



# Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 01:53 AM EST

PDB ID : 6U2J  
EMDB ID : EMD-20620  
Title : EM structure of MPEG-1 (L425K, alpha conformation) soluble pre-pore complex  
Authors : Pang, S.S.; Bayly-Jones, C.  
Deposited on : 2019-08-20  
Resolution : 2.37 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](mailto: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 (i) symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

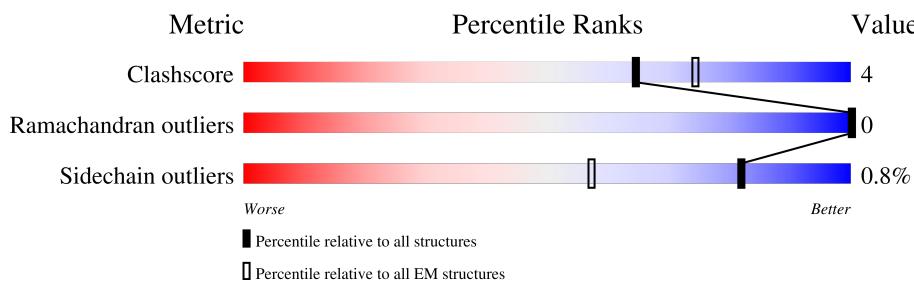
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : FAILED  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

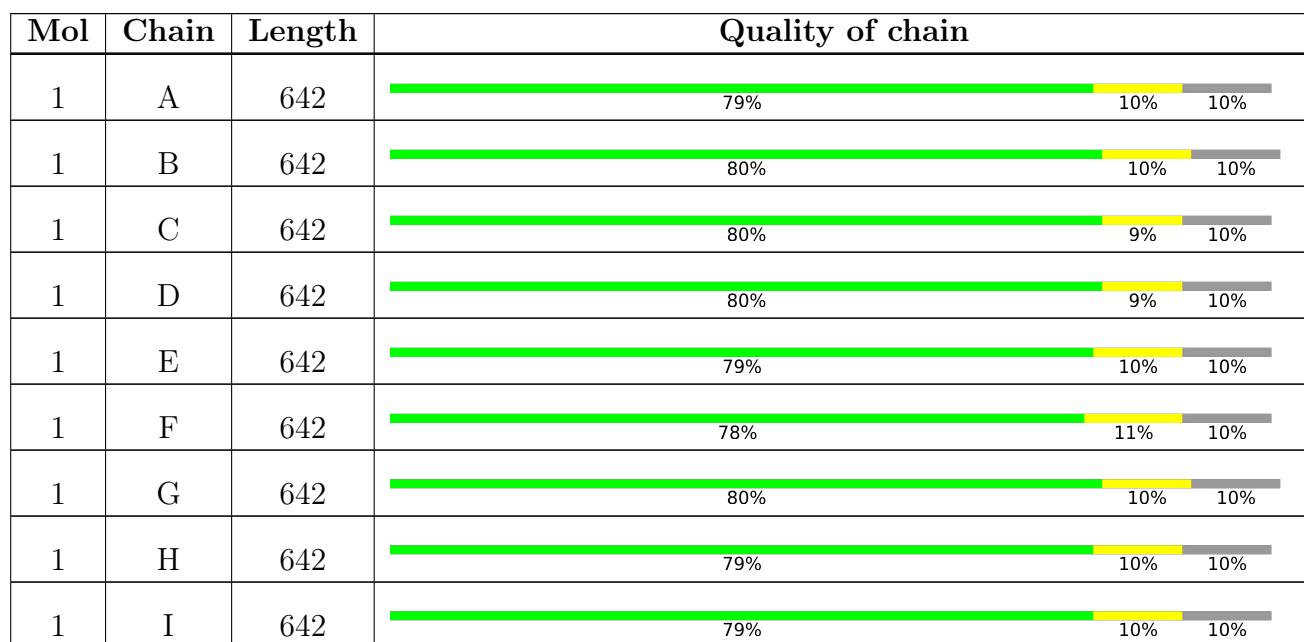
The reported resolution of this entry is 2.37 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%



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Mol	Chain	Length	Quality of chain		
1	J	642	80%	10%	10%
1	K	642	80%	10%	10%
1	L	642	79%	10%	10%
1	M	642	79%	10%	10%
1	N	642	79%	11%	10%
1	O	642	79%	10%	10%
1	P	642	79%	10%	10%
2	Q	2	100%		
2	R	2	100%		
2	S	2	100%		
2	T	2	100%		
2	U	2	100%		
2	V	2	100%		
2	W	2	100%		
2	X	2	100%		
2	Y	2	100%		
2	Z	2	100%		
2	a	2	100%		
2	b	2	100%		
2	c	2	100%		
2	d	2	100%		
2	e	2	100%		
2	f	2	100%		

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 71744 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	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	B	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	C	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	D	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	E	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	F	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	G	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	H	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	I	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	J	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	K	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	L	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	M	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	N	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	O	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		
1	P	575	Total	C	N	O	S	0	0
			4442	2811	763	843	25		

There are 112 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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



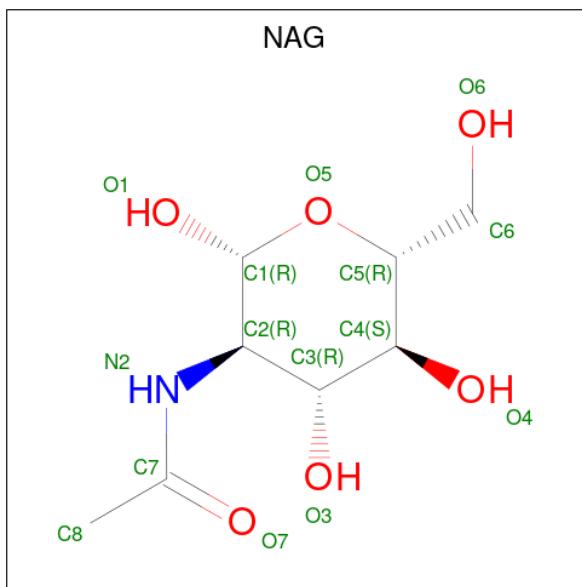
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
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		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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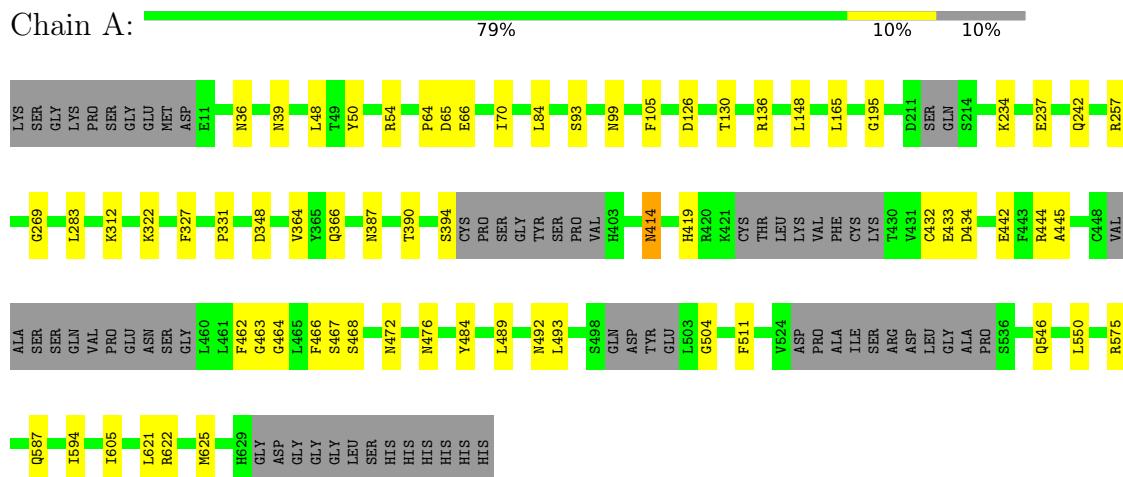
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Mol	Chain	Residues	Atoms	AltConf
3	O	1	Total C N O 14 8 1 5	0
3	P	1	Total C N O 14 8 1 5	0

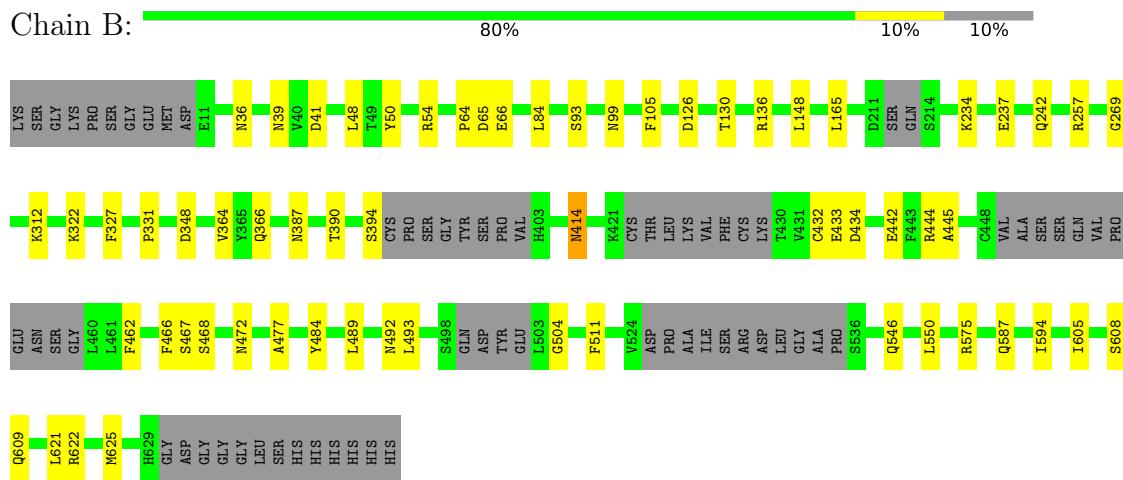
### 3 Residue-property plots

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

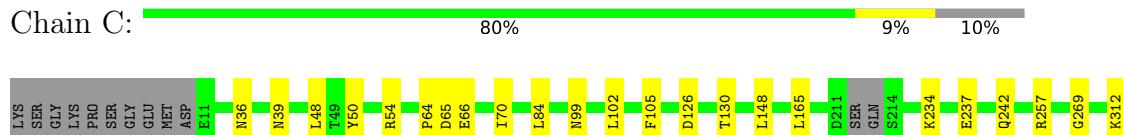
- Molecule 1: Macrophage-expressed gene 1 protein

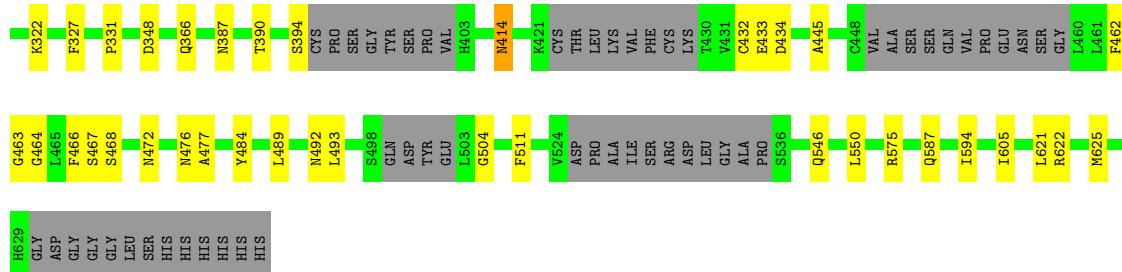


- Molecule 1: Macrophage-expressed gene 1 protein



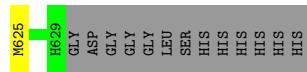
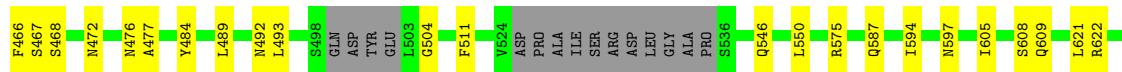
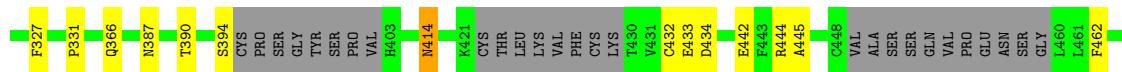
- Molecule 1: Macrophage-expressed gene 1 protein





