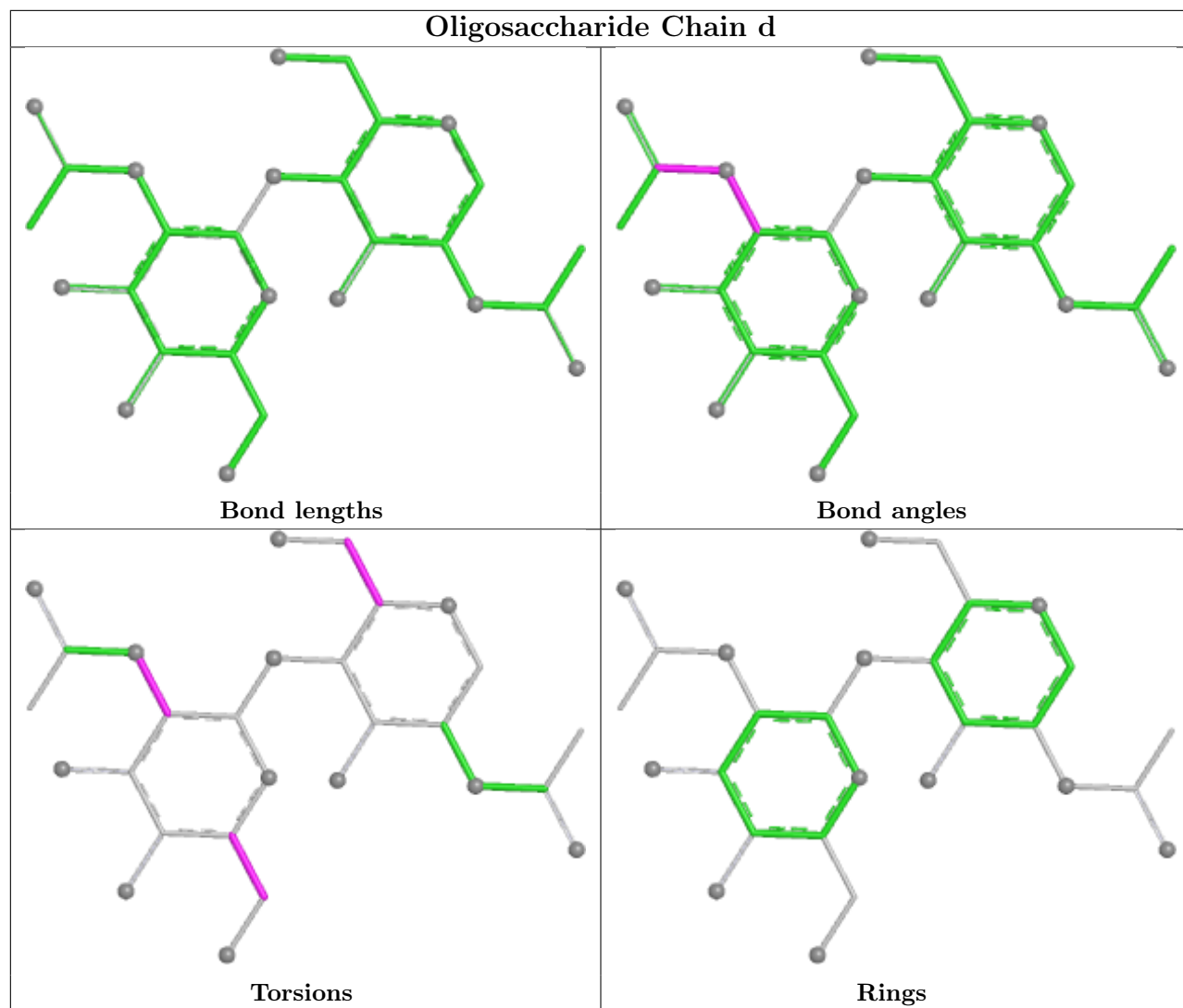


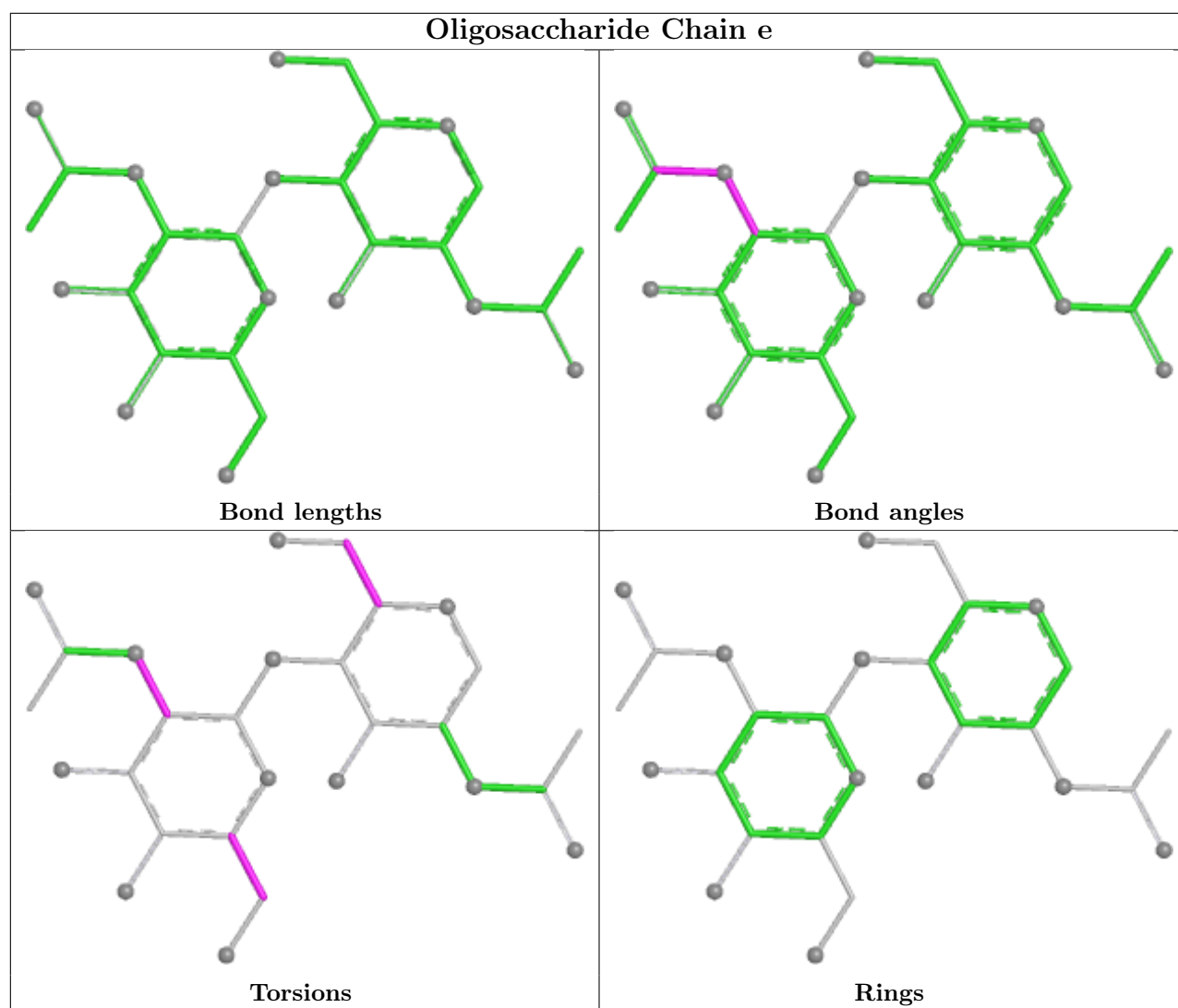


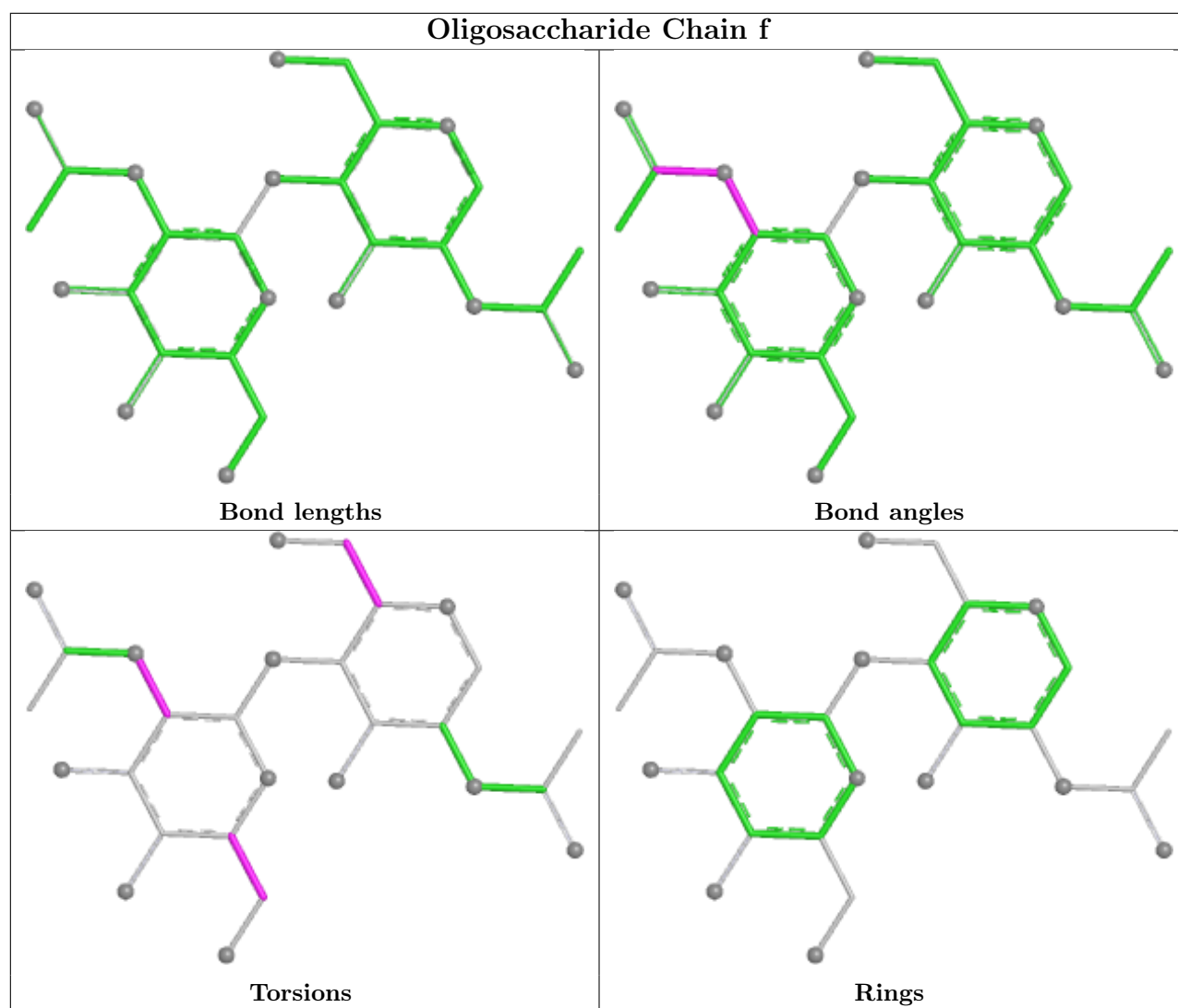


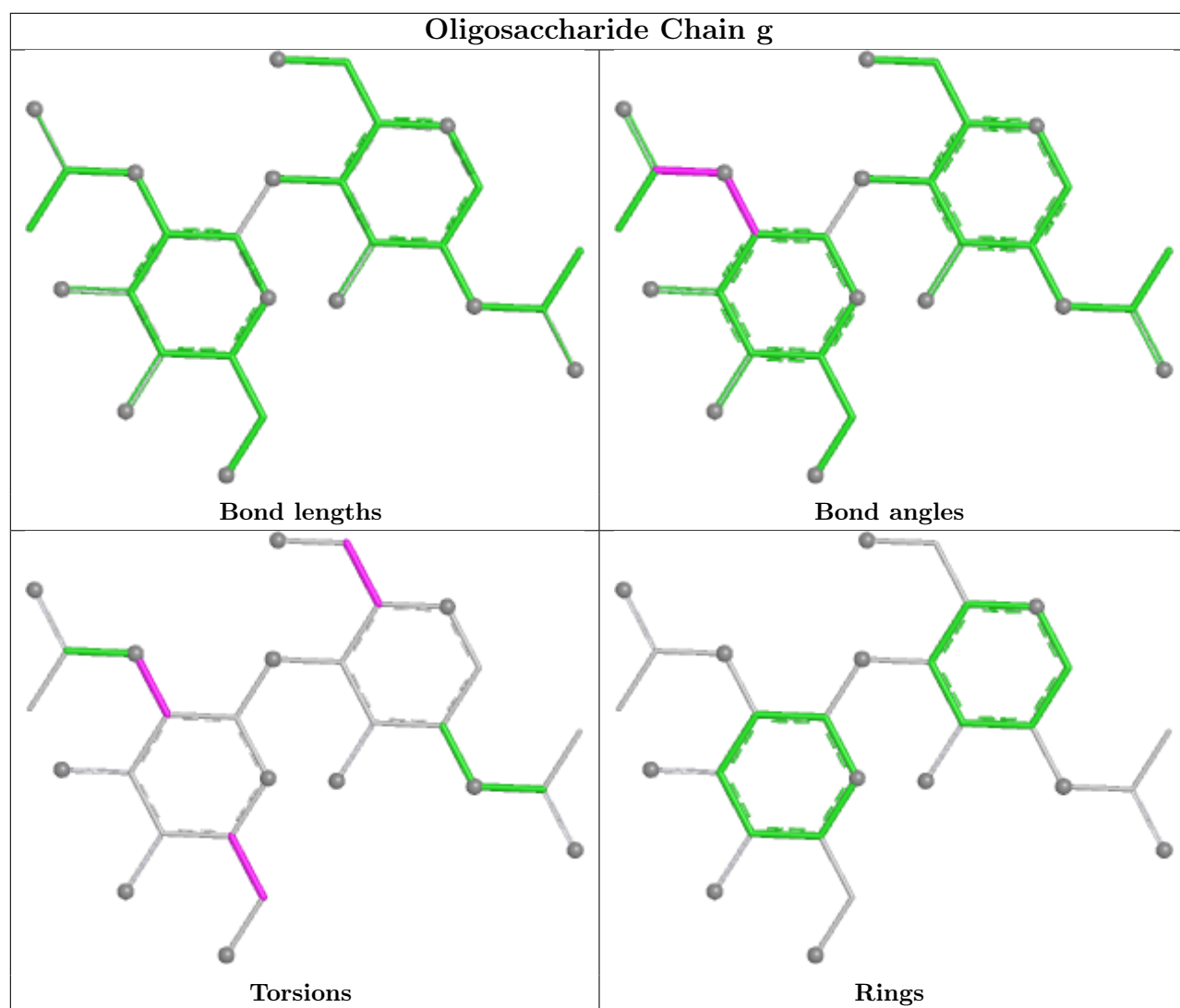


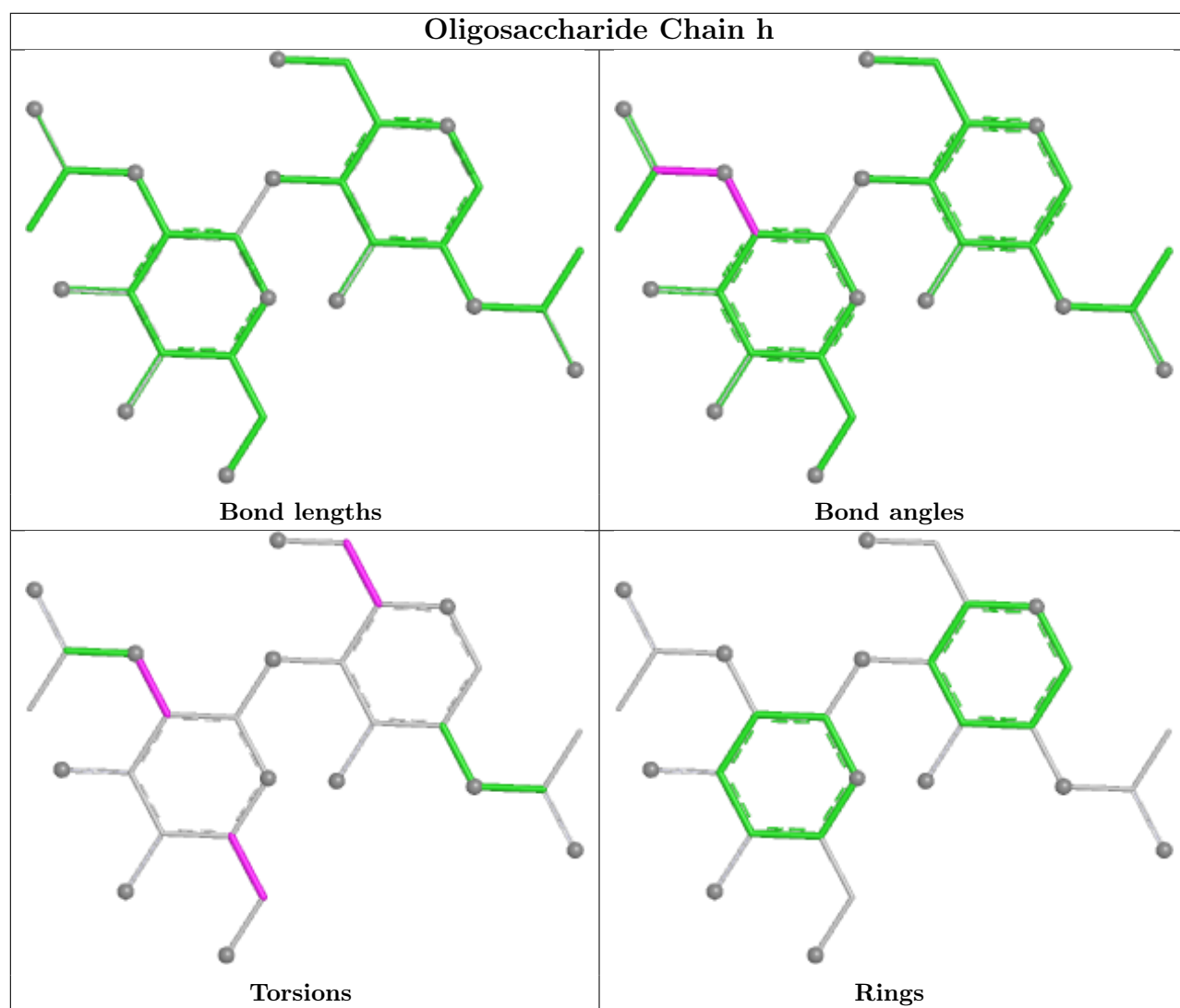


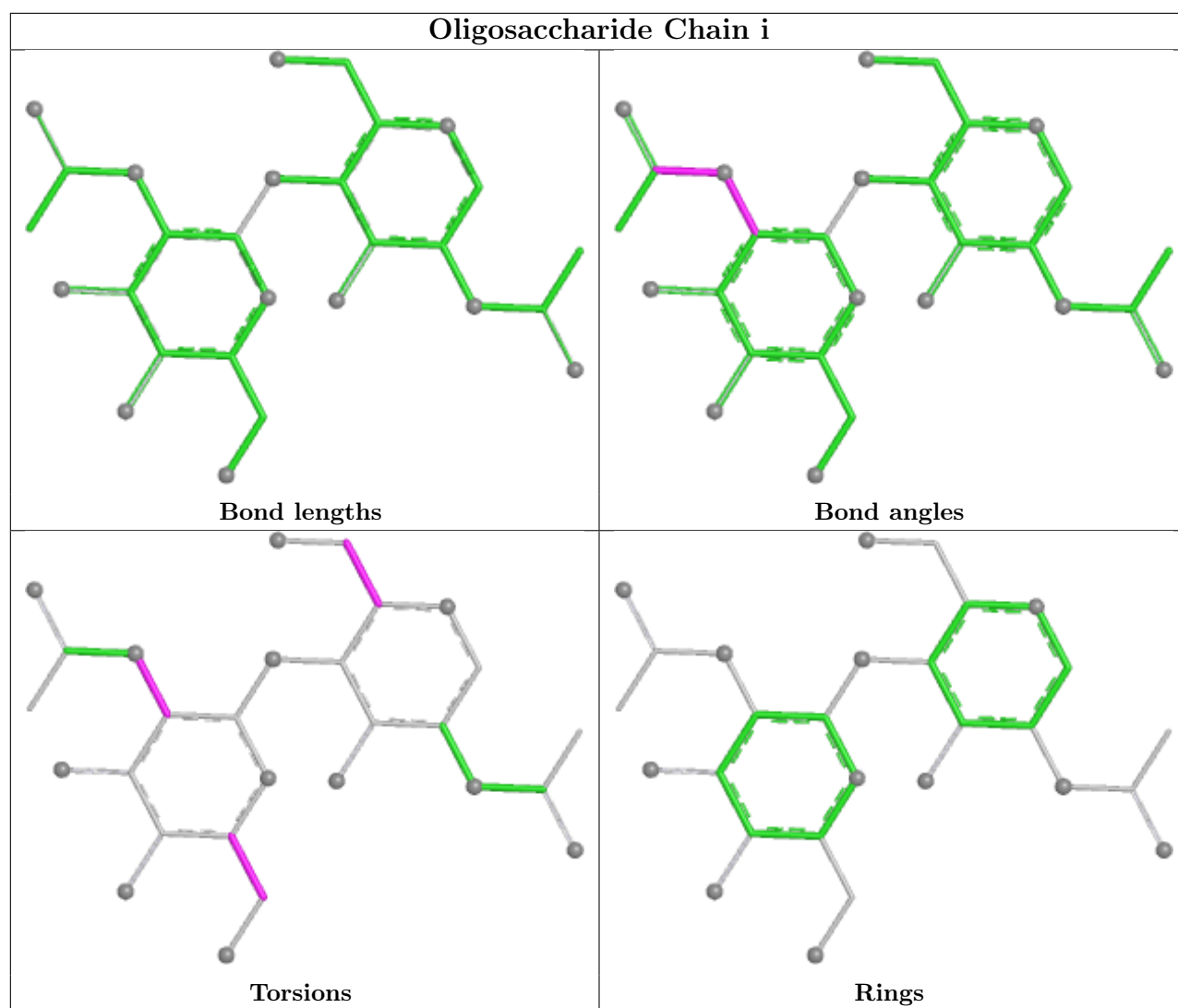


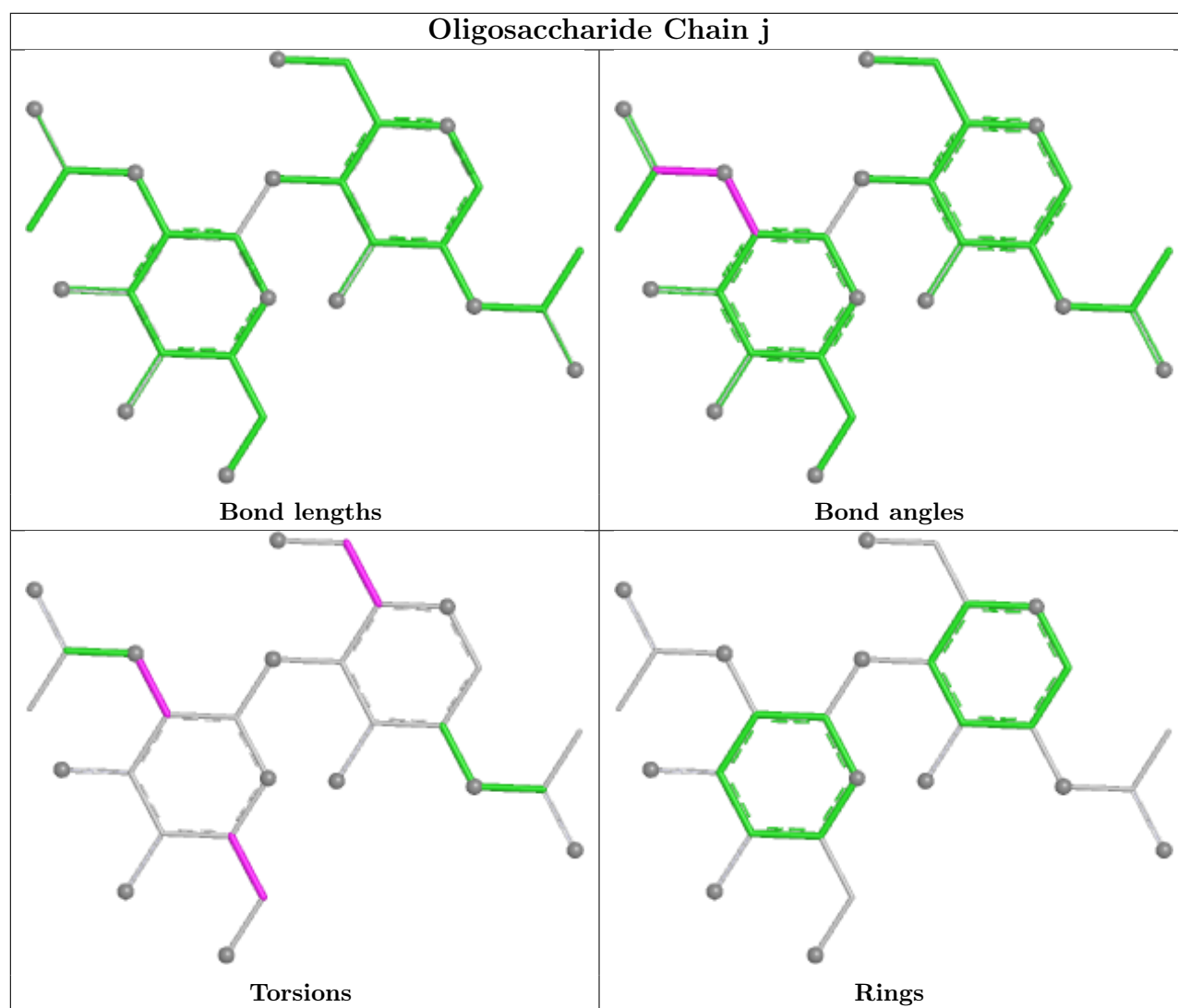


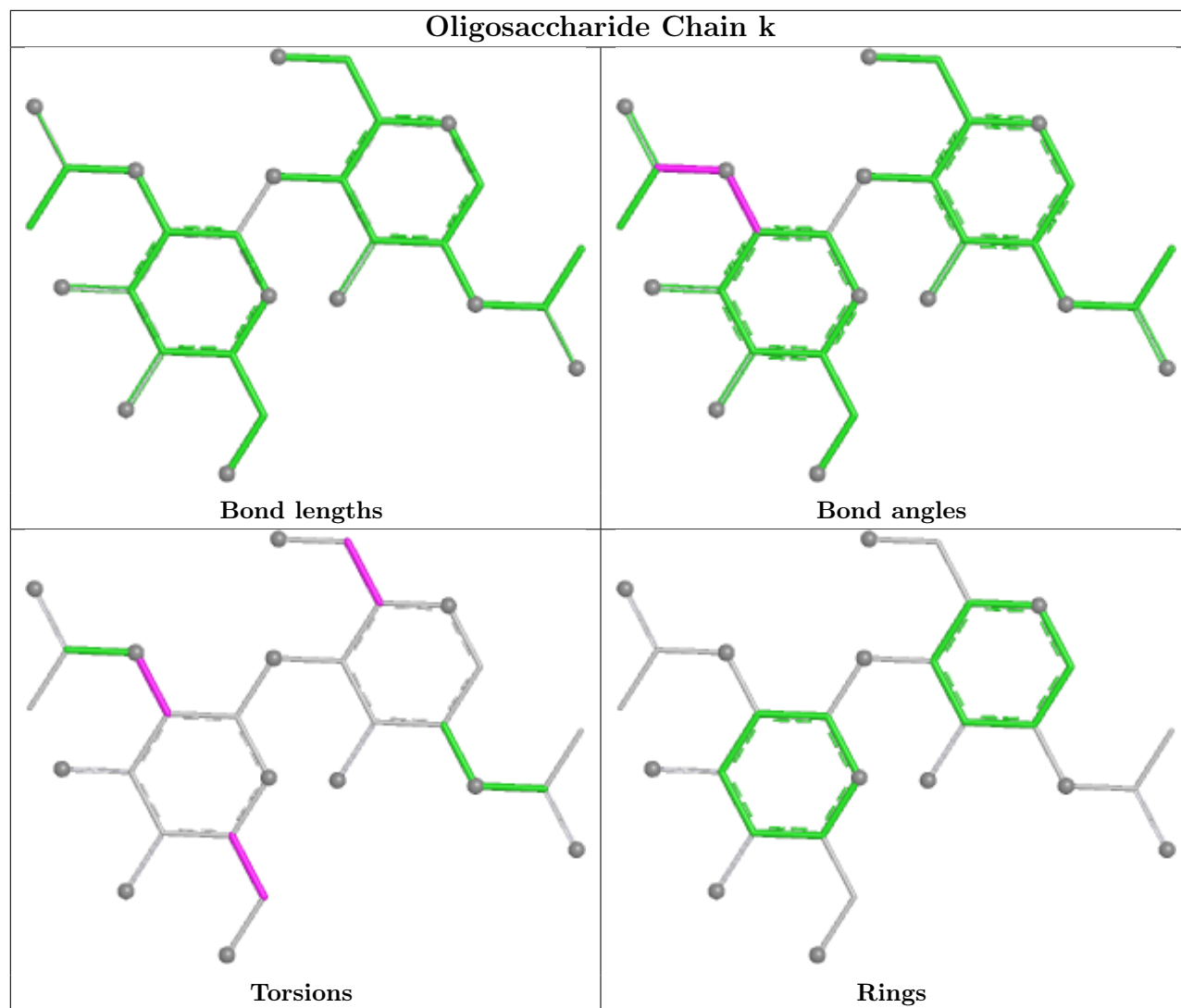


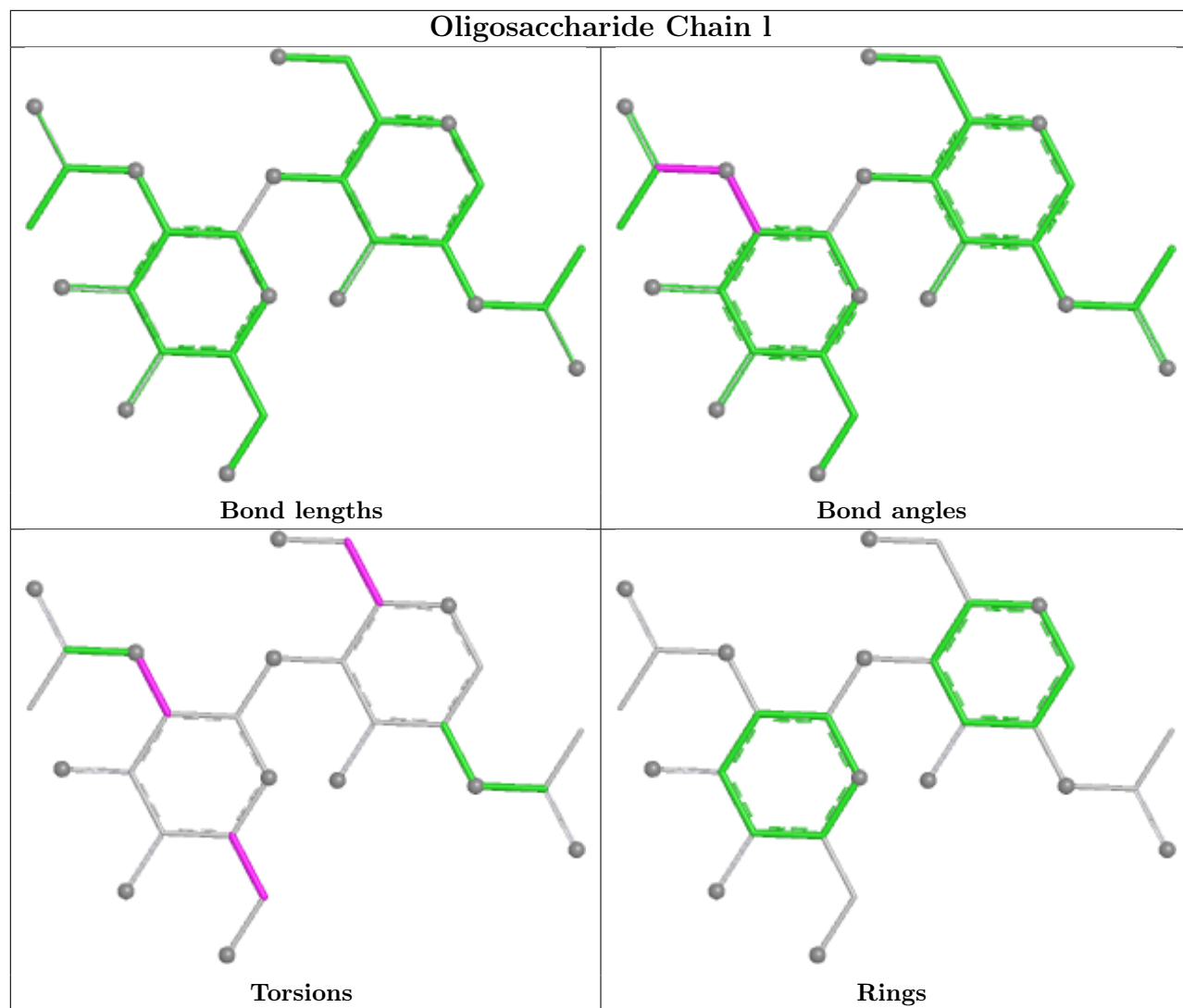


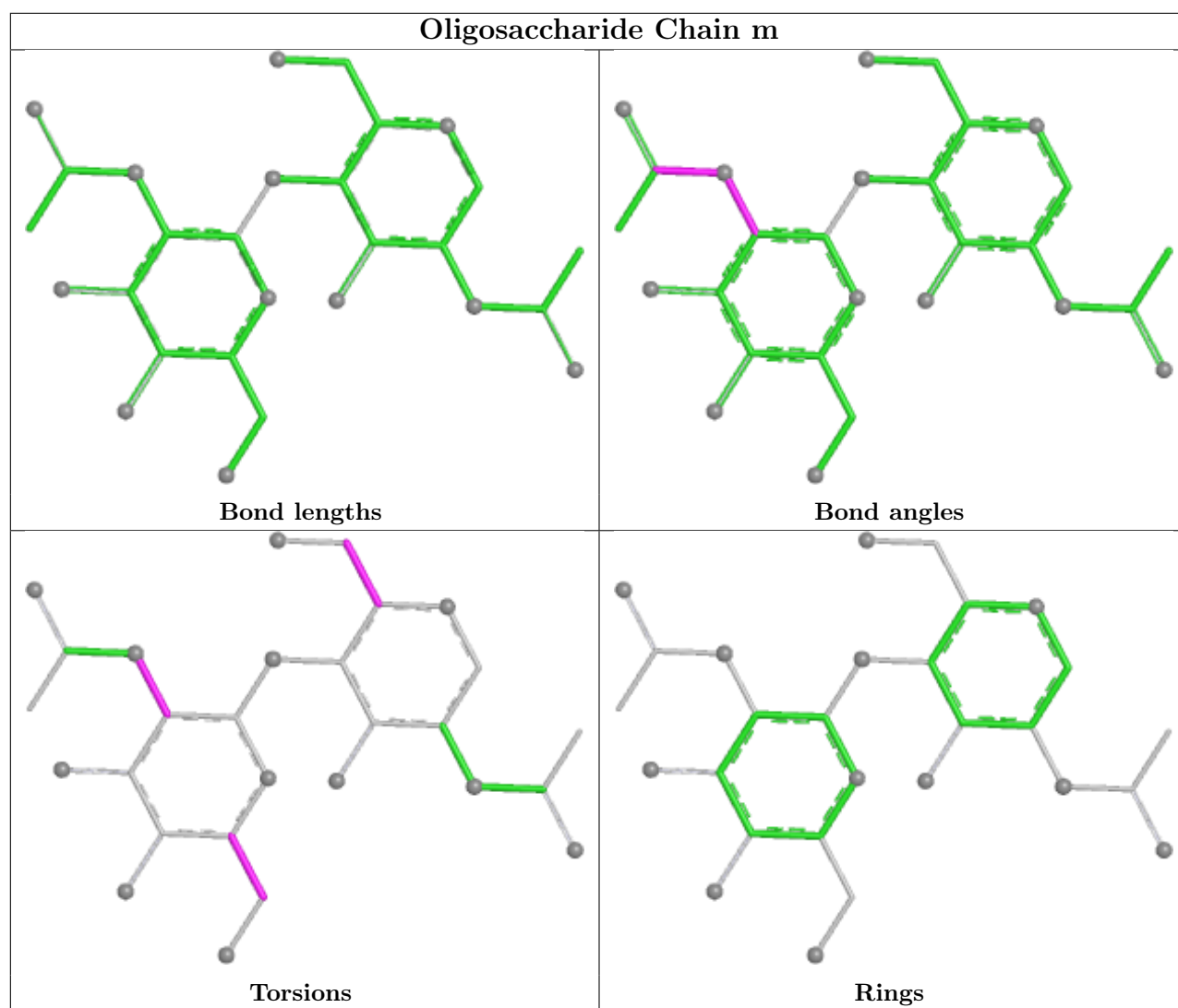


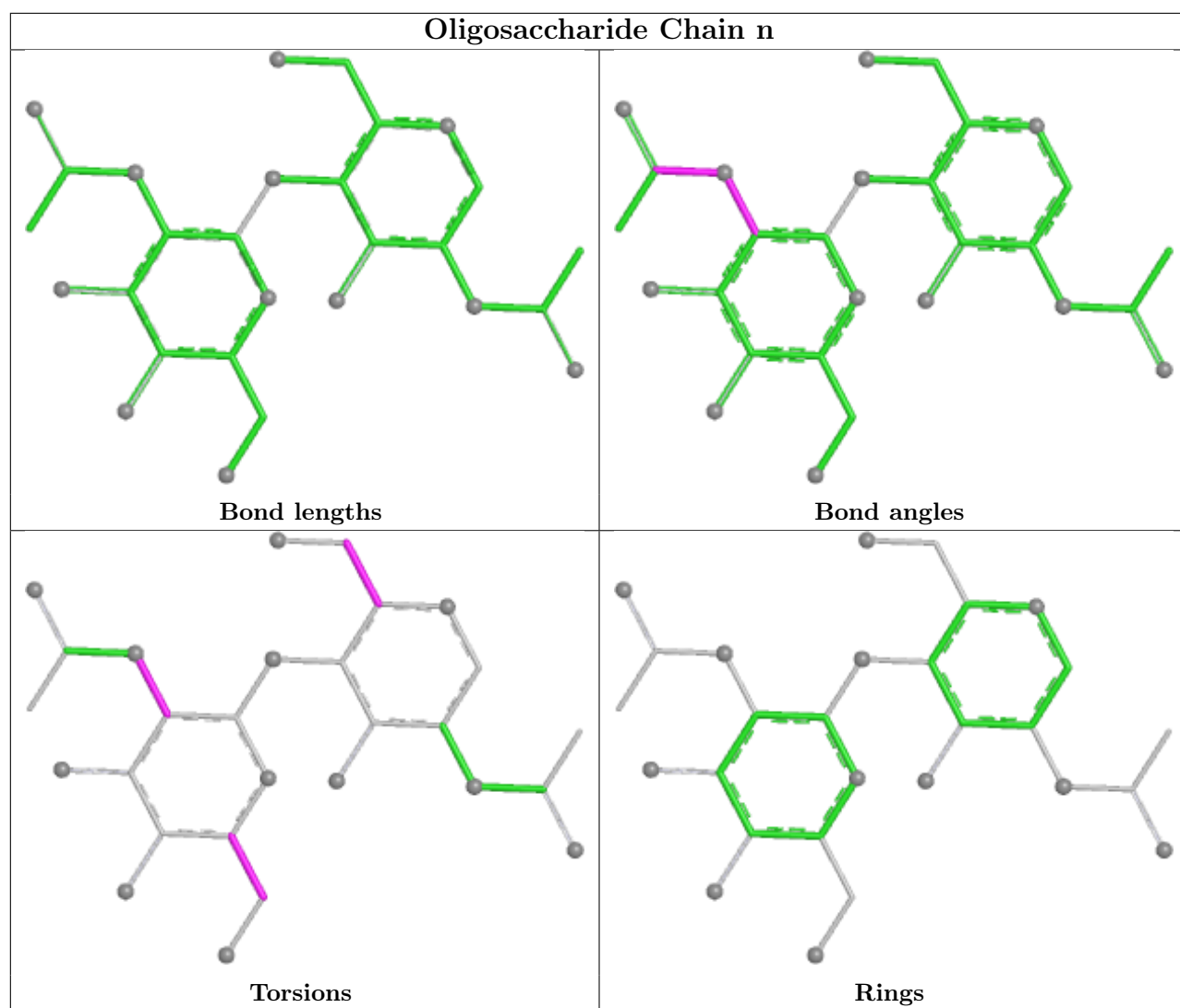


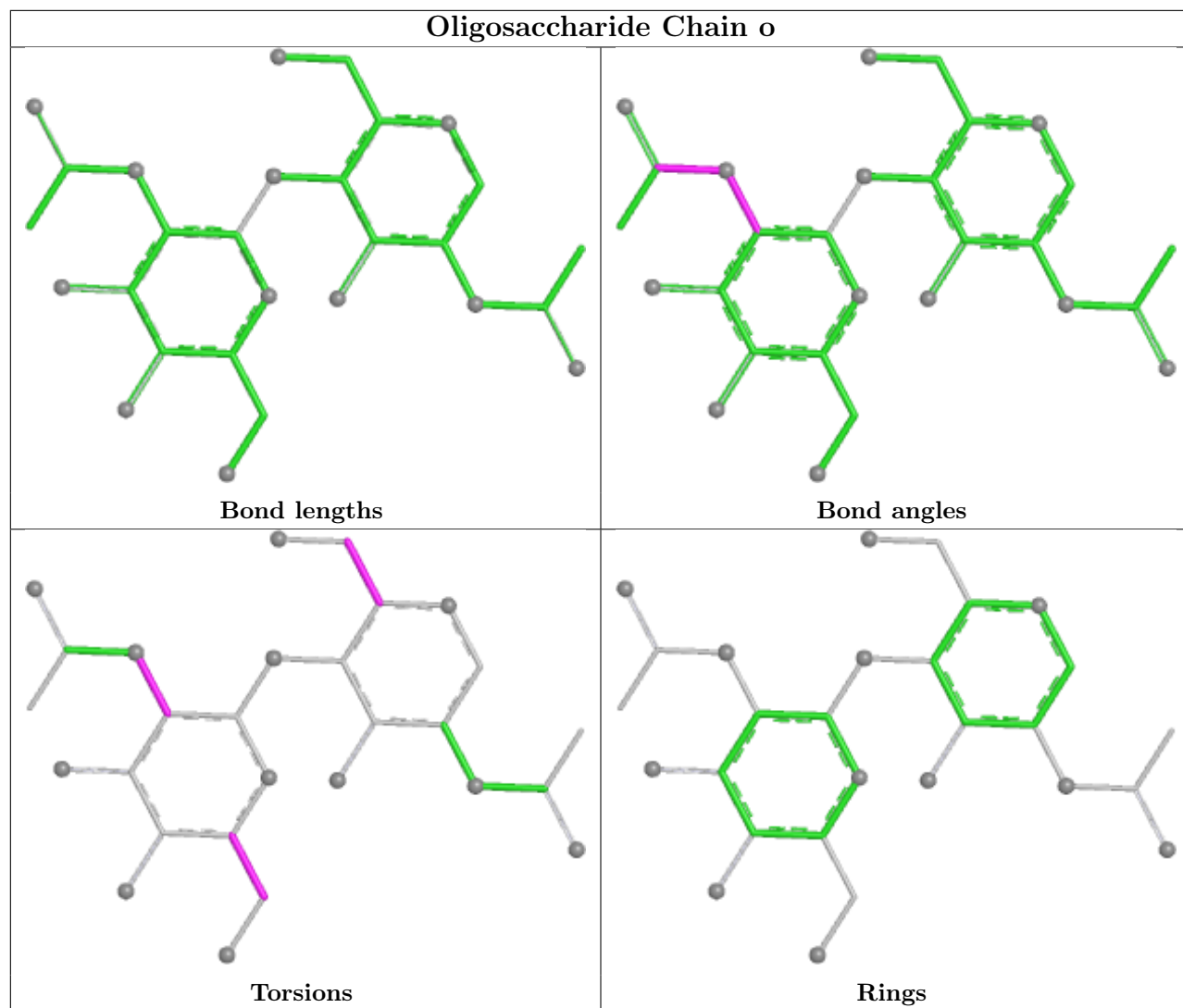


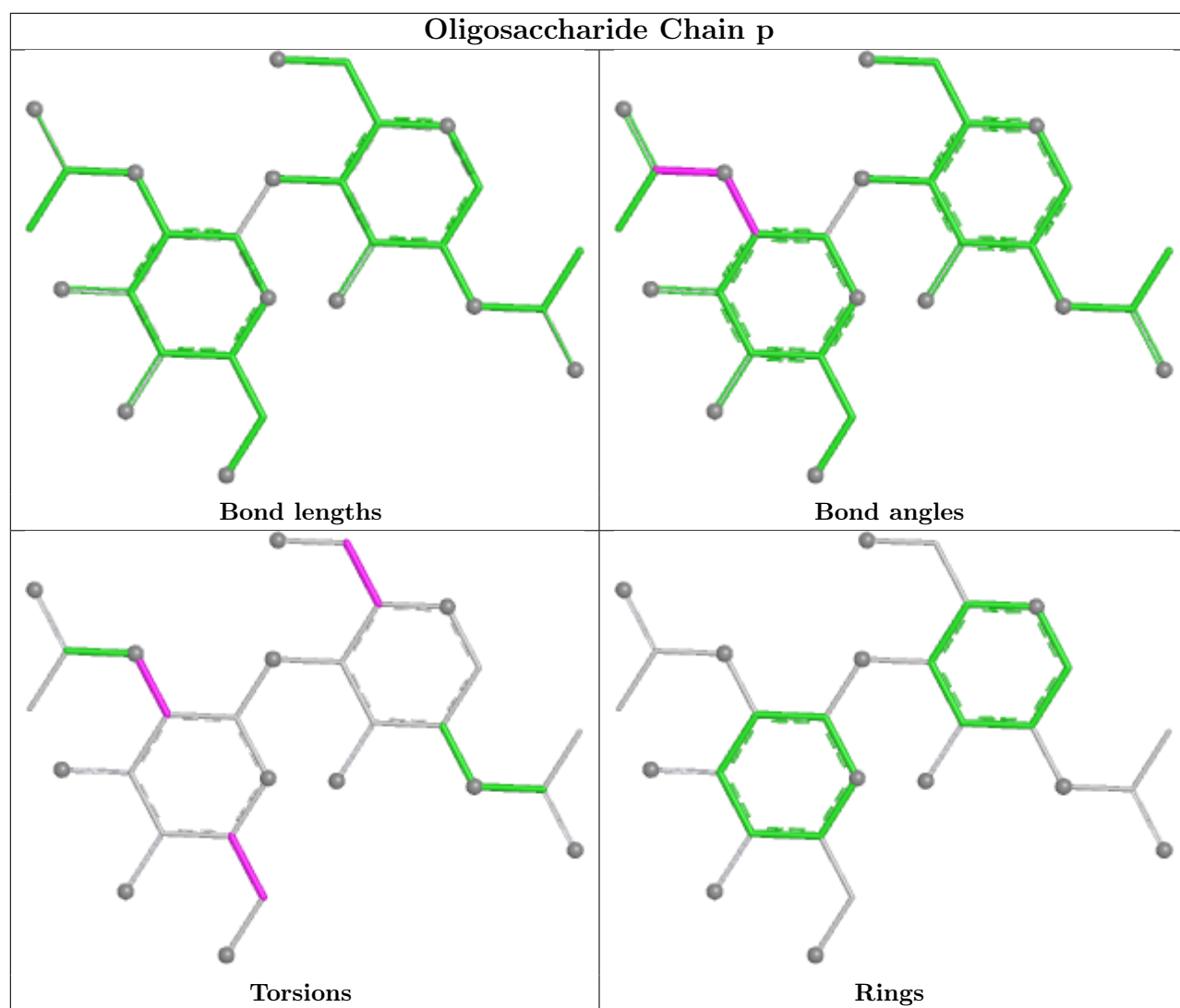


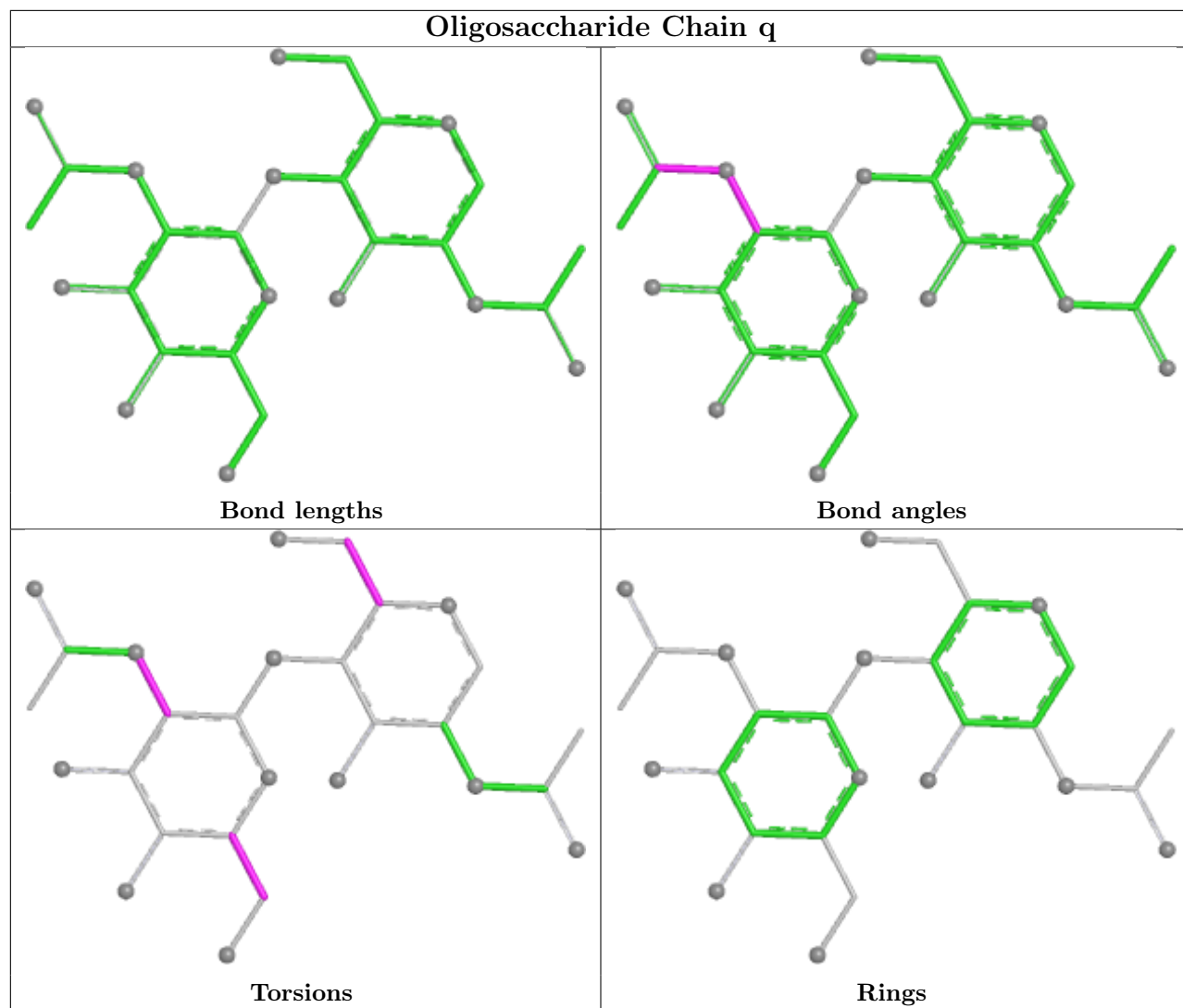


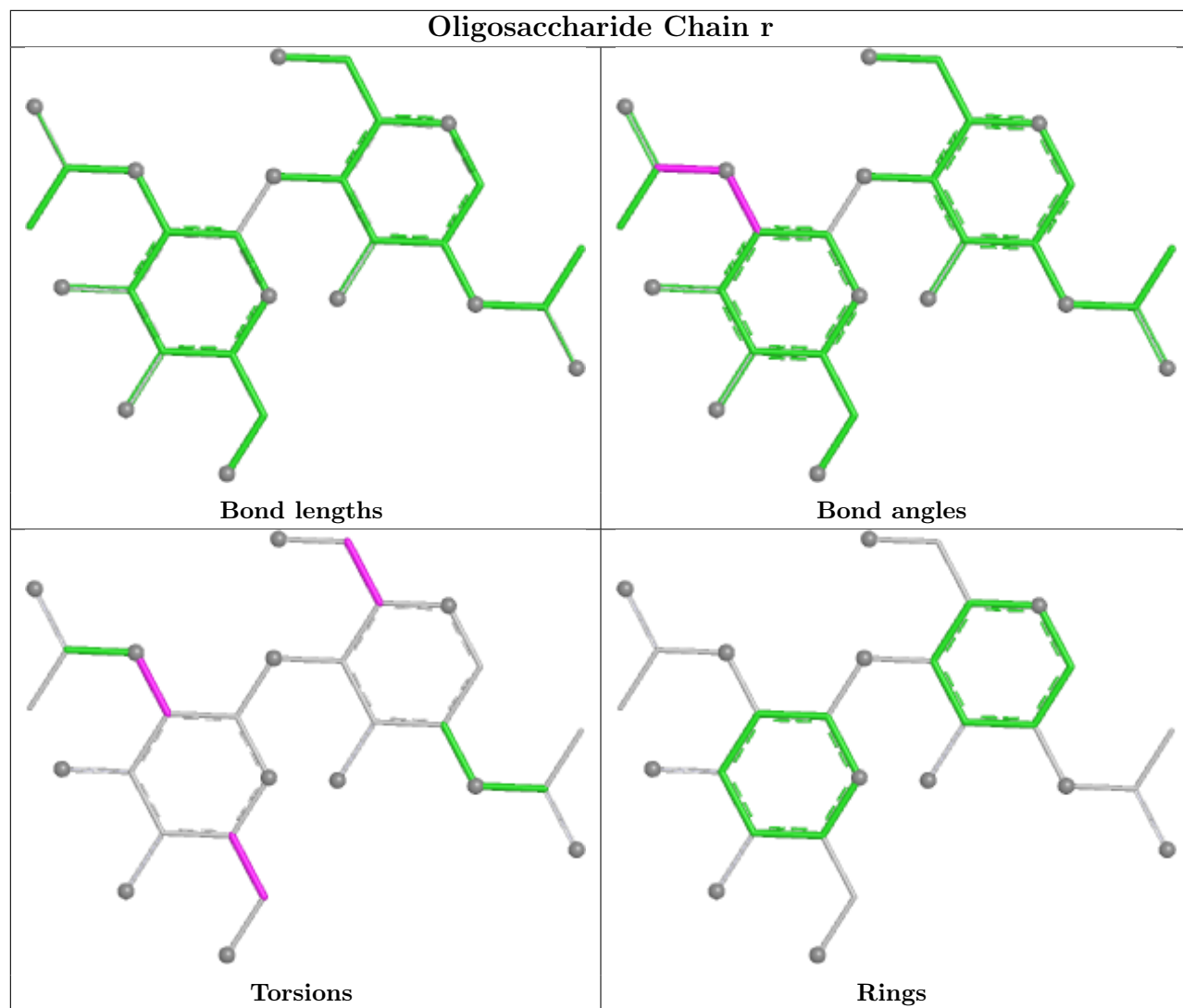


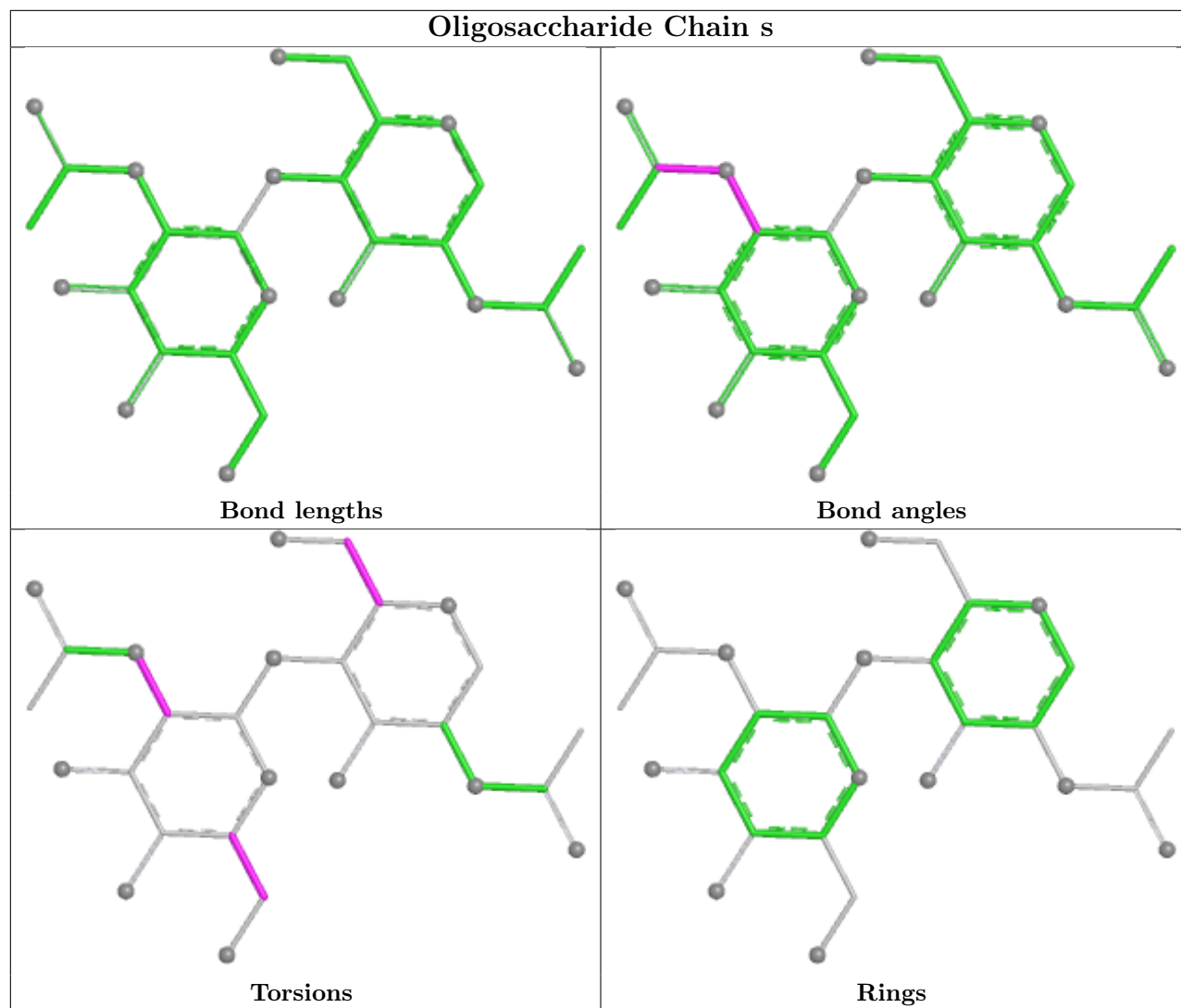


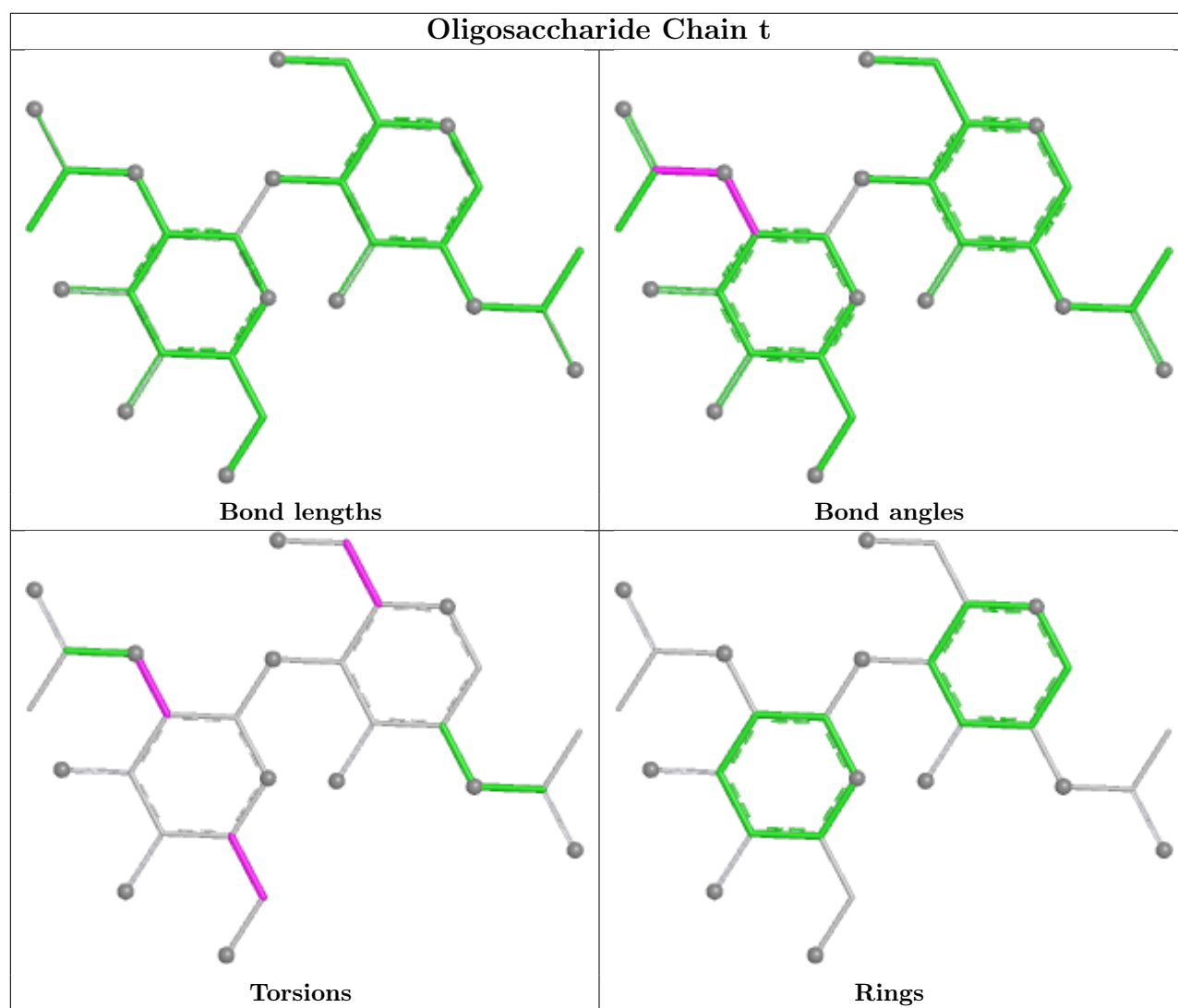


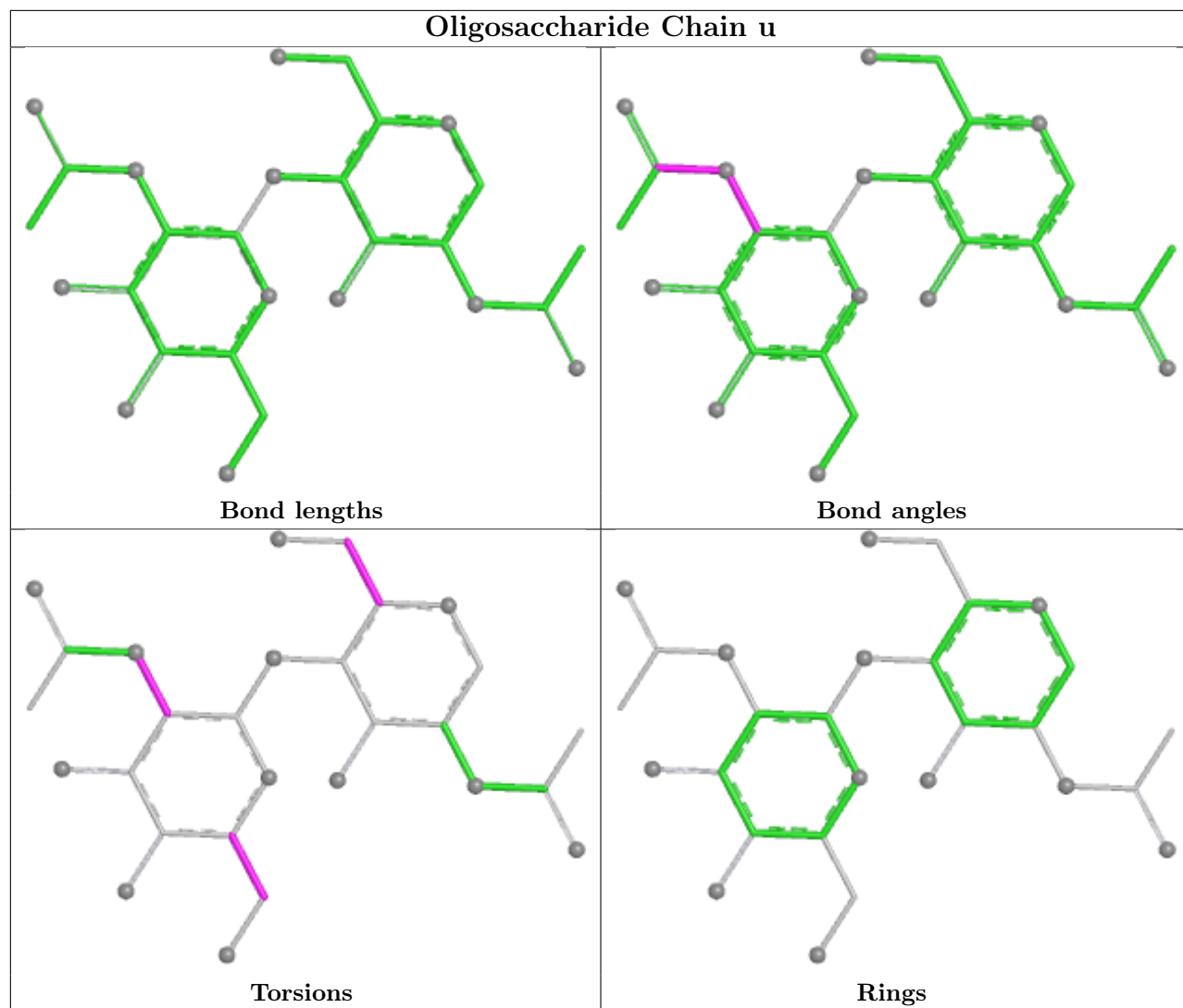


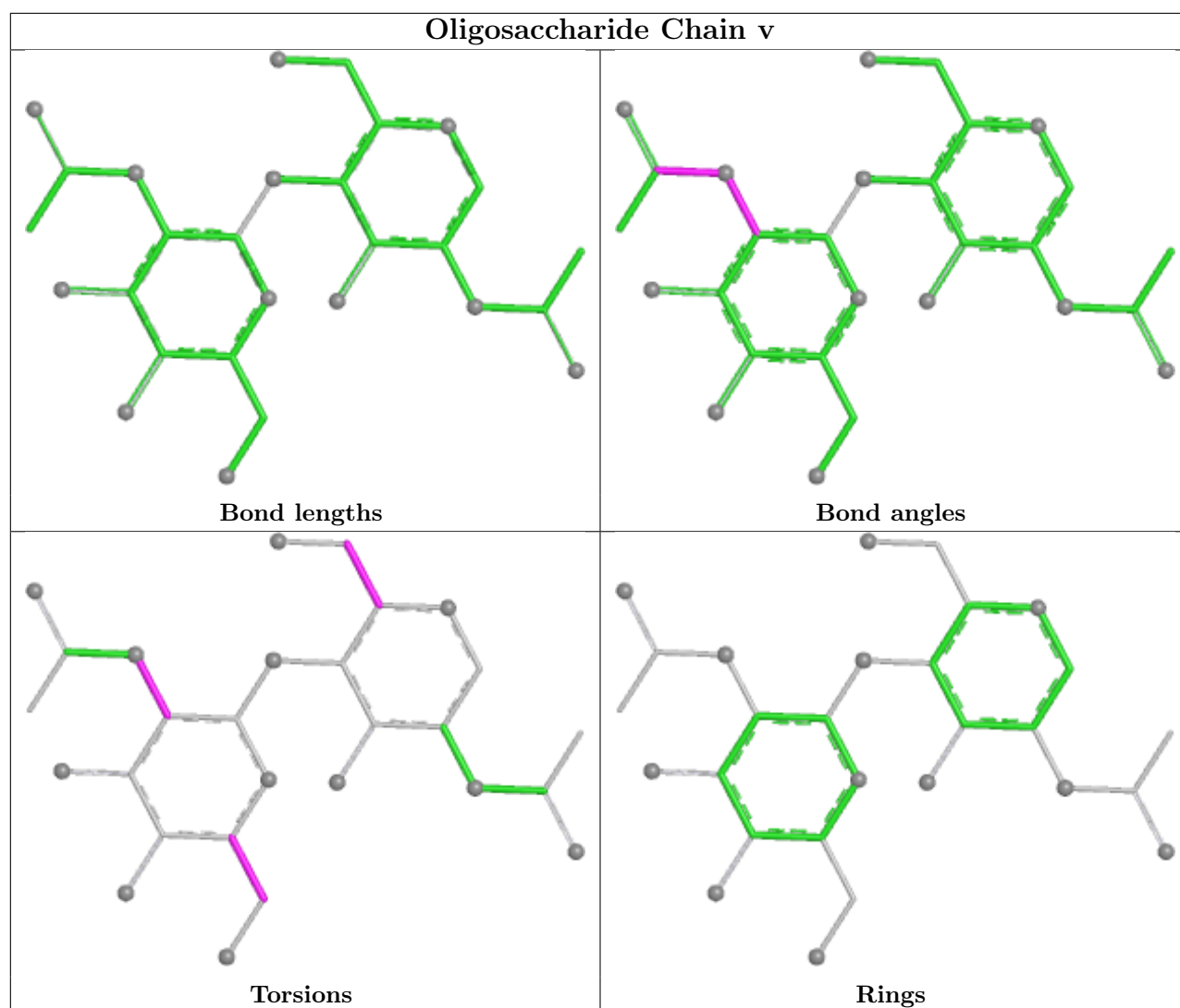












5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	FF	701	1	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	D	701	1	14,14,15	0.22	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	GG	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	LL	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	B	701	1	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	J	701	1	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	EE	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	CC	701	1	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	A	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	G	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	KK	701	1	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	MM	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	M	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	E	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	OO	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	H	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	II	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	JJ	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	F	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	I	701	1	14,14,15	0.22	0	17,19,21	0.54	0
3	NAG	BB	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	HH	701	1	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	AA	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	PP	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	N	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	L	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	NN	701	1	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	DD	701	1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	P	701	1	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	K	701	1	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	O	701	1	14,14,15	0.23	0	17,19,21	0.52	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	C	701	1	-	3/6/23/26	0/1/1/1
3	NAG	FF	701	1	-	3/6/23/26	0/1/1/1
3	NAG	D	701	1	-	3/6/23/26	0/1/1/1
3	NAG	GG	701	1	-	3/6/23/26	0/1/1/1
3	NAG	LL	701	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	701	1	-	3/6/23/26	0/1/1/1
3	NAG	J	701	1	-	3/6/23/26	0/1/1/1
3	NAG	EE	701	1	-	3/6/23/26	0/1/1/1
3	NAG	CC	701	1	-	3/6/23/26	0/1/1/1
3	NAG	A	701	1	-	3/6/23/26	0/1/1/1
3	NAG	G	701	1	-	3/6/23/26	0/1/1/1
3	NAG	KK	701	1	-	3/6/23/26	0/1/1/1
3	NAG	MM	701	1	-	3/6/23/26	0/1/1/1
3	NAG	M	701	1	-	3/6/23/26	0/1/1/1
3	NAG	E	701	1	-	3/6/23/26	0/1/1/1
3	NAG	OO	701	1	-	3/6/23/26	0/1/1/1
3	NAG	H	701	1	-	3/6/23/26	0/1/1/1
3	NAG	II	701	1	-	3/6/23/26	0/1/1/1
3	NAG	JJ	701	1	-	3/6/23/26	0/1/1/1
3	NAG	F	701	1	-	3/6/23/26	0/1/1/1
3	NAG	I	701	1	-	3/6/23/26	0/1/1/1
3	NAG	BB	701	1	-	3/6/23/26	0/1/1/1
3	NAG	HH	701	1	-	3/6/23/26	0/1/1/1
3	NAG	AA	701	1	-	3/6/23/26	0/1/1/1
3	NAG	PP	701	1	-	3/6/23/26	0/1/1/1
3	NAG	N	701	1	-	3/6/23/26	0/1/1/1
3	NAG	L	701	1	-	3/6/23/26	0/1/1/1
3	NAG	NN	701	1	-	3/6/23/26	0/1/1/1
3	NAG	DD	701	1	-	3/6/23/26	0/1/1/1
3	NAG	P	701	1	-	3/6/23/26	0/1/1/1