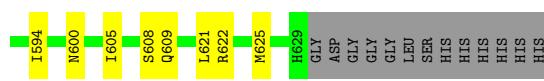
- Molecule 1: Macrophage-expressed gene 1 protein

Chain D:



- Molecule 1: Macrophage-expressed gene 1 protein

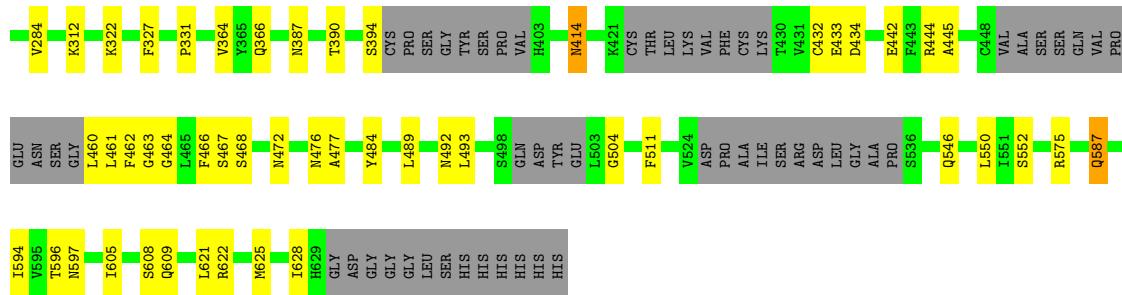
Chain E:



- Molecule 1: Macrophage-expressed gene 1 protein

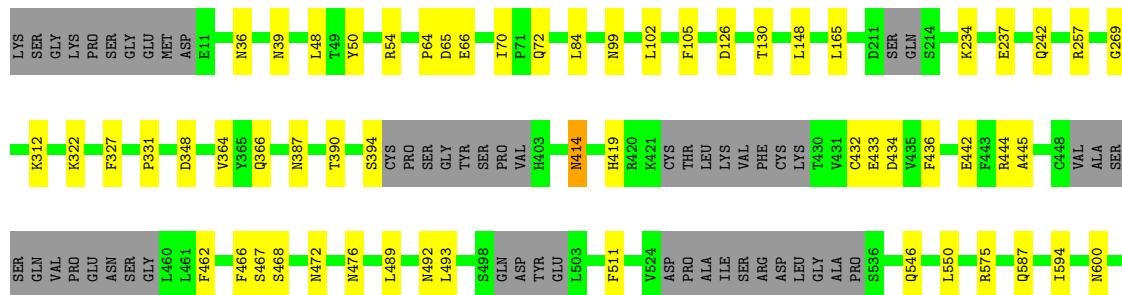
Chain F:





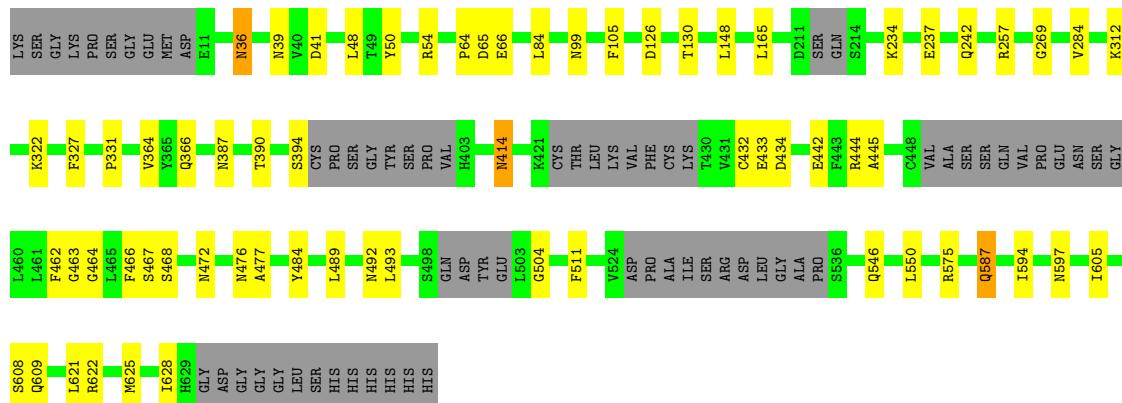
- Molecule 1: Macrophage-expressed gene 1 protein

Chain G:  80% 10% 10%



- Molecule 1: Macrophage-expressed gene 1 protein

Chain H:  79% 10% 10%



- Molecule 1: Macrophage-expressed gene 1 protein

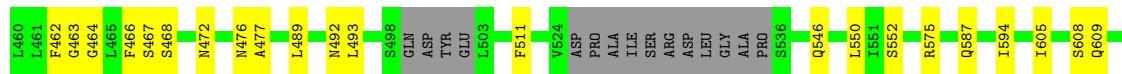
Chain I:  79% 10% 10%





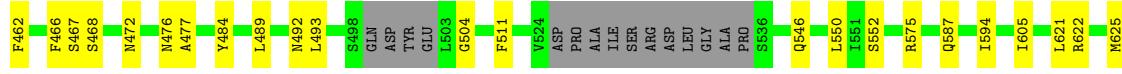
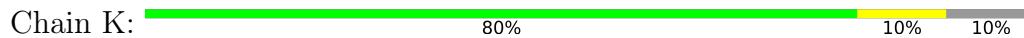
- Molecule 1: Macrophage-expressed gene 1 protein

Chain J:



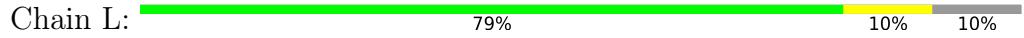
- Molecule 1: Macrophage-expressed gene 1 protein

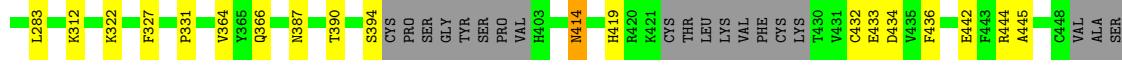
Chain K:



- Molecule 1: Macrophage-expressed gene 1 protein

### Chain L:

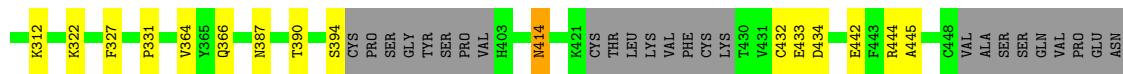






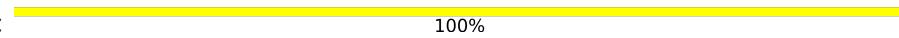
- Molecule 1: Macrophage-expressed gene 1 protein

Chain P:



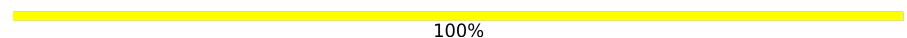
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



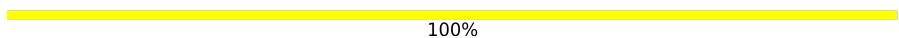
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

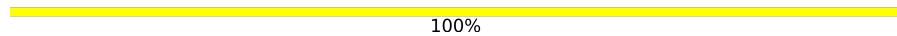


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

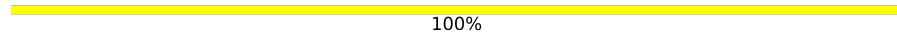


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

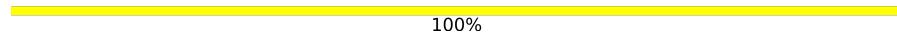


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

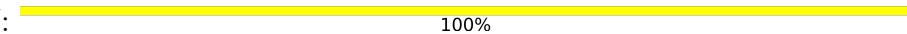


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

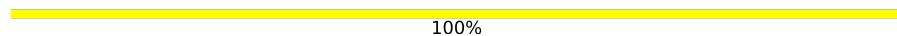


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

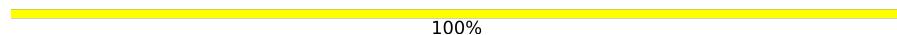


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

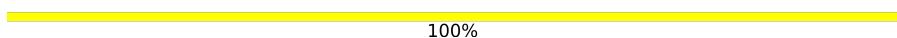


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

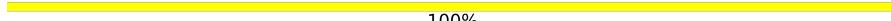


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

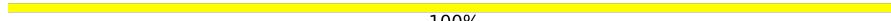
MAG1  
MAG2

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

Chain a:  100%

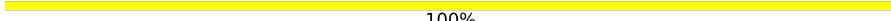
MAG1  
MAG2

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

Chain b:  100%

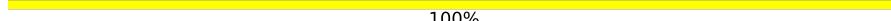
MAG1  
MAG2

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

Chain c:  100%

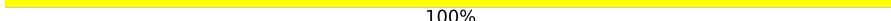
MAG1  
MAG2

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

Chain d:  100%

MAG1  
MAG2

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

Chain e:  100%

MAG1  
MAG2

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

Chain f:  100%

MAG1  
MAG2

## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C16	Depositor
Number of particles used	138422	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

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/4535	0.56	0/6153
1	B	0.35	0/4535	0.56	0/6153
1	C	0.35	0/4535	0.56	0/6153
1	D	0.35	0/4535	0.56	0/6153
1	E	0.35	0/4535	0.56	0/6153
1	F	0.35	0/4535	0.56	0/6153
1	G	0.35	0/4535	0.56	0/6153
1	H	0.35	0/4535	0.56	0/6153
1	I	0.35	0/4535	0.56	0/6153
1	J	0.35	0/4535	0.56	0/6153
1	K	0.35	0/4535	0.56	0/6153
1	L	0.35	0/4535	0.56	0/6153
1	M	0.35	0/4535	0.56	0/6153
1	N	0.35	0/4535	0.56	0/6153
1	O	0.35	0/4535	0.56	0/6153
1	P	0.35	0/4535	0.56	0/6153
All	All	0.35	0/72560	0.56	0/98448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4442	0	4318	39	0
1	B	4442	0	4318	36	0
1	C	4442	0	4318	35	0
1	D	4442	0	4318	36	0
1	E	4442	0	4318	42	0
1	F	4442	0	4318	47	0
1	G	4442	0	4318	40	0
1	H	4442	0	4318	42	0
1	I	4442	0	4318	39	0
1	J	4442	0	4318	38	0
1	K	4442	0	4318	36	0
1	L	4442	0	4318	39	0
1	M	4442	0	4318	43	0
1	N	4442	0	4318	45	0
1	O	4442	0	4318	40	0
1	P	4442	0	4318	39	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
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
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	0	0
3	J	14	0	13	0	0
3	K	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	14	0	13	0	0
3	M	14	0	13	0	0
3	N	14	0	13	0	0
3	O	14	0	13	0	0
3	P	14	0	13	0	0
All	All	71744	0	69696	591	0