3	NAG	K	701	1	-	3/6/23/26	0/1/1/1
3	NAG	O	701	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	701	NAG	O5-C5-C6-O6
3	C	701	NAG	O5-C5-C6-O6
3	D	701	NAG	O5-C5-C6-O6
3	E	701	NAG	O5-C5-C6-O6
3	F	701	NAG	O5-C5-C6-O6
3	G	701	NAG	O5-C5-C6-O6
3	H	701	NAG	O5-C5-C6-O6
3	I	701	NAG	O5-C5-C6-O6
3	J	701	NAG	O5-C5-C6-O6
3	K	701	NAG	O5-C5-C6-O6
3	L	701	NAG	O5-C5-C6-O6
3	M	701	NAG	O5-C5-C6-O6
3	N	701	NAG	O5-C5-C6-O6
3	O	701	NAG	O5-C5-C6-O6
3	P	701	NAG	O5-C5-C6-O6
3	AA	701	NAG	O5-C5-C6-O6
3	BB	701	NAG	O5-C5-C6-O6
3	CC	701	NAG	O5-C5-C6-O6
3	DD	701	NAG	O5-C5-C6-O6
3	EE	701	NAG	O5-C5-C6-O6
3	FF	701	NAG	O5-C5-C6-O6
3	GG	701	NAG	O5-C5-C6-O6
3	HH	701	NAG	O5-C5-C6-O6
3	II	701	NAG	O5-C5-C6-O6
3	JJ	701	NAG	O5-C5-C6-O6
3	KK	701	NAG	O5-C5-C6-O6
3	LL	701	NAG	O5-C5-C6-O6
3	MM	701	NAG	O5-C5-C6-O6
3	NN	701	NAG	O5-C5-C6-O6
3	OO	701	NAG	O5-C5-C6-O6
3	PP	701	NAG	O5-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	C	701	NAG	C4-C5-C6-O6
3	D	701	NAG	C4-C5-C6-O6
3	E	701	NAG	C4-C5-C6-O6
3	F	701	NAG	C4-C5-C6-O6
3	G	701	NAG	C4-C5-C6-O6
3	H	701	NAG	C4-C5-C6-O6
3	I	701	NAG	C4-C5-C6-O6
3	J	701	NAG	C4-C5-C6-O6
3	K	701	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	L	701	NAG	C4-C5-C6-O6
3	M	701	NAG	C4-C5-C6-O6
3	N	701	NAG	C4-C5-C6-O6
3	O	701	NAG	C4-C5-C6-O6
3	P	701	NAG	C4-C5-C6-O6
3	AA	701	NAG	C4-C5-C6-O6
3	BB	701	NAG	C4-C5-C6-O6
3	CC	701	NAG	C4-C5-C6-O6
3	DD	701	NAG	C4-C5-C6-O6
3	EE	701	NAG	C4-C5-C6-O6
3	FF	701	NAG	C4-C5-C6-O6
3	GG	701	NAG	C4-C5-C6-O6
3	HH	701	NAG	C4-C5-C6-O6
3	II	701	NAG	C4-C5-C6-O6
3	JJ	701	NAG	C4-C5-C6-O6
3	KK	701	NAG	C4-C5-C6-O6
3	LL	701	NAG	C4-C5-C6-O6
3	MM	701	NAG	C4-C5-C6-O6
3	NN	701	NAG	C4-C5-C6-O6
3	OO	701	NAG	C4-C5-C6-O6
3	PP	701	NAG	C4-C5-C6-O6
3	A	701	NAG	C1-C2-N2-C7
3	B	701	NAG	C1-C2-N2-C7
3	C	701	NAG	C1-C2-N2-C7
3	D	701	NAG	C1-C2-N2-C7
3	E	701	NAG	C1-C2-N2-C7
3	F	701	NAG	C1-C2-N2-C7
3	G	701	NAG	C1-C2-N2-C7
3	H	701	NAG	C1-C2-N2-C7
3	I	701	NAG	C1-C2-N2-C7
3	J	701	NAG	C1-C2-N2-C7
3	K	701	NAG	C1-C2-N2-C7
3	L	701	NAG	C1-C2-N2-C7
3	M	701	NAG	C1-C2-N2-C7
3	N	701	NAG	C1-C2-N2-C7
3	O	701	NAG	C1-C2-N2-C7
3	P	701	NAG	C1-C2-N2-C7
3	AA	701	NAG	C1-C2-N2-C7
3	BB	701	NAG	C1-C2-N2-C7
3	CC	701	NAG	C1-C2-N2-C7
3	DD	701	NAG	C1-C2-N2-C7
3	EE	701	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	FF	701	NAG	C1-C2-N2-C7
3	GG	701	NAG	C1-C2-N2-C7
3	HH	701	NAG	C1-C2-N2-C7
3	II	701	NAG	C1-C2-N2-C7
3	JJ	701	NAG	C1-C2-N2-C7
3	KK	701	NAG	C1-C2-N2-C7
3	LL	701	NAG	C1-C2-N2-C7
3	MM	701	NAG	C1-C2-N2-C7
3	NN	701	NAG	C1-C2-N2-C7
3	OO	701	NAG	C1-C2-N2-C7
3	PP	701	NAG	C1-C2-N2-C7

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.