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

All (591) 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:E:102:LEU:HD22	1:F:575:ARG:HG3	1.73	0.68
1:G:102:LEU:HD22	1:H:575:ARG:HG3	1.76	0.67
1:E:348:ASP:HB3	1:F:477:ALA:HB2	1.77	0.65
1:H:39:ASN:HD21	1:H:99:ASN:HD21	1.45	0.65
1:I:39:ASN:HD21	1:I:99:ASN:HD21	1.45	0.65
1:F:39:ASN:HD21	1:F:99:ASN:HD21	1.45	0.64
1:G:39:ASN:HD21	1:G:99:ASN:HD21	1.45	0.64
1:J:39:ASN:HD21	1:J:99:ASN:HD21	1.45	0.64
1:D:39:ASN:HD21	1:D:99:ASN:HD21	1.45	0.64
1:K:39:ASN:HD21	1:K:99:ASN:HD21	1.45	0.64
1:E:39:ASN:HD21	1:E:99:ASN:HD21	1.45	0.64
1:C:39:ASN:HD21	1:C:99:ASN:HD21	1.45	0.63
1:B:366:GLN:NE2	1:B:489:LEU:O	2.32	0.63
1:F:366:GLN:NE2	1:F:489:LEU:O	2.32	0.63
1:J:366:GLN:NE2	1:J:489:LEU:O	2.32	0.63
1:L:39:ASN:HD21	1:L:99:ASN:HD21	1.45	0.63
1:B:39:ASN:HD21	1:B:99:ASN:HD21	1.45	0.63
1:G:366:GLN:NE2	1:G:489:LEU:O	2.32	0.63
1:K:366:GLN:NE2	1:K:489:LEU:O	2.32	0.63
1:M:366:GLN:NE2	1:M:489:LEU:O	2.32	0.63
1:O:366:GLN:NE2	1:O:489:LEU:O	2.32	0.63
1:A:39:ASN:HD21	1:A:99:ASN:HD21	1.45	0.62
1:N:366:GLN:NE2	1:N:489:LEU:O	2.32	0.62
1:P:366:GLN:NE2	1:P:489:LEU:O	2.32	0.62
1:I:366:GLN:NE2	1:I:489:LEU:O	2.32	0.62
1:M:39:ASN:HD21	1:M:99:ASN:HD21	1.45	0.62
1:A:366:GLN:NE2	1:A:489:LEU:O	2.32	0.62
1:D:366:GLN:NE2	1:D:489:LEU:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:GLN:NE2	1:E:489:LEU:O	2.32	0.62
1:G:348:ASP:HB3	1:H:477:ALA:HB2	1.81	0.62
1:N:39:ASN:HD21	1:N:99:ASN:HD21	1.45	0.62
1:P:39:ASN:HD21	1:P:99:ASN:HD21	1.45	0.62
1:C:366:GLN:NE2	1:C:489:LEU:O	2.32	0.62
1:O:39:ASN:HD21	1:O:99:ASN:HD21	1.45	0.62
1:L:366:GLN:NE2	1:L:489:LEU:O	2.32	0.62
1:H:366:GLN:NE2	1:H:489:LEU:O	2.32	0.61
1:I:594:ILE:HG12	1:I:605:ILE:HG12	1.83	0.60
1:K:594:ILE:HG12	1:K:605:ILE:HG12	1.83	0.60
1:N:628:ILE:O	1:O:419:HIS:ND1	2.34	0.60
1:J:594:ILE:HG12	1:J:605:ILE:HG12	1.83	0.60
1:G:594:ILE:HG12	1:G:605:ILE:HG12	1.83	0.60
1:L:594:ILE:HG12	1:L:605:ILE:HG12	1.83	0.60
1:M:628:ILE:O	1:N:419:HIS:ND1	2.34	0.60
1:H:594:ILE:HG12	1:H:605:ILE:HG12	1.83	0.60
1:M:594:ILE:HG12	1:M:605:ILE:HG12	1.83	0.60
1:N:594:ILE:HG12	1:N:605:ILE:HG12	1.83	0.60
1:F:594:ILE:HG12	1:F:605:ILE:HG12	1.83	0.59
1:B:594:ILE:HG12	1:B:605:ILE:HG12	1.83	0.59
1:E:594:ILE:HG12	1:E:605:ILE:HG12	1.83	0.59
1:O:594:ILE:HG12	1:O:605:ILE:HG12	1.83	0.59
1:C:594:ILE:HG12	1:C:605:ILE:HG12	1.83	0.59
1:D:594:ILE:HG12	1:D:605:ILE:HG12	1.83	0.59
1:P:594:ILE:HG12	1:P:605:ILE:HG12	1.83	0.58
1:A:594:ILE:HG12	1:A:605:ILE:HG12	1.83	0.58
1:E:432:CYS:SG	1:E:433:GLU:N	2.77	0.58
1:D:432:CYS:SG	1:D:433:GLU:N	2.77	0.58
1:L:432:CYS:SG	1:L:433:GLU:N	2.76	0.58
1:M:432:CYS:SG	1:M:433:GLU:N	2.76	0.58
1:F:432:CYS:SG	1:F:433:GLU:N	2.76	0.58
1:K:432:CYS:SG	1:K:433:GLU:N	2.76	0.58
1:I:84:LEU:HB2	1:I:130:THR:HG23	1.86	0.58
1:L:84:LEU:HB2	1:L:130:THR:HG23	1.86	0.58
1:N:432:CYS:SG	1:N:433:GLU:N	2.77	0.58
1:C:432:CYS:SG	1:C:433:GLU:N	2.76	0.58
1:D:84:LEU:HB2	1:D:130:THR:HG23	1.86	0.58
1:G:432:CYS:SG	1:G:433:GLU:N	2.76	0.58
1:H:84:LEU:HB2	1:H:130:THR:HG23	1.86	0.58
1:P:84:LEU:HB2	1:P:130:THR:HG23	1.86	0.58
1:A:84:LEU:HB2	1:A:130:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HB2	1:C:130:THR:HG23	1.86	0.58
1:I:348:ASP:HB3	1:J:477:ALA:HB2	1.86	0.58
1:E:84:LEU:HB2	1:E:130:THR:HG23	1.86	0.58
1:M:84:LEU:HB2	1:M:130:THR:HG23	1.86	0.58
1:O:84:LEU:HB2	1:O:130:THR:HG23	1.86	0.57
1:B:432:CYS:SG	1:B:433:GLU:N	2.76	0.57
1:J:432:CYS:SG	1:J:433:GLU:N	2.77	0.57
1:O:432:CYS:SG	1:O:433:GLU:N	2.76	0.57
1:K:84:LEU:HB2	1:K:130:THR:HG23	1.86	0.57
1:G:84:LEU:HB2	1:G:130:THR:HG23	1.86	0.57
1:J:84:LEU:HB2	1:J:130:THR:HG23	1.86	0.57
1:A:432:CYS:SG	1:A:433:GLU:N	2.76	0.57
1:I:432:CYS:SG	1:I:433:GLU:N	2.76	0.57
1:P:432:CYS:SG	1:P:433:GLU:N	2.76	0.57
1:G:70:ILE:HD13	1:H:41:ASP:HB2	1.87	0.57
1:F:84:LEU:HB2	1:F:130:THR:HG23	1.86	0.56
1:A:419:HIS:ND1	1:P:628:ILE:O	2.39	0.56
1:B:84:LEU:HB2	1:B:130:THR:HG23	1.86	0.56
1:C:348:ASP:HB3	1:D:477:ALA:HB2	1.87	0.56
1:H:432:CYS:SG	1:H:433:GLU:N	2.76	0.56
1:L:348:ASP:HB3	1:M:477:ALA:HB2	1.87	0.56
1:N:84:LEU:HB2	1:N:130:THR:HG23	1.86	0.56
1:B:348:ASP:HB3	1:C:477:ALA:HB2	1.88	0.56
1:G:468:SER:HB3	1:G:492:ASN:HB3	1.89	0.55
1:K:468:SER:HB3	1:K:492:ASN:HB3	1.89	0.55
1:E:468:SER:HB3	1:E:492:ASN:HB3	1.89	0.55
1:F:468:SER:HB3	1:F:492:ASN:HB3	1.89	0.55
1:J:468:SER:HB3	1:J:492:ASN:HB3	1.89	0.55
1:H:468:SER:HB3	1:H:492:ASN:HB3	1.89	0.55
1:D:468:SER:HB3	1:D:492:ASN:HB3	1.89	0.55
1:I:468:SER:HB3	1:I:492:ASN:HB3	1.89	0.55
1:L:468:SER:HB3	1:L:492:ASN:HB3	1.89	0.55
1:B:414:ASN:HD21	1:B:434:ASP:HB2	1.72	0.55
1:M:468:SER:HB3	1:M:492:ASN:HB3	1.89	0.55
1:C:468:SER:HB3	1:C:492:ASN:HB3	1.89	0.55
1:M:414:ASN:HD21	1:M:434:ASP:HB2	1.72	0.55
1:N:414:ASN:HD21	1:N:434:ASP:HB2	1.72	0.54
1:A:414:ASN:HD21	1:A:434:ASP:HB2	1.72	0.54
1:N:468:SER:HB3	1:N:492:ASN:HB3	1.89	0.54
1:C:414:ASN:HD21	1:C:434:ASP:HB2	1.72	0.54
1:O:468:SER:HB3	1:O:492:ASN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:SER:HB3	1:B:492:ASN:HB3	1.89	0.54
1:L:414:ASN:HD21	1:L:434:ASP:HB2	1.72	0.54
1:A:468:SER:HB3	1:A:492:ASN:HB3	1.89	0.54
1:I:102:LEU:HD22	1:J:575:ARG:HG3	1.89	0.54
1:F:414:ASN:HD21	1:F:434:ASP:HB2	1.72	0.54
1:I:414:ASN:HD21	1:I:434:ASP:HB2	1.72	0.54
1:K:348:ASP:HB3	1:L:477:ALA:HB2	1.90	0.54
1:J:414:ASN:HD21	1:J:434:ASP:HB2	1.72	0.54
1:O:414:ASN:HD21	1:O:434:ASP:HB2	1.72	0.54
1:P:468:SER:HB3	1:P:492:ASN:HB3	1.89	0.54
1:G:414:ASN:HD21	1:G:434:ASP:HB2	1.72	0.53
1:H:414:ASN:HD21	1:H:434:ASP:HB2	1.72	0.53
1:N:165:LEU:HD22	1:N:312:LYS:HE3	1.91	0.53
1:E:414:ASN:HD21	1:E:434:ASP:HB2	1.72	0.53
1:P:414:ASN:HD21	1:P:434:ASP:HB2	1.72	0.53
1:K:165:LEU:HD22	1:K:312:LYS:HE3	1.91	0.53
1:O:165:LEU:HD22	1:O:312:LYS:HE3	1.91	0.53
1:D:414:ASN:HD21	1:D:434:ASP:HB2	1.72	0.53
1:B:165:LEU:HD22	1:B:312:LYS:HE3	1.91	0.53
1:A:165:LEU:HD22	1:A:312:LYS:HE3	1.91	0.53
1:H:327:PHE:O	1:H:575:ARG:NH2	2.42	0.53
1:I:327:PHE:O	1:I:575:ARG:NH2	2.42	0.53
1:J:165:LEU:HD22	1:J:312:LYS:HE3	1.91	0.53
1:J:327:PHE:O	1:J:575:ARG:NH2	2.42	0.53
1:G:327:PHE:O	1:G:575:ARG:NH2	2.42	0.52
1:K:414:ASN:HD21	1:K:434:ASP:HB2	1.72	0.52
1:K:467:SER:HA	1:K:493:LEU:HA	1.92	0.52
1:L:165:LEU:HD22	1:L:312:LYS:HE3	1.91	0.52
1:M:165:LEU:HD22	1:M:312:LYS:HE3	1.91	0.52
1:G:467:SER:HA	1:G:493:LEU:HA	1.92	0.52
1:J:467:SER:HA	1:J:493:LEU:HA	1.91	0.52
1:L:467:SER:HA	1:L:493:LEU:HA	1.92	0.52
1:C:165:LEU:HD22	1:C:312:LYS:HE3	1.91	0.52
1:H:467:SER:HA	1:H:493:LEU:HA	1.92	0.52
1:J:348:ASP:HB3	1:K:477:ALA:HB2	1.91	0.52
1:O:327:PHE:O	1:O:575:ARG:NH2	2.42	0.52
1:P:327:PHE:O	1:P:575:ARG:NH2	2.42	0.52
1:A:327:PHE:O	1:A:575:ARG:NH2	2.42	0.52
1:F:467:SER:HA	1:F:493:LEU:HA	1.92	0.52
1:I:467:SER:HA	1:I:493:LEU:HA	1.92	0.52
1:K:327:PHE:O	1:K:575:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:467:SER:HA	1:M:493:LEU:HA	1.92	0.52
1:F:327:PHE:O	1:F:575:ARG:NH2	2.42	0.52
1:N:327:PHE:O	1:N:575:ARG:NH2	2.42	0.52
1:P:165:LEU:HD22	1:P:312:LYS:HE3	1.91	0.52
1:E:70:ILE:HD13	1:F:41:ASP:HB2	1.91	0.52
1:F:597:ASN:HB3	1:G:436:PHE:HB2	1.90	0.52
1:G:165:LEU:HD22	1:G:312:LYS:HE3	1.91	0.52
1:B:327:PHE:O	1:B:575:ARG:NH2	2.42	0.52
1:E:327:PHE:O	1:E:575:ARG:NH2	2.42	0.52
1:N:467:SER:HA	1:N:493:LEU:HA	1.92	0.52
1:E:467:SER:HA	1:E:493:LEU:HA	1.92	0.52
1:F:165:LEU:HD22	1:F:312:LYS:HE3	1.91	0.52
1:L:327:PHE:O	1:L:575:ARG:NH2	2.42	0.52
1:M:327:PHE:O	1:M:575:ARG:NH2	2.42	0.52
1:C:327:PHE:O	1:C:575:ARG:NH2	2.42	0.52
1:D:327:PHE:O	1:D:575:ARG:NH2	2.42	0.52
1:D:467:SER:HA	1:D:493:LEU:HA	1.91	0.52
1:G:105:PHE:HZ	1:G:322:LYS:HG3	1.75	0.52
1:H:165:LEU:HD22	1:H:312:LYS:HE3	1.91	0.52
1:K:105:PHE:HZ	1:K:322:LYS:HG3	1.75	0.52
1:F:105:PHE:HZ	1:F:322:LYS:HG3	1.75	0.51
1:L:105:PHE:HZ	1:L:322:LYS:HG3	1.76	0.51
1:O:467:SER:HA	1:O:493:LEU:HA	1.91	0.51
1:C:105:PHE:HZ	1:C:322:LYS:HG3	1.75	0.51
1:E:165:LEU:HD22	1:E:312:LYS:HE3	1.91	0.51
1:I:165:LEU:HD22	1:I:312:LYS:HE3	1.91	0.51
1:O:105:PHE:HZ	1:O:322:LYS:HG3	1.75	0.51
1:P:105:PHE:HZ	1:P:322:LYS:HG3	1.75	0.51
1:F:628:ILE:O	1:G:419:HIS:ND1	2.43	0.51
1:O:348:ASP:HB3	1:P:477:ALA:HB2	1.93	0.51
1:C:467:SER:HA	1:C:493:LEU:HA	1.92	0.51
1:P:467:SER:HA	1:P:493:LEU:HA	1.91	0.51
1:B:467:SER:HA	1:B:493:LEU:HA	1.92	0.51
1:D:165:LEU:HD22	1:D:312:LYS:HE3	1.91	0.51
1:H:105:PHE:HZ	1:H:322:LYS:HG3	1.75	0.51
1:J:105:PHE:HZ	1:J:322:LYS:HG3	1.75	0.51
1:M:105:PHE:HZ	1:M:322:LYS:HG3	1.75	0.51
1:M:462:PHE:HE2	1:M:511:PHE:HB2	1.76	0.51
1:N:462:PHE:HE2	1:N:511:PHE:HB2	1.76	0.51
1:B:105:PHE:HZ	1:B:322:LYS:HG3	1.76	0.51
1:A:467:SER:HA	1:A:493:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:PHE:HZ	1:D:322:LYS:HG3	1.75	0.50
1:I:462:PHE:HE2	1:I:511:PHE:HB2	1.76	0.50
1:J:462:PHE:HE2	1:J:511:PHE:HB2	1.76	0.50
1:E:105:PHE:HZ	1:E:322:LYS:HG3	1.76	0.50
1:K:462:PHE:HE2	1:K:511:PHE:HB2	1.76	0.50
1:A:462:PHE:HE2	1:A:511:PHE:HB2	1.76	0.50
1:O:462:PHE:HE2	1:O:511:PHE:HB2	1.76	0.50
1:I:390:THR:HG21	1:I:394:SER:HB2	1.94	0.50
1:J:390:THR:HG21	1:J:394:SER:HB2	1.94	0.50
1:N:105:PHE:HZ	1:N:322:LYS:HG3	1.75	0.50
1:O:390:THR:HG21	1:O:394:SER:HB2	1.94	0.50
1:P:390:THR:HG21	1:P:394:SER:HB2	1.94	0.50
1:A:105:PHE:HZ	1:A:322:LYS:HG3	1.75	0.50
1:H:390:THR:HG21	1:H:394:SER:HB2	1.94	0.50
1:A:390:THR:HG21	1:A:394:SER:HB2	1.94	0.50
1:B:462:PHE:HE2	1:B:511:PHE:HB2	1.76	0.50
1:E:462:PHE:HE2	1:E:511:PHE:HB2	1.76	0.50
1:E:600:ASN:ND2	1:F:587:GLN:O	2.45	0.50
1:L:390:THR:HG21	1:L:394:SER:HB2	1.94	0.50
1:M:390:THR:HG21	1:M:394:SER:HB2	1.94	0.50
1:D:390:THR:HG21	1:D:394:SER:HB2	1.94	0.50
1:E:390:THR:HG21	1:E:394:SER:HB2	1.94	0.50
1:G:390:THR:HG21	1:G:394:SER:HB2	1.94	0.50
1:K:390:THR:HG21	1:K:394:SER:HB2	1.94	0.50
1:L:462:PHE:HE2	1:L:511:PHE:HB2	1.76	0.50
1:N:390:THR:HG21	1:N:394:SER:HB2	1.94	0.50
1:C:390:THR:HG21	1:C:394:SER:HB2	1.94	0.50
1:F:390:THR:HG21	1:F:394:SER:HB2	1.94	0.50
1:G:462:PHE:HE2	1:G:511:PHE:HB2	1.76	0.50
1:B:54:ARG:HD3	1:B:65:ASP:HA	1.94	0.49
1:B:390:THR:HG21	1:B:394:SER:HB2	1.94	0.49
1:D:54:ARG:HD3	1:D:65:ASP:HA	1.94	0.49
1:I:105:PHE:HZ	1:I:322:LYS:HG3	1.76	0.49
1:C:462:PHE:HE2	1:C:511:PHE:HB2	1.76	0.49
1:A:54:ARG:HD3	1:A:65:ASP:HA	1.94	0.49
1:C:54:ARG:HD3	1:C:65:ASP:HA	1.94	0.49
1:E:54:ARG:HD3	1:E:65:ASP:HA	1.94	0.49
1:P:462:PHE:HE2	1:P:511:PHE:HB2	1.76	0.49
1:F:462:PHE:HE2	1:F:511:PHE:HB2	1.76	0.49
1:K:54:ARG:HD3	1:K:65:ASP:HA	1.94	0.49
1:H:462:PHE:HE2	1:H:511:PHE:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:ARG:HD3	1:L:65:ASP:HA	1.94	0.49
1:D:462:PHE:HE2	1:D:511:PHE:HB2	1.76	0.49
1:F:54:ARG:HD3	1:F:65:ASP:HA	1.94	0.49
1:P:54:ARG:HD3	1:P:65:ASP:HA	1.94	0.49
1:J:54:ARG:HD3	1:J:65:ASP:HA	1.94	0.48
1:G:54:ARG:HD3	1:G:65:ASP:HA	1.94	0.48
1:O:54:ARG:HD3	1:O:65:ASP:HA	1.94	0.48
1:H:54:ARG:HD3	1:H:65:ASP:HA	1.94	0.48
1:M:348:ASP:HB3	1:N:477:ALA:HB2	1.96	0.48
1:N:54:ARG:HD3	1:N:65:ASP:HA	1.94	0.48
1:M:54:ARG:HD3	1:M:65:ASP:HA	1.94	0.47
1:I:54:ARG:HD3	1:I:65:ASP:HA	1.94	0.47
1:J:331:PRO:HD2	1:J:546:GLN:HE21	1.79	0.47
1:L:331:PRO:HD2	1:L:546:GLN:HE21	1.79	0.47
1:H:434:ASP:OD1	1:H:434:ASP:N	2.47	0.47
1:I:434:ASP:OD1	1:I:434:ASP:N	2.46	0.47
1:K:48:LEU:HA	1:K:66:GLU:OE2	2.15	0.47
1:M:48:LEU:HA	1:M:66:GLU:OE2	2.15	0.47
1:D:48:LEU:HA	1:D:66:GLU:OE2	2.15	0.47
1:G:48:LEU:HA	1:G:66:GLU:OE2	2.15	0.47
1:G:434:ASP:OD1	1:G:434:ASP:N	2.47	0.47
1:A:463:GLY:HA3	1:A:464:GLY:HA2	1.68	0.47
1:C:48:LEU:HA	1:C:66:GLU:OE2	2.15	0.47
1:D:597:ASN:HB3	1:E:436:PHE:HB2	1.97	0.47
1:E:72:GLN:O	1:F:284:VAL:HG11	2.14	0.47
1:F:434:ASP:OD1	1:F:434:ASP:N	2.47	0.47
1:G:331:PRO:HD2	1:G:546:GLN:HE21	1.80	0.47
1:H:331:PRO:HD2	1:H:546:GLN:HE21	1.80	0.47
1:J:434:ASP:N	1:J:434:ASP:OD1	2.47	0.47
1:K:434:ASP:OD1	1:K:434:ASP:N	2.47	0.47
1:L:434:ASP:N	1:L:434:ASP:OD1	2.47	0.47
1:M:434:ASP:OD1	1:M:434:ASP:N	2.47	0.47
1:O:48:LEU:HA	1:O:66:GLU:OE2	2.15	0.47
1:I:48:LEU:HA	1:I:66:GLU:OE2	2.15	0.47
1:I:331:PRO:HD2	1:I:546:GLN:HE21	1.80	0.47
1:N:434:ASP:OD1	1:N:434:ASP:N	2.47	0.47
1:P:48:LEU:HA	1:P:66:GLU:OE2	2.15	0.47
1:E:331:PRO:HD2	1:E:546:GLN:HE21	1.80	0.47
1:N:48:LEU:HA	1:N:66:GLU:OE2	2.15	0.47
1:N:331:PRO:HD2	1:N:546:GLN:HE21	1.80	0.47
1:E:434:ASP:N	1:E:434:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:LEU:HA	1:H:66:GLU:OE2	2.15	0.47
1:K:331:PRO:HD2	1:K:546:GLN:HE21	1.80	0.47
1:O:434:ASP:N	1:O:434:ASP:OD1	2.47	0.47
1:P:434:ASP:OD1	1:P:434:ASP:N	2.46	0.47
1:B:48:LEU:HA	1:B:66:GLU:OE2	2.15	0.46
1:L:48:LEU:HA	1:L:66:GLU:OE2	2.15	0.46
1:A:48:LEU:HA	1:A:66:GLU:OE2	2.15	0.46
1:A:331:PRO:HD2	1:A:546:GLN:HE21	1.79	0.46
1:D:434:ASP:OD1	1:D:434:ASP:N	2.47	0.46
1:F:48:LEU:HA	1:F:66:GLU:OE2	2.15	0.46
1:J:50:TYR:HE1	1:J:64:PRO:HG3	1.81	0.46
1:C:50:TYR:HE1	1:C:64:PRO:HG3	1.81	0.46
1:E:48:LEU:HA	1:E:66:GLU:OE2	2.15	0.46
1:H:628:ILE:O	1:I:419:HIS:ND1	2.48	0.46
1:A:434:ASP:OD1	1:A:434:ASP:N	2.47	0.46
1:C:331:PRO:HD2	1:C:546:GLN:HE21	1.80	0.46
1:C:434:ASP:OD1	1:C:434:ASP:N	2.47	0.46
1:F:50:TYR:HE1	1:F:64:PRO:HG3	1.81	0.46
1:F:331:PRO:HD2	1:F:546:GLN:HE21	1.79	0.46
1:H:442:GLU:OE2	1:H:444:ARG:NH1	2.47	0.46
1:K:442:GLU:OE2	1:K:444:ARG:NH1	2.47	0.46
1:M:331:PRO:HD2	1:M:546:GLN:HE21	1.80	0.46
1:A:387:ASN:ND2	1:A:394:SER:O	2.49	0.46
1:B:434:ASP:N	1:B:434:ASP:OD1	2.47	0.46
1:I:50:TYR:HE1	1:I:64:PRO:HG3	1.81	0.46
1:N:387:ASN:ND2	1:N:394:SER:O	2.49	0.46
1:P:331:PRO:HD2	1:P:546:GLN:HE21	1.79	0.46
1:B:50:TYR:HE1	1:B:64:PRO:HG3	1.81	0.46
1:G:50:TYR:HE1	1:G:64:PRO:HG3	1.81	0.46
1:H:597:ASN:HB3	1:I:436:PHE:HB2	1.97	0.46
1:J:48:LEU:HA	1:J:66:GLU:OE2	2.15	0.46
1:J:608:SER:HA	1:J:609:GLN:HA	1.72	0.46
1:L:102:LEU:HD22	1:M:575:ARG:HG3	1.97	0.46
1:M:50:TYR:HE1	1:M:64:PRO:HG3	1.81	0.46
1:B:331:PRO:HD2	1:B:546:GLN:HE21	1.79	0.46
1:B:387:ASN:ND2	1:B:394:SER:O	2.49	0.46
1:M:387:ASN:ND2	1:M:394:SER:O	2.49	0.46
1:P:387:ASN:ND2	1:P:394:SER:O	2.49	0.46
1:L:50:TYR:HE1	1:L:64:PRO:HG3	1.81	0.46
1:P:50:TYR:HE1	1:P:64:PRO:HG3	1.81	0.46
1:C:102:LEU:HD22	1:D:575:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:GLY:HA3	1:E:464:GLY:HA2	1.68	0.46
1:P:463:GLY:HA3	1:P:464:GLY:HA2	1.68	0.46
1:E:50:TYR:HE1	1:E:64:PRO:HG3	1.81	0.45
1:K:387:ASN:ND2	1:K:394:SER:O	2.49	0.45
1:L:387:ASN:ND2	1:L:394:SER:O	2.49	0.45
1:O:50:TYR:HE1	1:O:64:PRO:HG3	1.81	0.45
1:O:331:PRO:HD2	1:O:546:GLN:HE21	1.79	0.45
1:O:600:ASN:HD21	1:P:585:MET:HG3	1.82	0.45
1:I:70:ILE:HD13	1:J:41:ASP:HB2	1.98	0.45
1:O:387:ASN:ND2	1:O:394:SER:O	2.49	0.45
1:C:387:ASN:ND2	1:C:394:SER:O	2.49	0.45
1:D:331:PRO:HD2	1:D:546:GLN:HE21	1.79	0.45
1:N:484:TYR:OH	1:N:504:GLY:O	2.34	0.45
1:I:463:GLY:HA3	1:I:464:GLY:HA2	1.68	0.45
1:J:387:ASN:ND2	1:J:394:SER:O	2.49	0.45
1:A:575:ARG:HG3	1:P:102:LEU:HD22	1.98	0.45
1:D:387:ASN:ND2	1:D:394:SER:O	2.49	0.45
1:D:50:TYR:HE1	1:D:64:PRO:HG3	1.81	0.45
1:E:466:PHE:HB3	1:E:472:ASN:HB2	1.99	0.45
1:F:484:TYR:OH	1:F:504:GLY:O	2.34	0.45
1:I:484:TYR:OH	1:I:504:GLY:O	2.34	0.45
1:L:484:TYR:OH	1:L:504:GLY:O	2.34	0.45
1:F:442:GLU:OE2	1:F:444:ARG:NH1	2.47	0.45
1:F:608:SER:HA	1:F:609:GLN:HA	1.72	0.45
1:K:50:TYR:HE1	1:K:64:PRO:HG3	1.81	0.45
1:G:387:ASN:ND2	1:G:394:SER:O	2.49	0.45
1:H:50:TYR:HE1	1:H:64:PRO:HG3	1.81	0.45
1:I:387:ASN:ND2	1:I:394:SER:O	2.49	0.45
1:N:50:TYR:HE1	1:N:64:PRO:HG3	1.81	0.45
1:A:50:TYR:HE1	1:A:64:PRO:HG3	1.81	0.45
1:F:466:PHE:HB3	1:F:472:ASN:HB2	1.99	0.45
1:H:387:ASN:ND2	1:H:394:SER:O	2.49	0.45
1:D:466:PHE:HB3	1:D:472:ASN:HB2	1.99	0.45
1:D:237:GLU:OE2	1:D:242:GLN:NE2	2.51	0.44
1:G:237:GLU:OE2	1:G:242:GLN:NE2	2.51	0.44
1:O:493:LEU:HB2	1:O:550:LEU:HD13	2.00	0.44
1:D:493:LEU:HB2	1:D:550:LEU:HD13	2.00	0.44
1:H:493:LEU:HB2	1:H:550:LEU:HD13	2.00	0.44
1:A:484:TYR:OH	1:A:504:GLY:O	2.34	0.44
1:B:484:TYR:OH	1:B:504:GLY:O	2.34	0.44
1:E:387:ASN:ND2	1:E:394:SER:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ASN:ND2	1:F:394:SER:O	2.49	0.44
1:L:66:GLU:HG3	1:L:148:LEU:HD13	2.00	0.44
1:A:466:PHE:HB3	1:A:472:ASN:HB2	1.99	0.44
1:B:66:GLU:HG3	1:B:148:LEU:HD13	2.00	0.44
1:C:463:GLY:HA3	1:C:464:GLY:HA2	1.68	0.44
1:C:493:LEU:HB2	1:C:550:LEU:HD13	2.00	0.44
1:D:66:GLU:HG3	1:D:148:LEU:HD13	2.00	0.44
1:D:442:GLU:OE2	1:D:444:ARG:NH1	2.47	0.44
1:E:66:GLU:HG3	1:E:148:LEU:HD13	2.00	0.44
1:N:66:GLU:HG3	1:N:148:LEU:HD13	2.00	0.44
1:P:484:TYR:OH	1:P:504:GLY:O	2.34	0.44
1:A:66:GLU:HG3	1:A:148:LEU:HD13	2.00	0.44
1:A:237:GLU:OE2	1:A:242:GLN:NE2	2.51	0.44
1:E:493:LEU:HB2	1:E:550:LEU:HD13	2.00	0.44
1:G:66:GLU:HG3	1:G:148:LEU:HD13	2.00	0.44
1:G:466:PHE:HB3	1:G:472:ASN:HB2	1.99	0.44
1:I:442:GLU:OE2	1:I:444:ARG:NH1	2.47	0.44
1:K:493:LEU:HB2	1:K:550:LEU:HD13	2.00	0.44
1:N:493:LEU:HB2	1:N:550:LEU:HD13	2.00	0.44
1:E:237:GLU:OE2	1:E:242:GLN:NE2	2.51	0.44
1:E:605:ILE:HD11	1:E:621:LEU:HD23	2.00	0.44
1:G:493:LEU:HB2	1:G:550:LEU:HD13	2.00	0.44
1:I:466:PHE:HB3	1:I:472:ASN:HB2	1.99	0.44
1:J:237:GLU:OE2	1:J:242:GLN:NE2	2.51	0.44
1:J:466:PHE:HB3	1:J:472:ASN:HB2	1.99	0.44
1:M:66:GLU:HG3	1:M:148:LEU:HD13	2.00	0.44
1:N:442:GLU:OE2	1:N:444:ARG:NH1	2.47	0.44
1:O:66:GLU:HG3	1:O:148:LEU:HD13	2.00	0.44
1:P:442:GLU:OE2	1:P:444:ARG:NH1	2.47	0.44
1:B:493:LEU:HB2	1:B:550:LEU:HD13	2.00	0.44
1:C:66:GLU:HG3	1:C:148:LEU:HD13	2.00	0.44
1:F:66:GLU:HG3	1:F:148:LEU:HD13	2.00	0.44
1:F:237:GLU:OE2	1:F:242:GLN:NE2	2.51	0.44
1:F:605:ILE:HD11	1:F:621:LEU:HD23	2.00	0.44
1:G:608:SER:HA	1:G:609:GLN:HA	1.72	0.44
1:H:605:ILE:HD11	1:H:621:LEU:HD23	2.00	0.44
1:I:66:GLU:HG3	1:I:148:LEU:HD13	2.00	0.44
1:J:66:GLU:HG3	1:J:148:LEU:HD13	2.00	0.44
1:K:66:GLU:HG3	1:K:148:LEU:HD13	2.00	0.44
1:B:442:GLU:OE2	1:B:444:ARG:NH1	2.47	0.44
1:G:605:ILE:HD11	1:G:621:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:GLU:OE2	1:H:242:GLN:NE2	2.51	0.44
1:J:605:ILE:HD11	1:J:621:LEU:HD23	2.00	0.44
1:N:102:LEU:HD22	1:O:575:ARG:HG3	2.00	0.44
1:B:466:PHE:HB3	1:B:472:ASN:HB2	1.99	0.43
1:C:237:GLU:OE2	1:C:242:GLN:NE2	2.51	0.43
1:C:466:PHE:HB3	1:C:472:ASN:HB2	1.99	0.43
1:H:66:GLU:HG3	1:H:148:LEU:HD13	2.00	0.43
1:K:237:GLU:OE2	1:K:242:GLN:NE2	2.51	0.43
1:L:493:LEU:HB2	1:L:550:LEU:HD13	2.00	0.43
1:M:126:ASP:OD1	1:M:126:ASP:N	2.51	0.43
1:O:463:GLY:HA3	1:O:464:GLY:HA2	1.68	0.43
1:P:66:GLU:HG3	1:P:148:LEU:HD13	2.00	0.43
1:P:466:PHE:HB3	1:P:472:ASN:HB2	1.99	0.43
1:C:605:ILE:HD11	1:C:621:LEU:HD23	2.00	0.43
1:E:484:TYR:OH	1:E:504:GLY:O	2.34	0.43
1:G:600:ASN:ND2	1:H:587:GLN:O	2.51	0.43
1:H:126:ASP:N	1:H:126:ASP:OD1	2.52	0.43
1:I:237:GLU:OE2	1:I:242:GLN:NE2	2.51	0.43
1:I:493:LEU:HB2	1:I:550:LEU:HD13	2.00	0.43
1:L:126:ASP:N	1:L:126:ASP:OD1	2.51	0.43
1:L:237:GLU:OE2	1:L:242:GLN:NE2	2.51	0.43
1:O:237:GLU:OE2	1:O:242:GLN:NE2	2.51	0.43
1:P:493:LEU:HB2	1:P:550:LEU:HD13	2.00	0.43
1:A:348:ASP:HB3	1:B:477:ALA:HB2	2.00	0.43
1:D:126:ASP:OD1	1:D:126:ASP:N	2.51	0.43
1:E:126:ASP:N	1:E:126:ASP:OD1	2.51	0.43