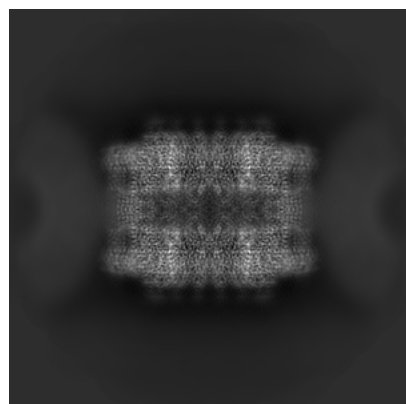
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20623. These allow visual inspection of the internal detail of the map and identification of artifacts.

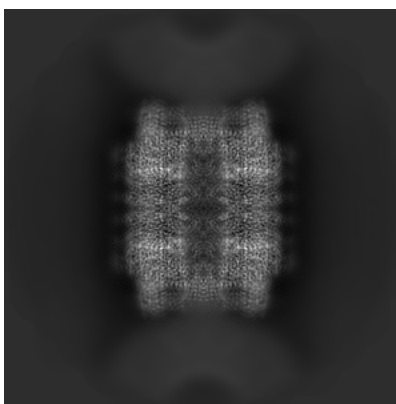
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

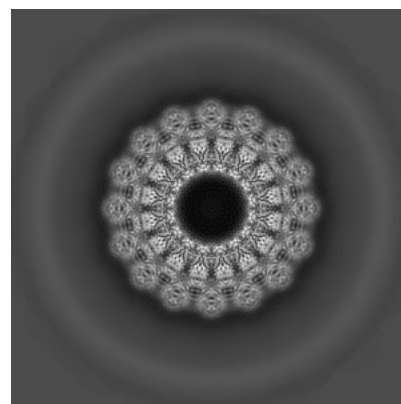
6.1.1 Primary map



X

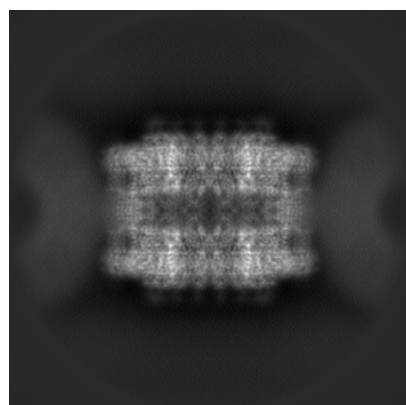


Y

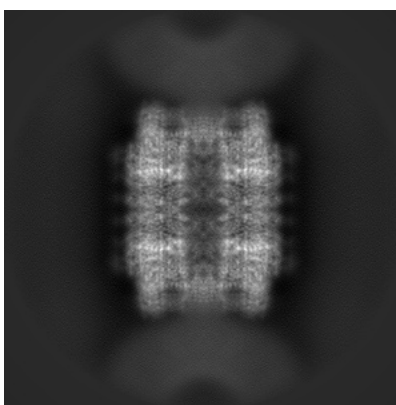


Z

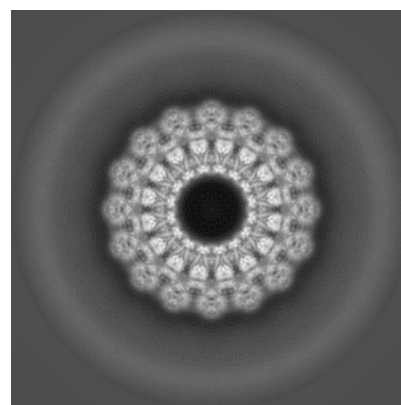
6.1.2 Raw map



X



Y

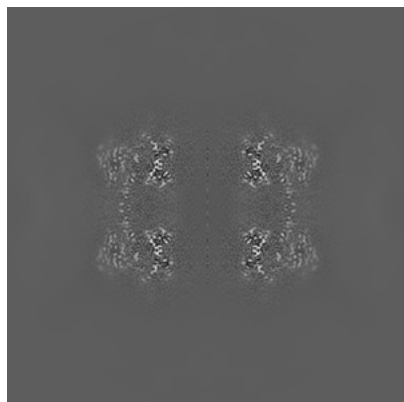


Z

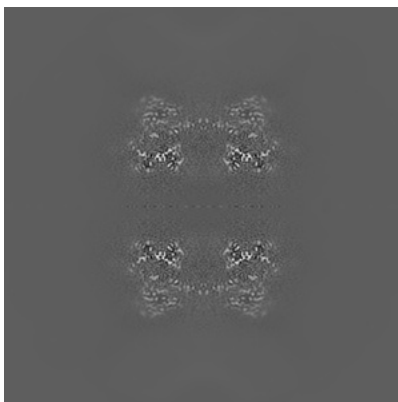
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

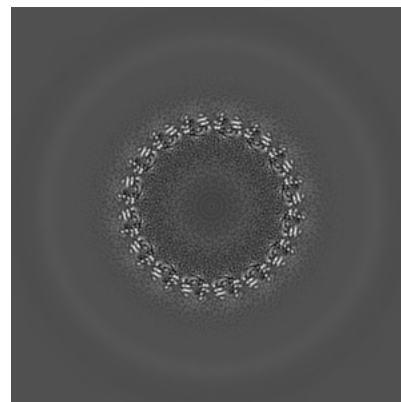
6.2.1 Primary map



X Index: 200

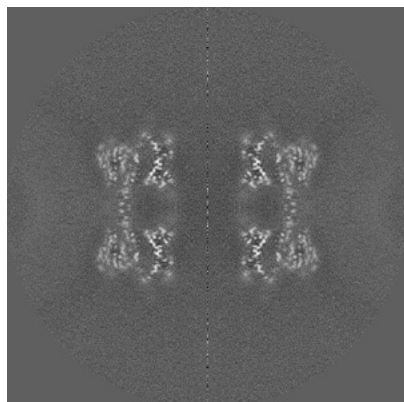


Y Index: 200

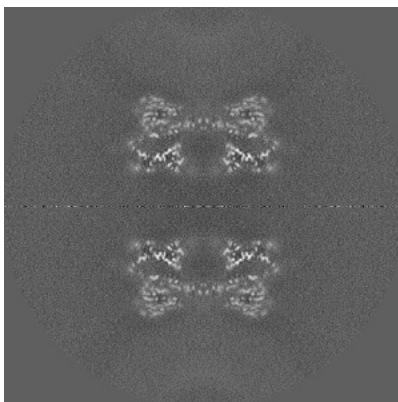


Z Index: 200

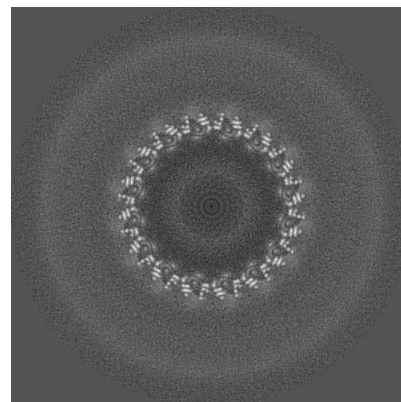
6.2.2 Raw map



X Index: 200



Y Index: 200

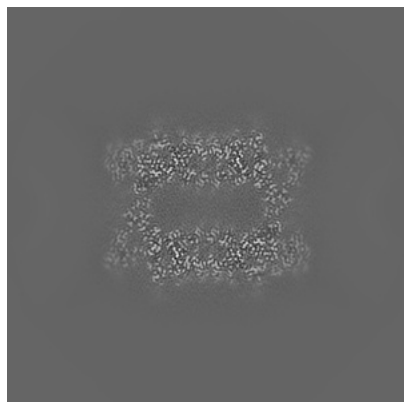


Z Index: 200

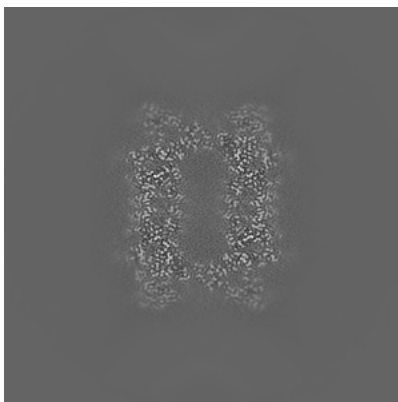
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

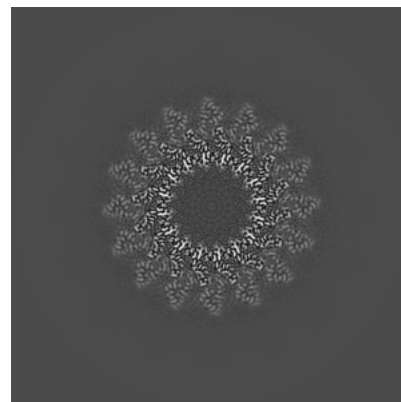
6.3.1 Primary map



X Index: 162

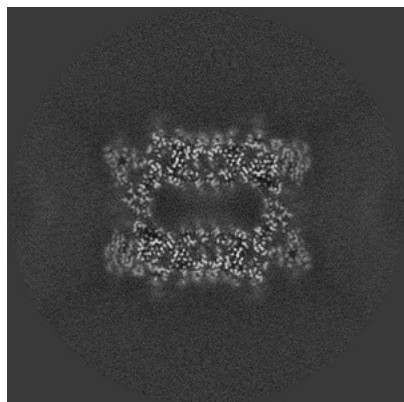


Y Index: 162

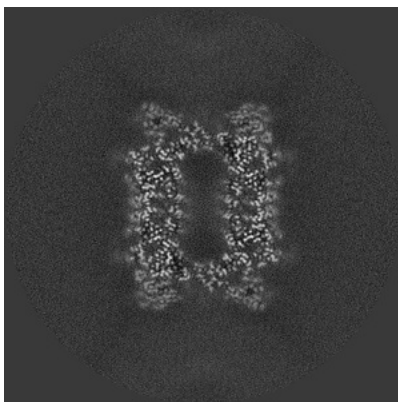


Z Index: 241

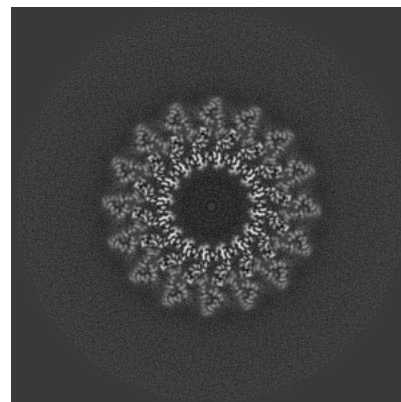
6.3.2 Raw map



X Index: 238



Y Index: 162

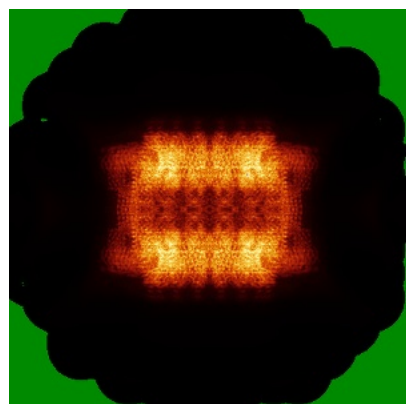


Z Index: 157

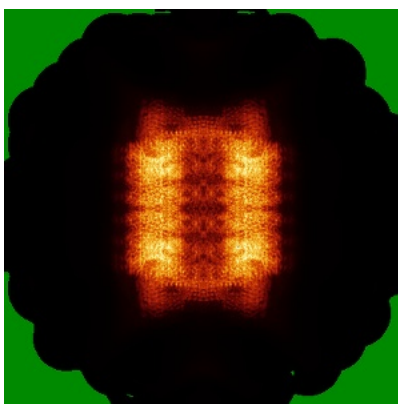
The images above show the largest variance slices of the map in three orthogonal directions.

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

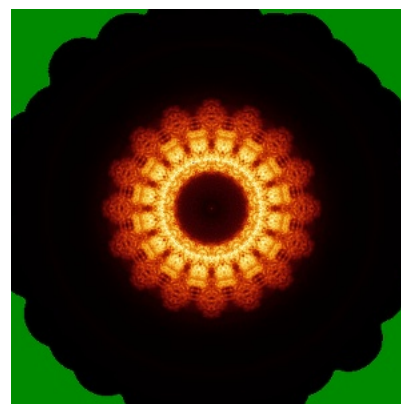
6.4.1 Primary map



X

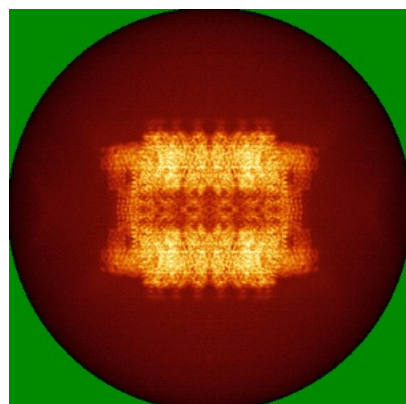


Y

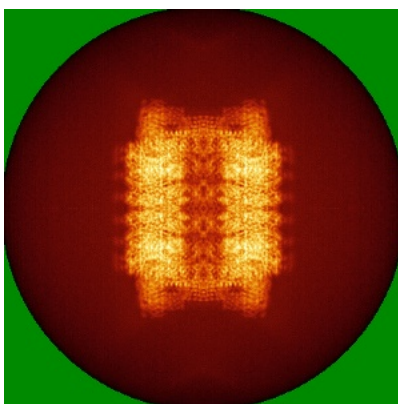


Z

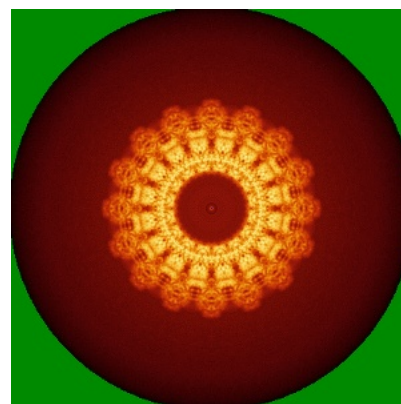
6.4.2 Raw map



X



Y

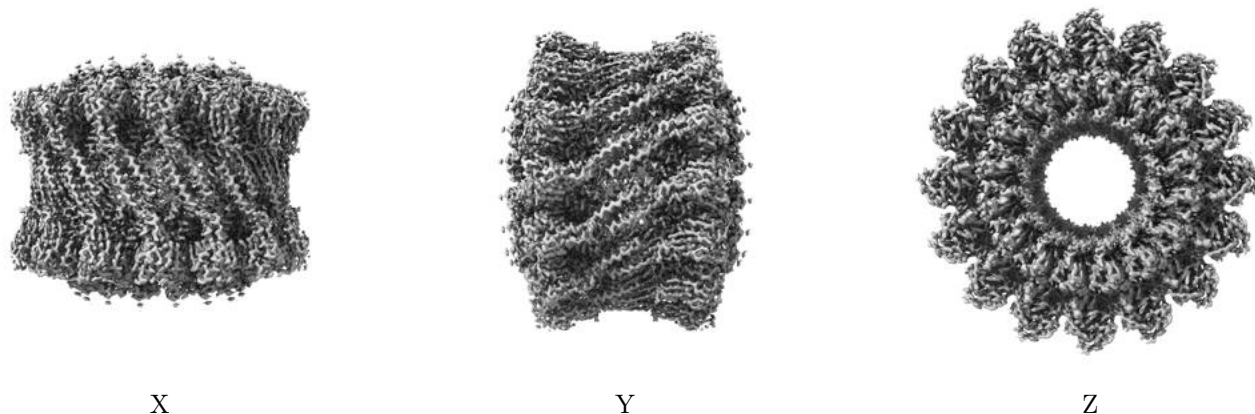


Z

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.