1:O:484:TYR:OH	1:O:504:GLY:O	2.34	0.43
1:P:237:GLU:OE2	1:P:242:GLN:NE2	2.51	0.43
1:B:237:GLU:OE2	1:B:242:GLN:NE2	2.51	0.43
1:D:605:ILE:HD11	1:D:621:LEU:HD23	2.00	0.43
1:F:126:ASP:OD1	1:F:126:ASP:N	2.51	0.43
1:I:605:ILE:HD11	1:I:621:LEU:HD23	2.00	0.43
1:N:126:ASP:OD1	1:N:126:ASP:N	2.52	0.43
1:N:237:GLU:OE2	1:N:242:GLN:NE2	2.51	0.43
1:F:36:ASN:HD22	1:F:36:ASN:HA	1.61	0.43
1:H:466:PHE:HB3	1:H:472:ASN:HB2	1.99	0.43
1:I:126:ASP:N	1:I:126:ASP:OD1	2.51	0.43
1:K:605:ILE:HD11	1:K:621:LEU:HD23	2.00	0.43
1:L:466:PHE:HB3	1:L:472:ASN:HB2	1.99	0.43
1:M:237:GLU:OE2	1:M:242:GLN:NE2	2.51	0.43
1:M:466:PHE:HB3	1:M:472:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HB2	1:A:550:LEU:HD13	2.00	0.43
1:M:597:ASN:HB3	1:N:436:PHE:HB2	2.01	0.43
1:N:466:PHE:HB3	1:N:472:ASN:HB2	1.99	0.43
1:C:70:ILE:HD13	1:D:41:ASP:HB2	2.01	0.43
1:C:126:ASP:N	1:C:126:ASP:OD1	2.51	0.43
1:E:608:SER:HA	1:E:609:GLN:HA	1.72	0.43
1:L:442:GLU:OE2	1:L:444:ARG:NH1	2.47	0.43
1:L:605:ILE:HD11	1:L:621:LEU:HD23	2.00	0.43
1:B:605:ILE:HD11	1:B:621:LEU:HD23	2.00	0.43
1:F:493:LEU:HB2	1:F:550:LEU:HD13	2.00	0.43
1:J:493:LEU:HB2	1:J:550:LEU:HD13	2.00	0.43
1:K:484:TYR:OH	1:K:504:GLY:O	2.34	0.43
1:M:608:SER:HA	1:M:609:GLN:HA	1.72	0.43
1:O:126:ASP:OD1	1:O:126:ASP:N	2.51	0.43
1:H:484:TYR:OH	1:H:504:GLY:O	2.34	0.43
1:K:466:PHE:HB3	1:K:472:ASN:HB2	1.99	0.43
1:L:463:GLY:HA3	1:L:464:GLY:HA2	1.68	0.43
1:M:493:LEU:HB2	1:M:550:LEU:HD13	2.00	0.43
1:O:466:PHE:HB3	1:O:472:ASN:HB2	1.99	0.43
1:A:234:LYS:HD2	1:A:269:GLY:HA3	2.01	0.42
1:B:126:ASP:OD1	1:B:126:ASP:N	2.51	0.42
1:N:234:LYS:HD2	1:N:269:GLY:HA3	2.01	0.42
1:P:234:LYS:HD2	1:P:269:GLY:HA3	2.01	0.42
1:B:366:GLN:HG2	1:B:445:ALA:HA	2.02	0.42
1:F:366:GLN:HG2	1:F:445:ALA:HA	2.02	0.42
1:K:102:LEU:HD22	1:L:575:ARG:HG3	2.00	0.42
1:M:605:ILE:HD11	1:M:621:LEU:HD23	2.00	0.42
1:N:463:GLY:HA3	1:N:464:GLY:HA2	1.68	0.42
1:O:234:LYS:HD2	1:O:269:GLY:HA3	2.01	0.42
1:C:622:ARG:HA	1:C:625:MET:HB2	2.01	0.42
1:D:484:TYR:OH	1:D:504:GLY:O	2.34	0.42
1:I:366:GLN:HG2	1:I:445:ALA:HA	2.02	0.42
1:J:366:GLN:HG2	1:J:445:ALA:HA	2.02	0.42
1:M:70:ILE:HD13	1:N:41:ASP:HB2	2.01	0.42
1:O:605:ILE:HD11	1:O:621:LEU:HD23	2.00	0.42
1:P:605:ILE:HD11	1:P:621:LEU:HD23	2.00	0.42
1:A:366:GLN:HG2	1:A:445:ALA:HA	2.02	0.42
1:A:605:ILE:HD11	1:A:621:LEU:HD23	2.00	0.42
1:B:234:LYS:HD2	1:B:269:GLY:HA3	2.01	0.42
1:E:366:GLN:HG2	1:E:445:ALA:HA	2.02	0.42
1:E:622:ARG:HA	1:E:625:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLY:HA3	1:F:464:GLY:HA2	1.68	0.42
1:K:622:ARG:HA	1:K:625:MET:HB2	2.01	0.42
1:C:366:GLN:HG2	1:C:445:ALA:HA	2.02	0.42
1:L:622:ARG:HA	1:L:625:MET:HB2	2.01	0.42
1:M:234:LYS:HD2	1:M:269:GLY:HA3	2.01	0.42
1:M:463:GLY:HA3	1:M:464:GLY:HA2	1.68	0.42
1:P:126:ASP:OD1	1:P:126:ASP:N	2.51	0.42
1:A:126:ASP:OD1	1:A:126:ASP:N	2.51	0.42
1:C:234:LYS:HD2	1:C:269:GLY:HA3	2.01	0.42
1:F:596:THR:HG22	1:G:433:GLU:OE2	2.20	0.42
1:M:622:ARG:HA	1:M:625:MET:HB2	2.01	0.42
1:N:597:ASN:HB3	1:O:436:PHE:HB2	2.02	0.42
1:I:608:SER:HA	1:I:609:GLN:HA	1.72	0.42
1:J:622:ARG:HA	1:J:625:MET:HB2	2.01	0.42
1:L:472:ASN:O	1:L:476:ASN:N	2.53	0.42
1:M:472:ASN:O	1:M:476:ASN:N	2.53	0.42
1:N:366:GLN:HG2	1:N:445:ALA:HA	2.02	0.42
1:B:608:SER:HA	1:B:609:GLN:HA	1.72	0.42
1:F:234:LYS:HD2	1:F:269:GLY:HA3	2.01	0.42
1:I:234:LYS:HD2	1:I:269:GLY:HA3	2.01	0.42
1:M:366:GLN:HG2	1:M:445:ALA:HA	2.02	0.42
1:N:472:ASN:O	1:N:476:ASN:N	2.53	0.42
1:N:605:ILE:HD11	1:N:621:LEU:HD23	2.00	0.42
1:N:622:ARG:HA	1:N:625:MET:HB2	2.01	0.42
1:O:366:GLN:HG2	1:O:445:ALA:HA	2.02	0.42
1:O:442:GLU:OE2	1:O:444:ARG:NH1	2.47	0.42
1:G:366:GLN:HG2	1:G:445:ALA:HA	2.02	0.42
1:H:234:LYS:HD2	1:H:269:GLY:HA3	2.01	0.42
1:I:622:ARG:HA	1:I:625:MET:HB2	2.01	0.42
1:J:126:ASP:N	1:J:126:ASP:OD1	2.52	0.42
1:L:234:LYS:HD2	1:L:269:GLY:HA3	2.01	0.42
1:A:622:ARG:HA	1:A:625:MET:HB2	2.01	0.41
1:B:93:SER:O	1:B:136:ARG:NH1	2.48	0.41
1:B:622:ARG:HA	1:B:625:MET:HB2	2.01	0.41
1:C:472:ASN:O	1:C:476:ASN:N	2.53	0.41
1:K:472:ASN:O	1:K:476:ASN:N	2.53	0.41
1:G:442:GLU:OE2	1:G:444:ARG:NH1	2.47	0.41
1:H:364:VAL:HG21	1:H:489:LEU:HD11	2.02	0.41
1:H:366:GLN:HG2	1:H:445:ALA:HA	2.02	0.41
1:I:364:VAL:HG21	1:I:489:LEU:HD11	2.03	0.41
1:J:364:VAL:HG21	1:J:489:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:364:VAL:HG21	1:K:489:LEU:HD11	2.02	0.41
1:K:366:GLN:HG2	1:K:445:ALA:HA	2.02	0.41
1:O:472:ASN:O	1:O:476:ASN:N	2.53	0.41
1:O:622:ARG:HA	1:O:625:MET:HB2	2.01	0.41
1:E:73:LYS:HB2	1:F:262:GLY:HA2	2.03	0.41
1:P:622:ARG:HA	1:P:625:MET:HB2	2.01	0.41
1:A:93:SER:O	1:A:136:ARG:NH1	2.48	0.41
1:D:234:LYS:HD2	1:D:269:GLY:HA3	2.01	0.41
1:D:472:ASN:O	1:D:476:ASN:N	2.53	0.41
1:G:364:VAL:HG21	1:G:489:LEU:HD11	2.03	0.41
1:K:234:LYS:HD2	1:K:269:GLY:HA3	2.01	0.41
1:L:364:VAL:HG21	1:L:489:LEU:HD11	2.03	0.41
1:M:364:VAL:HG21	1:M:489:LEU:HD11	2.02	0.41
1:M:592:THR:HA	1:N:432:CYS:HB3	2.02	0.41
1:G:234:LYS:HD2	1:G:269:GLY:HA3	2.01	0.41
1:D:608:SER:HA	1:D:609:GLN:HA	1.72	0.41
1:G:126:ASP:N	1:G:126:ASP:OD1	2.52	0.41
1:H:622:ARG:HA	1:H:625:MET:HB2	2.01	0.41
1:J:472:ASN:O	1:J:476:ASN:N	2.53	0.41
1:M:442:GLU:OE2	1:M:444:ARG:NH1	2.47	0.41
1:N:364:VAL:HG21	1:N:489:LEU:HD11	2.02	0.41
1:E:472:ASN:O	1:E:476:ASN:N	2.53	0.41
1:F:364:VAL:HG21	1:F:489:LEU:HD11	2.02	0.41
1:F:622:ARG:HA	1:F:625:MET:HB2	2.01	0.41
1:G:622:ARG:HA	1:G:625:MET:HB2	2.01	0.41
1:L:366:GLN:HG2	1:L:445:ALA:HA	2.02	0.41
1:P:472:ASN:O	1:P:476:ASN:N	2.53	0.41
1:H:463:GLY:HA3	1:H:464:GLY:HA2	1.68	0.41
1:L:571:LEU:HA	1:L:572:PRO:HD3	1.96	0.41
1:D:366:GLN:HG2	1:D:445:ALA:HA	2.02	0.41
1:D:622:ARG:HA	1:D:625:MET:HB2	2.01	0.41
1:E:234:LYS:HD2	1:E:269:GLY:HA3	2.01	0.41
1:F:460:LEU:HB3	1:F:461:LEU:H	1.76	0.41
1:G:72:GLN:O	1:H:284:VAL:HG11	2.20	0.41
1:I:472:ASN:O	1:I:476:ASN:N	2.53	0.41
1:L:550:LEU:HD23	1:L:552:SER:HB3	2.03	0.41
1:M:550:LEU:HD23	1:M:552:SER:HB3	2.03	0.41
1:M:592:THR:HG22	1:N:432:CYS:SG	2.61	0.41
1:N:550:LEU:HD23	1:N:552:SER:HB3	2.03	0.41
1:O:93:SER:O	1:O:136:ARG:NH1	2.48	0.41
1:O:364:VAL:HG21	1:O:489:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:93:SER:O	1:P:136:ARG:NH1	2.48	0.41
1:P:366:GLN:HG2	1:P:445:ALA:HA	2.02	0.41
1:E:364:VAL:HG21	1:E:489:LEU:HD11	2.03	0.41
1:F:472:ASN:O	1:F:476:ASN:N	2.53	0.41
1:H:36:ASN:HD22	1:H:36:ASN:HA	1.61	0.41
1:J:234:LYS:HD2	1:J:269:GLY:HA3	2.01	0.41
1:K:460:LEU:HB3	1:K:461:LEU:H	1.75	0.41
1:P:364:VAL:HG21	1:P:489:LEU:HD11	2.02	0.41
1:H:472:ASN:O	1:H:476:ASN:N	2.53	0.40
1:K:550:LEU:HD23	1:K:552:SER:HB3	2.03	0.40
1:G:472:ASN:O	1:G:476:ASN:N	2.53	0.40
1:H:608:SER:HA	1:H:609:GLN:HA	1.72	0.40
1:N:608:SER:HA	1:N:609:GLN:HA	1.72	0.40
1:O:550:LEU:HD23	1:O:552:SER:HB3	2.03	0.40
1:A:364:VAL:HG21	1:A:489:LEU:HD11	2.03	0.40
1:E:550:LEU:HD23	1:E:552:SER:HB3	2.03	0.40
1:P:550:LEU:HD23	1:P:552:SER:HB3	2.03	0.40
1:A:70:ILE:HD13	1:B:41:ASP:HB2	2.04	0.40
1:A:195:GLY:HA2	1:A:283:LEU:HD22	2.03	0.40
1:A:472:ASN:O	1:A:476:ASN:N	2.53	0.40
1:C:484:TYR:OH	1:C:504:GLY:O	2.34	0.40
1:F:550:LEU:HD23	1:F:552:SER:HB3	2.03	0.40
1:J:442:GLU:OE2	1:J:444:ARG:NH1	2.47	0.40
1:J:463:GLY:HA3	1:J:464:GLY:HA2	1.68	0.40
1:J:550:LEU:HD23	1:J:552:SER:HB3	2.03	0.40
1:A:442:GLU:OE2	1:A:444:ARG:NH1	2.47	0.40
1:B:364:VAL:HG21	1:B:489:LEU:HD11	2.03	0.40
1:E:75:SER:HB3	1:F:260:SER:HB3	2.03	0.40
1:M:571:LEU:HA	1:M:572:PRO:HD3	1.96	0.40
1:N:195:GLY:HA2	1:N:283:LEU:HD22	2.04	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	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	B	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	C	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	D	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	E	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	F	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	G	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	H	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	I	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	J	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	K	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	L	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	M	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	N	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	O	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
1	P	561/642 (87%)	534 (95%)	27 (5%)	0	100 100
All	All	8976/10272 (87%)	8544 (95%)	432 (5%)	0	100 100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	491/562 (87%)	487 (99%)	4 (1%)	81 91
1	B	491/562 (87%)	487 (99%)	4 (1%)	81 91
1	C	491/562 (87%)	487 (99%)	4 (1%)	81 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	E	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	F	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	G	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	H	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	I	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	J	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	K	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	L	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	M	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	N	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	O	491/562 (87%)	487 (99%)	4 (1%)	81	91
1	P	491/562 (87%)	487 (99%)	4 (1%)	81	91
All	All	7856/8992 (87%)	7792 (99%)	64 (1%)	82	91

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	257	ARG
1	A	414	ASN
1	A	587	GLN
1	B	36	ASN
1	B	257	ARG
1	B	414	ASN
1	B	587	GLN
1	C	36	ASN
1	C	257	ARG
1	C	414	ASN
1	C	587	GLN
1	D	36	ASN
1	D	257	ARG
1	D	414	ASN
1	D	587	GLN
1	E	36	ASN
1	E	257	ARG
1	E	414	ASN

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Mol	Chain	Res	Type
1	E	587	GLN
1	F	36	ASN
1	F	257	ARG
1	F	414	ASN
1	F	587	GLN
1	G	36	ASN
1	G	257	ARG
1	G	414	ASN
1	G	587	GLN
1	H	36	ASN
1	H	257	ARG
1	H	414	ASN
1	H	587	GLN
1	I	36	ASN
1	I	257	ARG
1	I	414	ASN
1	I	587	GLN
1	J	36	ASN
1	J	257	ARG
1	J	414	ASN
1	J	587	GLN
1	K	36	ASN
1	K	257	ARG
1	K	414	ASN
1	K	587	GLN
1	L	36	ASN
1	L	257	ARG
1	L	414	ASN
1	L	587	GLN
1	M	36	ASN
1	M	257	ARG
1	M	414	ASN
1	M	587	GLN
1	N	36	ASN
1	N	257	ARG
1	N	414	ASN
1	N	587	GLN
1	O	36	ASN
1	O	257	ARG
1	O	414	ASN
1	O	587	GLN
1	P	36	ASN