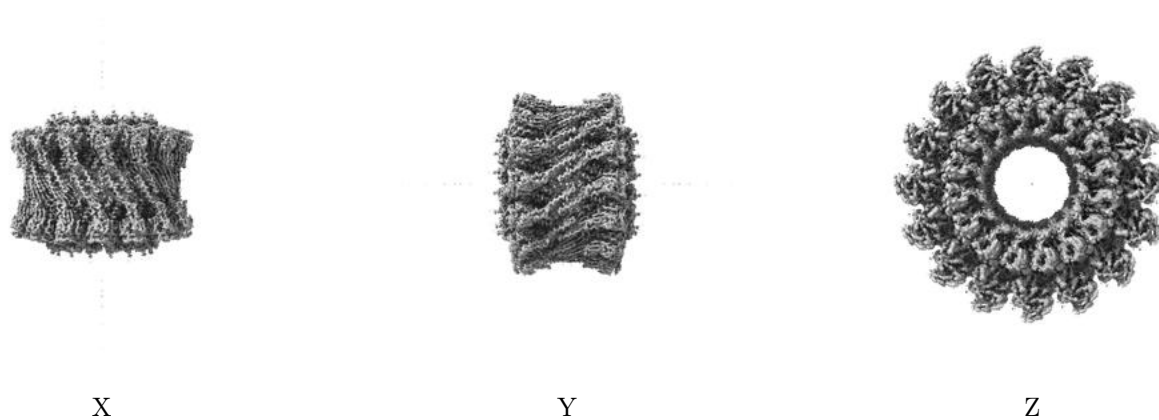
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0328. 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.

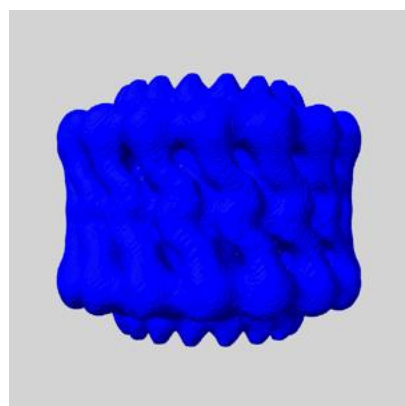
6.6 Mask visualisation [i](#)

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

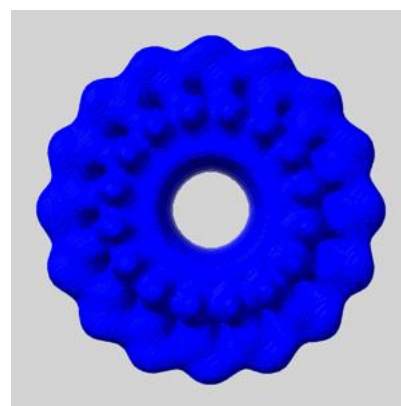
6.6.1 emd_20623_msk_1.map [i](#)



X



Y

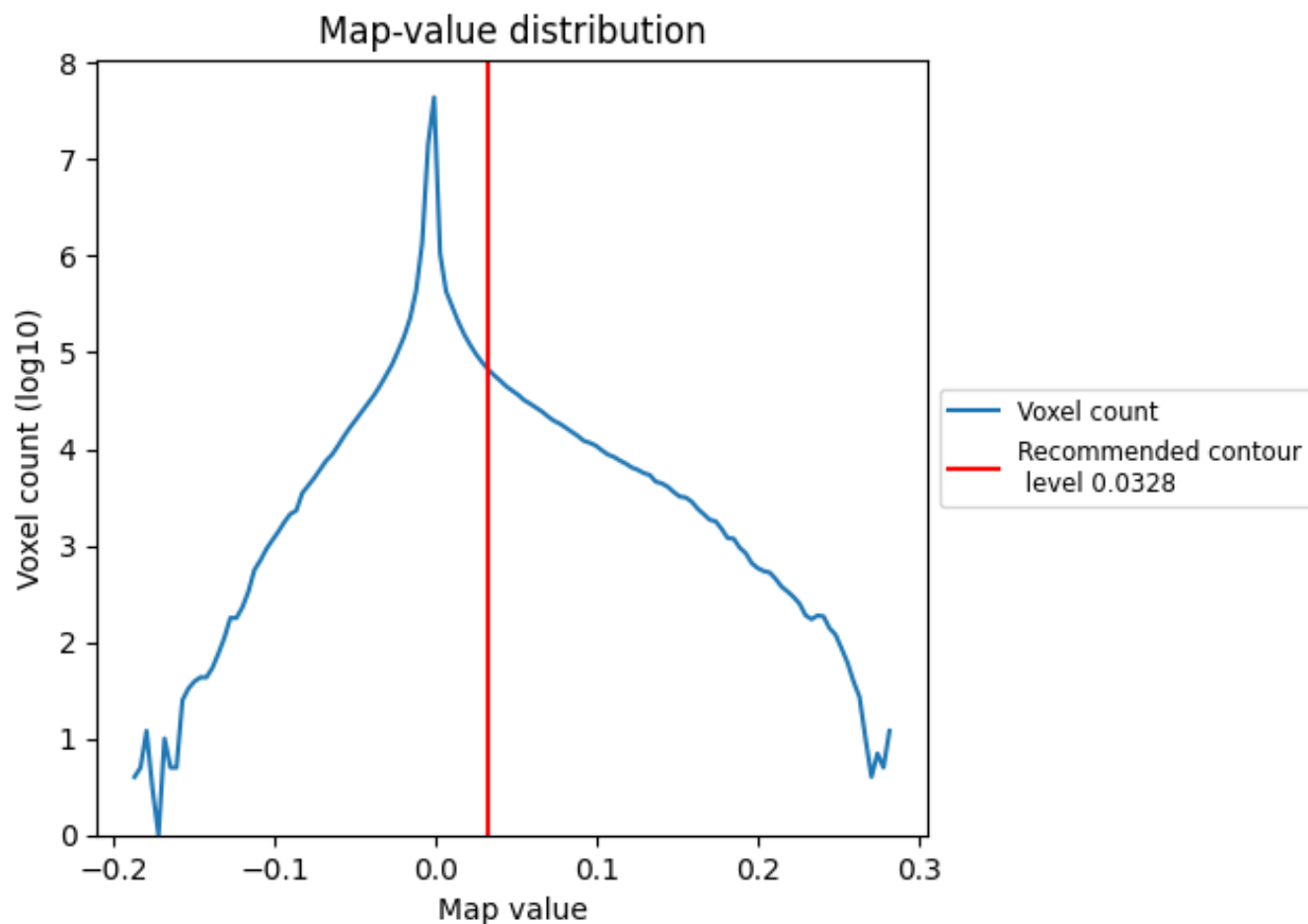


Z

7 Map analysis [i](#)

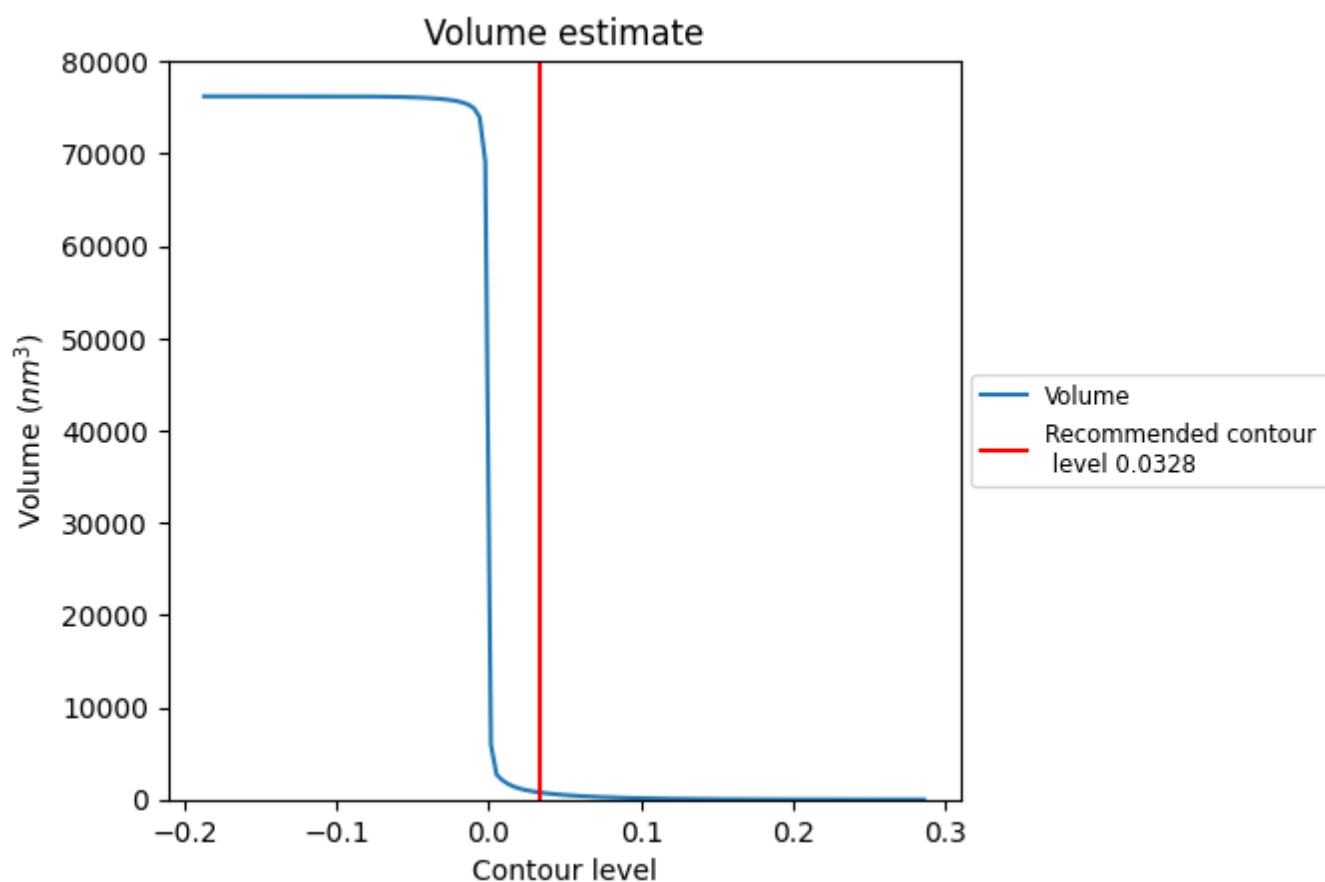
This section contains the results of statistical analysis of the map.

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.

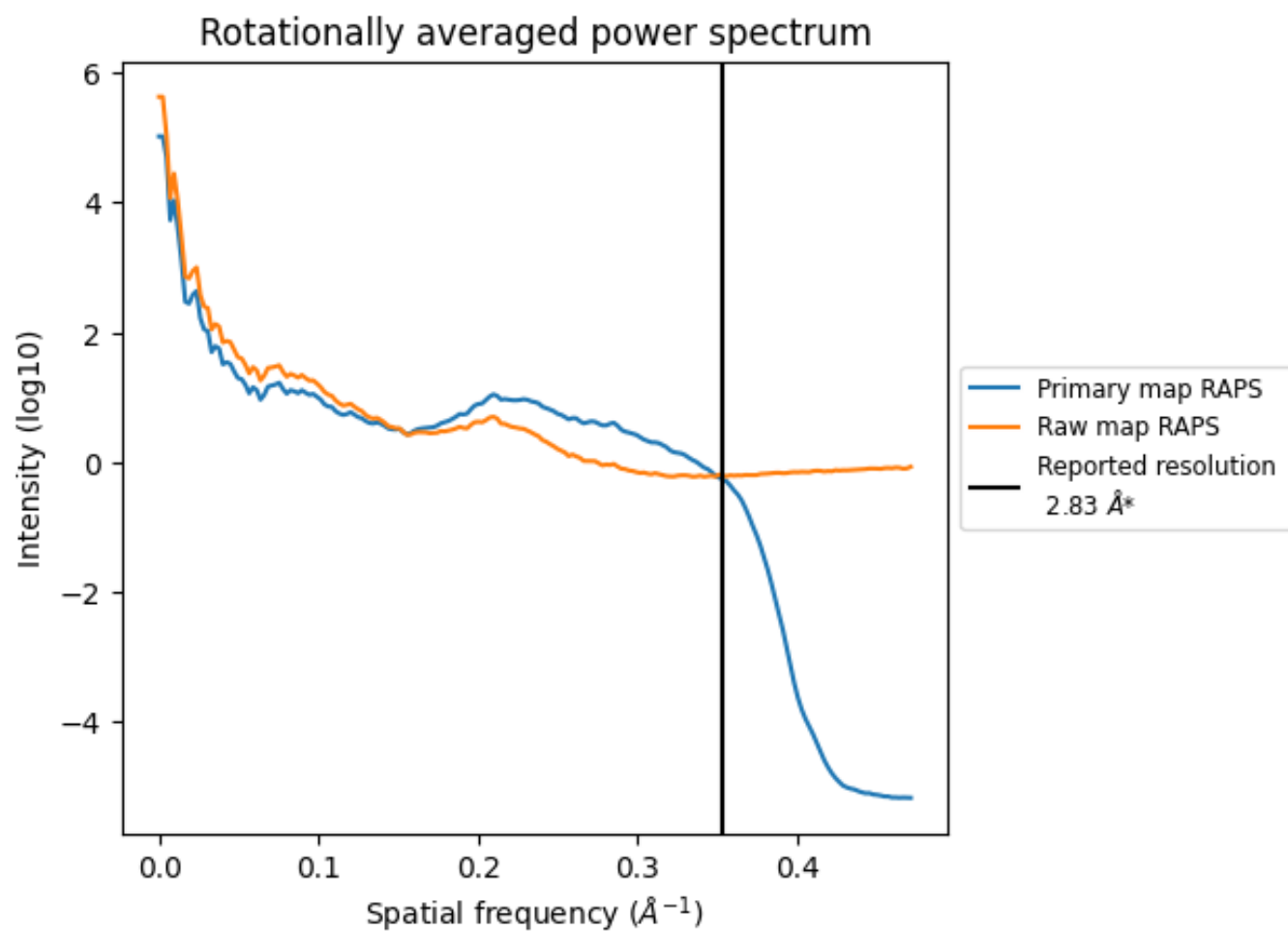
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 782 nm³; this corresponds to an approximate mass of 707 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 ⓘ