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Mol	Chain	Res	Type
1	P	257	ARG
1	P	414	ASN
1	P	587	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	99	ASN
1	A	137	ASN
1	A	187	HIS
1	A	203	HIS
1	A	366	GLN
1	A	387	ASN
1	A	414	ASN
1	A	478	GLN
1	B	36	ASN
1	B	99	ASN
1	B	187	HIS
1	B	203	HIS
1	B	366	GLN
1	B	387	ASN
1	B	414	ASN
1	C	36	ASN
1	C	99	ASN
1	C	187	HIS
1	C	203	HIS
1	C	366	GLN
1	C	387	ASN
1	C	414	ASN
1	D	36	ASN
1	D	99	ASN
1	D	187	HIS
1	D	203	HIS
1	D	366	GLN
1	D	387	ASN
1	D	414	ASN
1	E	36	ASN
1	E	99	ASN
1	E	137	ASN
1	E	187	HIS
1	E	203	HIS

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Mol	Chain	Res	Type
1	E	366	GLN
1	E	387	ASN
1	E	414	ASN
1	F	36	ASN
1	F	99	ASN
1	F	187	HIS
1	F	203	HIS
1	F	366	GLN
1	F	387	ASN
1	F	414	ASN
1	G	36	ASN
1	G	99	ASN
1	G	137	ASN
1	G	187	HIS
1	G	203	HIS
1	G	366	GLN
1	G	387	ASN
1	G	414	ASN
1	H	36	ASN
1	H	99	ASN
1	H	187	HIS
1	H	203	HIS
1	H	366	GLN
1	H	387	ASN
1	H	414	ASN
1	I	36	ASN
1	I	99	ASN
1	I	137	ASN
1	I	187	HIS
1	I	203	HIS
1	I	366	GLN
1	I	387	ASN
1	I	414	ASN
1	J	36	ASN
1	J	99	ASN
1	J	187	HIS
1	J	203	HIS
1	J	366	GLN
1	J	387	ASN
1	J	414	ASN
1	K	36	ASN
1	K	99	ASN

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Mol	Chain	Res	Type
1	K	187	HIS
1	K	203	HIS
1	K	366	GLN
1	K	387	ASN
1	K	414	ASN
1	L	36	ASN
1	L	99	ASN
1	L	187	HIS
1	L	203	HIS
1	L	366	GLN
1	L	387	ASN
1	L	414	ASN
1	M	36	ASN
1	M	99	ASN
1	M	187	HIS
1	M	203	HIS
1	M	366	GLN
1	M	387	ASN
1	M	414	ASN
1	N	36	ASN
1	N	99	ASN
1	N	187	HIS
1	N	203	HIS
1	N	366	GLN
1	N	387	ASN
1	N	414	ASN
1	O	36	ASN
1	O	99	ASN
1	O	137	ASN
1	O	187	HIS
1	O	203	HIS
1	O	366	GLN
1	O	387	ASN
1	O	414	ASN
1	O	478	GLN
1	P	36	ASN
1	P	99	ASN
1	P	187	HIS
1	P	203	HIS
1	P	366	GLN
1	P	387	ASN
1	P	414	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

32 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	0.62	0	17,19,21	0.83	1 (5%)
2	NAG	Q	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
2	NAG	R	2	2	14,14,15	0.49	0	17,19,21	0.95	1 (5%)
2	NAG	S	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	S	2	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
2	NAG	T	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	T	2	2	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
2	NAG	U	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	U	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	V	1	1,2	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
2	NAG	V	2	2	14,14,15	0.50	0	17,19,21	0.96	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	W	2	2	14,14,15	0.49	0	17,19,21	0.95	1 (5%)
2	NAG	X	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	X	2	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
2	NAG	Y	1	1,2	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
2	NAG	Y	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	Z	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	Z	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	a	1	1,2	14,14,15	0.63	0	17,19,21	0.83	1 (5%)
2	NAG	a	2	2	14,14,15	0.47	0	17,19,21	0.96	1 (5%)
2	NAG	b	1	1,2	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
2	NAG	b	2	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
2	NAG	c	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	c	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	d	1	1,2	14,14,15	0.62	0	17,19,21	0.83	1 (5%)
2	NAG	d	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	e	1	1,2	14,14,15	0.63	0	17,19,21	0.82	1 (5%)
2	NAG	e	2	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
2	NAG	f	1	1,2	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
2	NAG	f	2	2	14,14,15	0.47	0	17,19,21	0.96	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	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	3/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	3/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	3/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	3/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	3/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	3/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	3/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	3/6/23/26	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	3/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	3/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	3/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	3/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	3/6/23/26	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	Y	2	NAG	C2-N2-C7	3.14	127.38	122.90
2	X	2	NAG	C2-N2-C7	3.14	127.37	122.90
2	T	2	NAG	C2-N2-C7	3.14	127.37	122.90
2	S	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	c	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	b	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	d	2	NAG	C2-N2-C7	3.13	127.36	122.90
2	f	2	NAG	C2-N2-C7	3.12	127.35	122.90
2	e	2	NAG	C2-N2-C7	3.12	127.35	122.90
2	a	2	NAG	C2-N2-C7	3.11	127.34	122.90
2	V	2	NAG	C2-N2-C7	3.11	127.33	122.90
2	Z	2	NAG	C2-N2-C7	3.10	127.32	122.90
2	Q	2	NAG	C2-N2-C7	3.10	127.31	122.90
2	W	2	NAG	C2-N2-C7	3.10	127.31	122.90
2	U	2	NAG	C2-N2-C7	3.09	127.31	122.90
2	R	2	NAG	C2-N2-C7	3.09	127.30	122.90
2	R	1	NAG	C1-O5-C5	2.93	116.16	112.19
2	d	1	NAG	C1-O5-C5	2.91	116.14	112.19
2	Q	1	NAG	C1-O5-C5	2.91	116.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	1	NAG	C1-O5-C5	2.90	116.13	112.19
2	Z	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	X	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	a	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	c	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	S	1	NAG	C1-O5-C5	2.89	116.11	112.19
2	V	1	NAG	C1-O5-C5	2.89	116.10	112.19
2	U	1	NAG	C1-O5-C5	2.88	116.10	112.19
2	f	1	NAG	C1-O5-C5	2.88	116.10	112.19
2	e	1	NAG	C1-O5-C5	2.88	116.09	112.19
2	b	1	NAG	C1-O5-C5	2.88	116.09	112.19
2	T	1	NAG	C1-O5-C5	2.88	116.09	112.19
2	Y	1	NAG	C1-O5-C5	2.86	116.07	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	U	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
2	e	2	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6