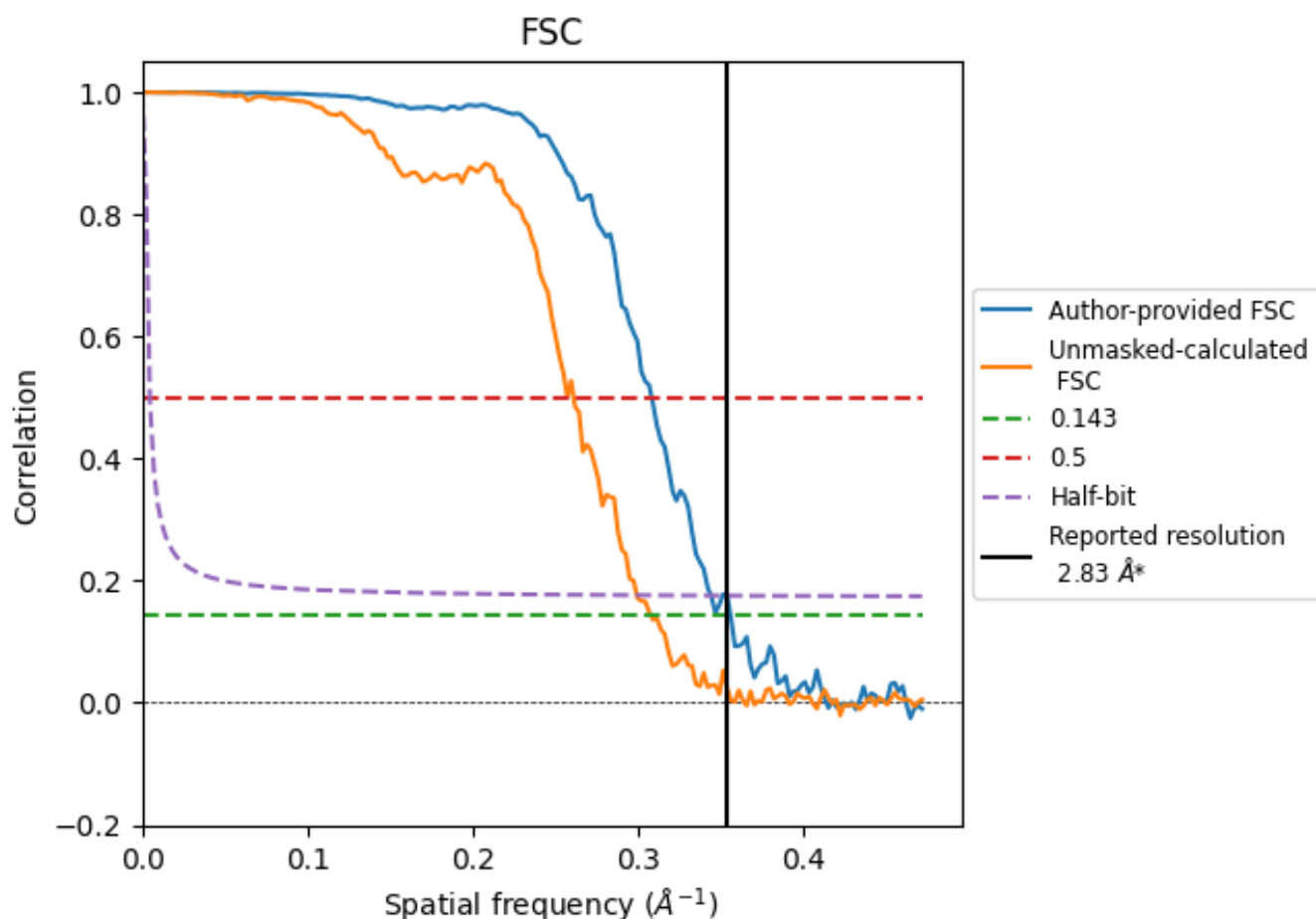


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 $0.353 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

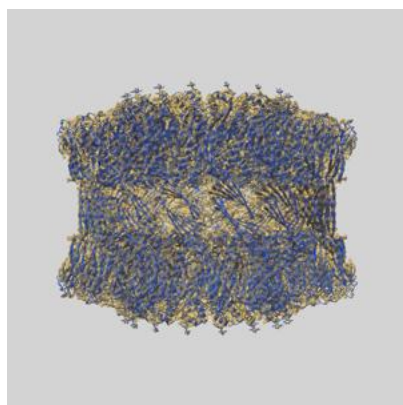
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.81	3.25	2.91
Unmasked-calculated*	3.25	3.83	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.83 by more than 10 %

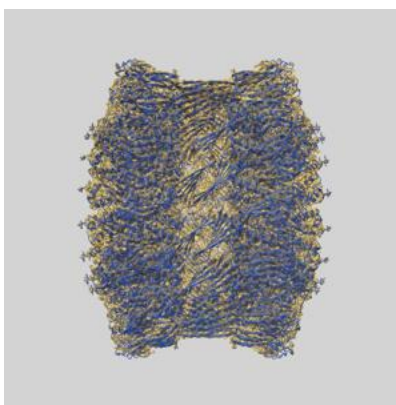
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20623 and PDB model 6U2L. Per-residue inclusion information can be found in section [3](#) on page [17](#).

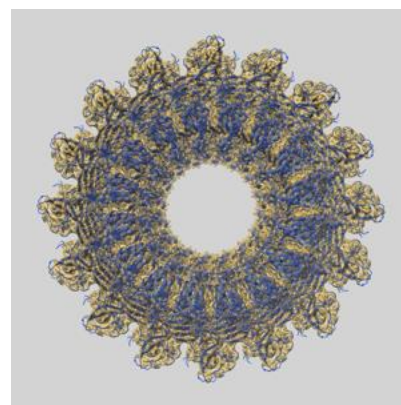
9.1 Map-model overlay [i](#)



X



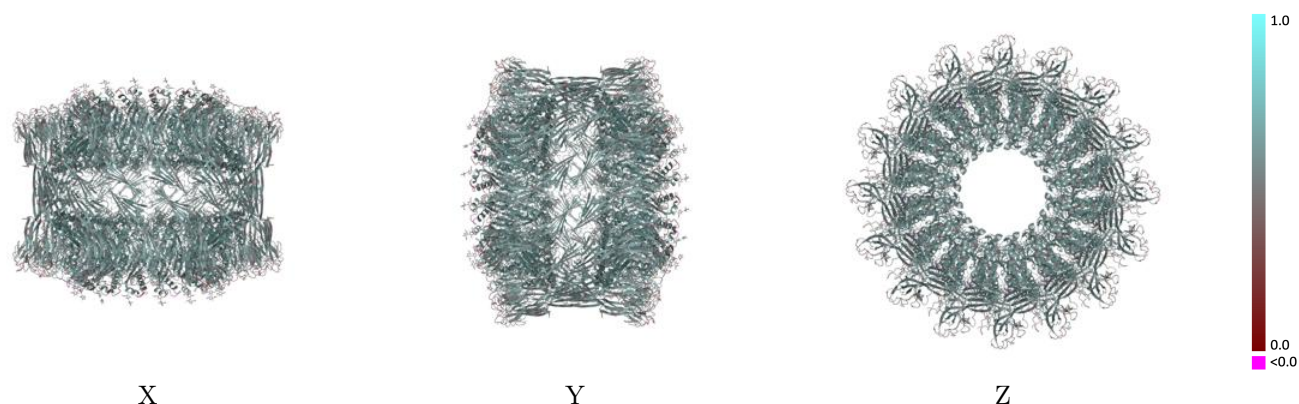
Y



Z

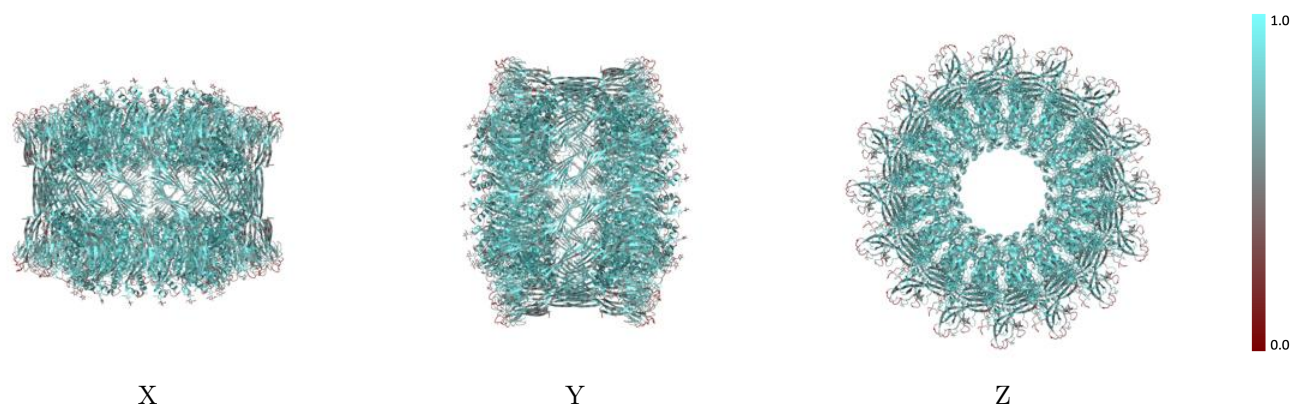
The images above show the 3D surface view of the map at the recommended contour level 0.0328 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



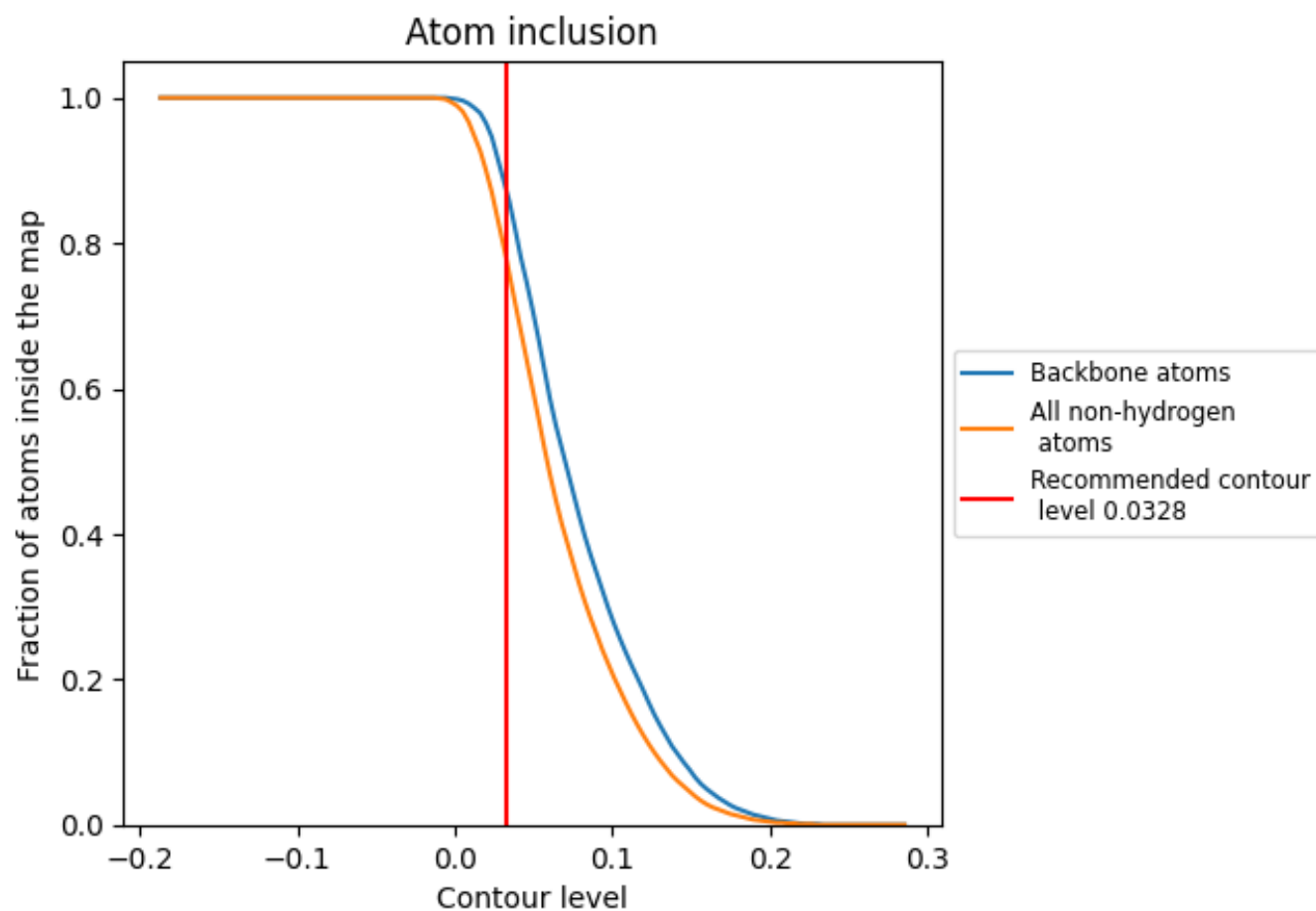
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0328).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.0328) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.5580
A	 0.7800	 0.5590
AA	 0.7820	 0.5590
B	 0.7800	 0.5590
BB	 0.7790	 0.5580
C	 0.7770	 0.5580
CC	 0.7780	 0.5600
D	 0.7770	 0.5590
DD	 0.7830	 0.5600
E	 0.7800	 0.5590
EE	 0.7800	 0.5600
F	 0.7800	 0.5590
FF	 0.7800	 0.5600
G	 0.7770	 0.5590
GG	 0.7780	 0.5600
H	 0.7790	 0.5600
HH	 0.7810	 0.5610
I	 0.7800	 0.5600
II	 0.7810	 0.5600
J	 0.7760	 0.5600
JJ	 0.7820	 0.5590
K	 0.7780	 0.5590
KK	 0.7810	 0.5590
L	 0.7810	 0.5600
LL	 0.7800	 0.5590
M	 0.7790	 0.5600
MM	 0.7790	 0.5570
N	 0.7790	 0.5600
NN	 0.7750	 0.5550
O	 0.7790	 0.5570
OO	 0.7790	 0.5570
P	 0.7790	 0.5560
PP	 0.7800	 0.5580
Q	 0.4640	 0.4220
R	 0.4290	 0.4250



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Chain	Atom inclusion	Q-score
S	 0.4640	 0.4290
T	 0.5000	 0.4230
U	 0.4640	 0.4310
V	 0.4640	 0.4360
W	 0.5000	 0.4230
X	 0.4640	 0.4270
Y	 0.4640	 0.4160
Z	 0.4290	 0.4370
a	 0.4640	 0.4350
b	 0.4640	 0.4120
c	 0.4640	 0.4070
d	 0.4640	 0.4210
e	 0.4640	 0.4240
f	 0.5000	 0.4180
g	 0.4640	 0.4280
h	 0.5360	 0.4450
i	 0.5000	 0.4460
j	 0.4640	 0.4260
k	 0.4640	 0.4320
l	 0.4640	 0.4340
m	 0.5000	 0.4250
n	 0.4640	 0.4160
o	 0.4640	 0.4290
p	 0.4640	 0.4340
q	 0.4640	 0.4340
r	 0.4640	 0.4110
s	 0.4640	 0.4300
t	 0.4640	 0.4440
u	 0.4640	 0.4350
v	 0.4640	 0.4260