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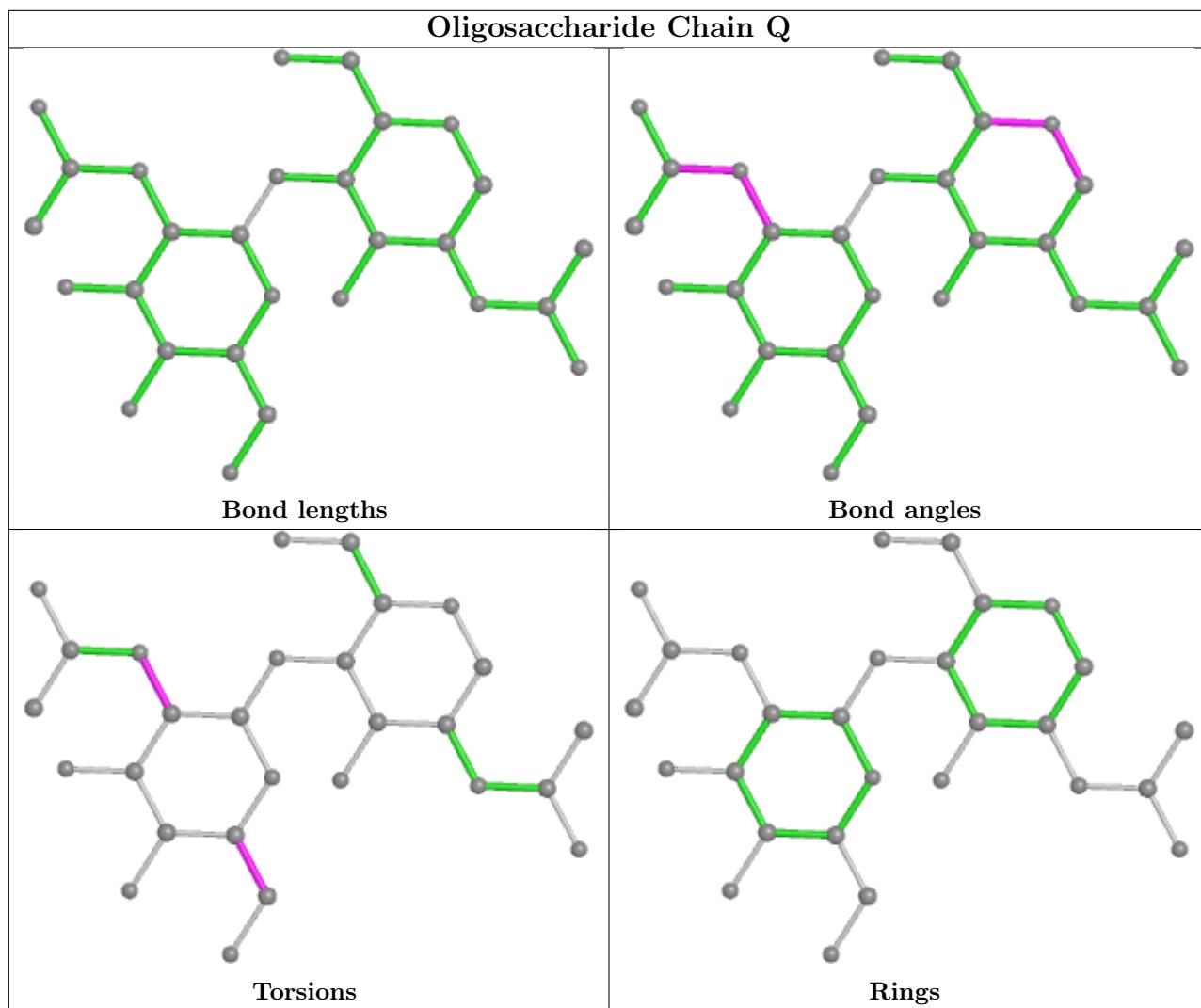
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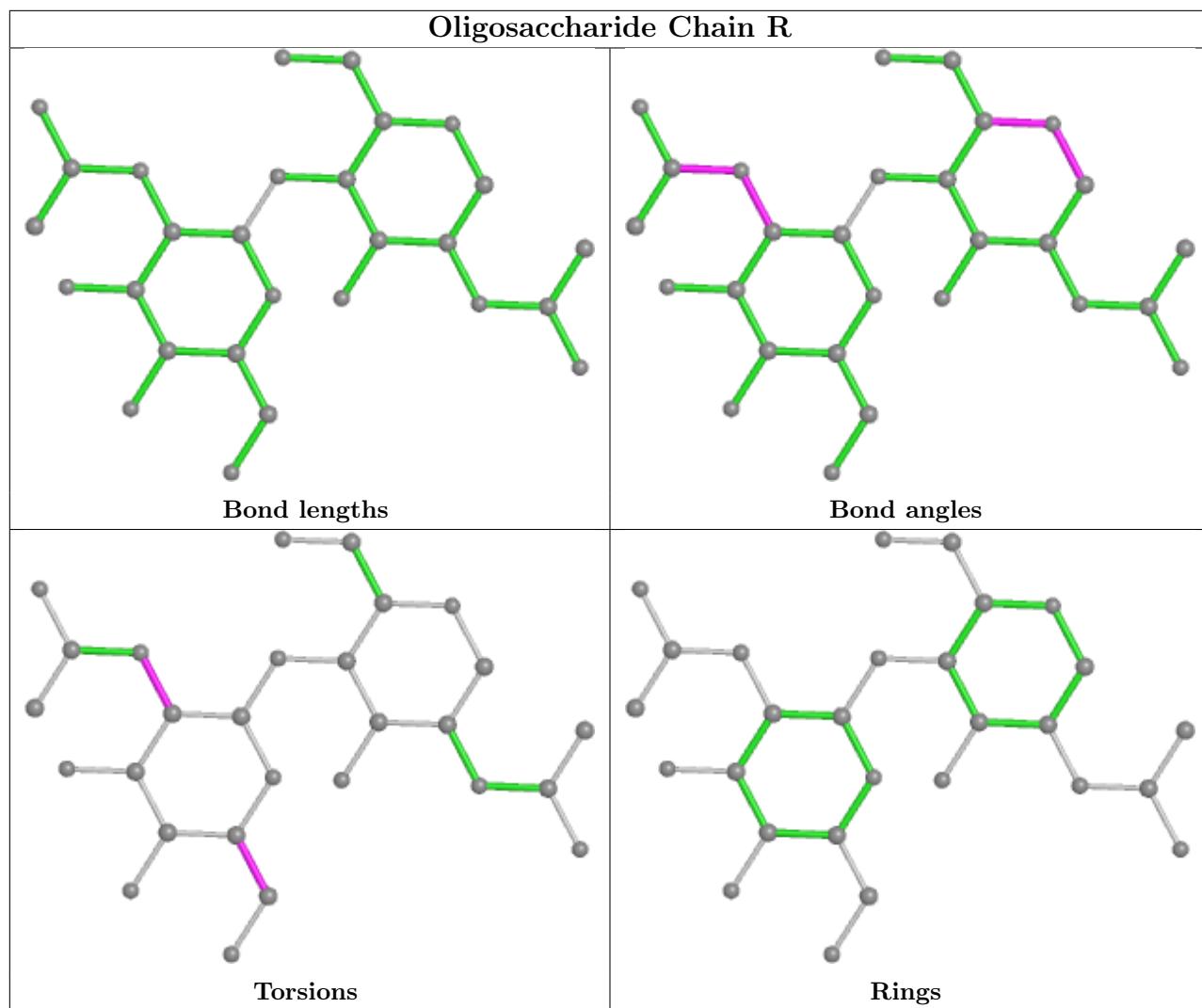
Mol	Chain	Res	Type	Atoms
2	Y	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C3-C2-N2-C7
2	R	2	NAG	C3-C2-N2-C7
2	S	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C3-C2-N2-C7
2	U	2	NAG	C3-C2-N2-C7
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

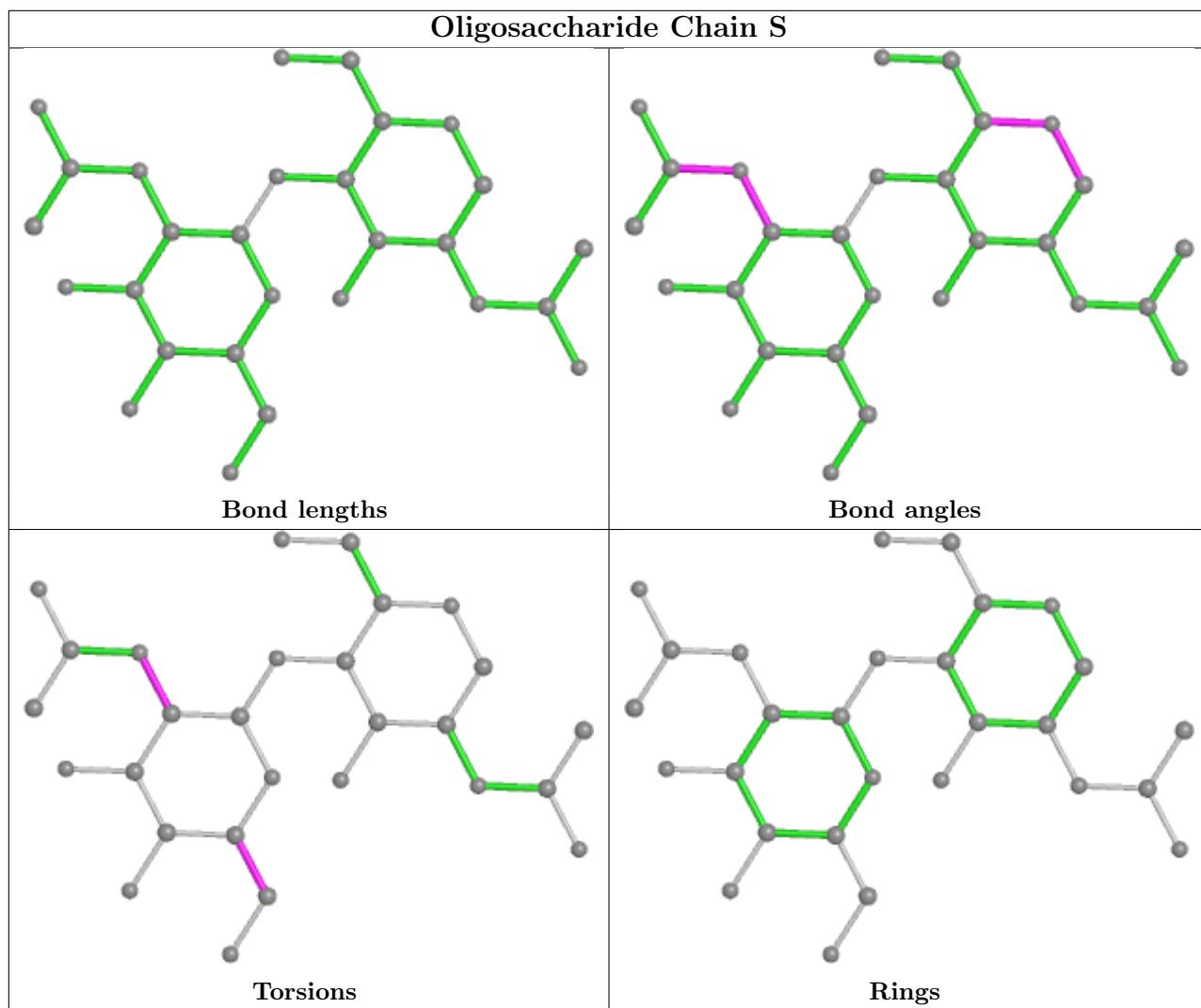
There are no ring outliers.

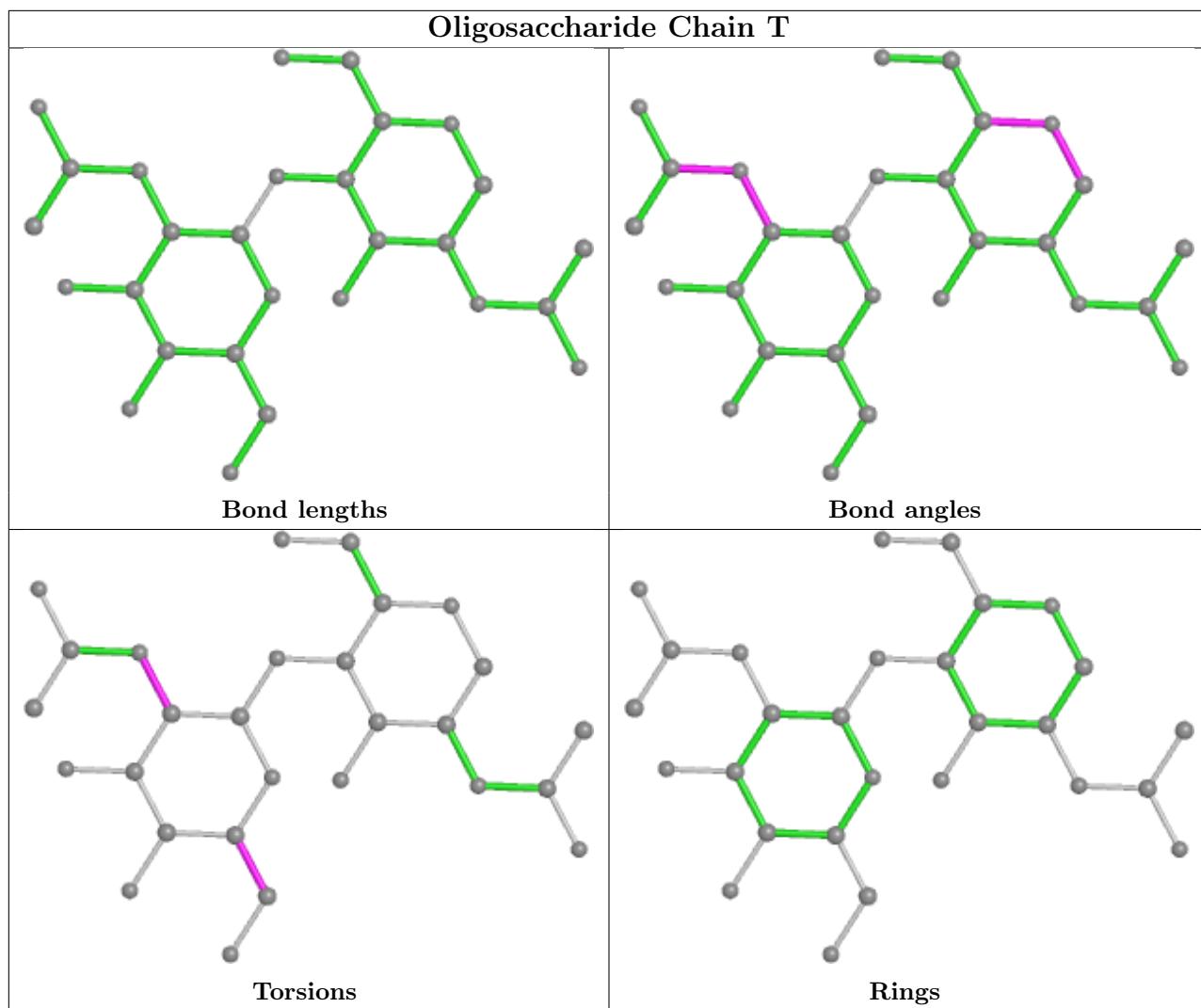
No monomer is involved in short contacts.

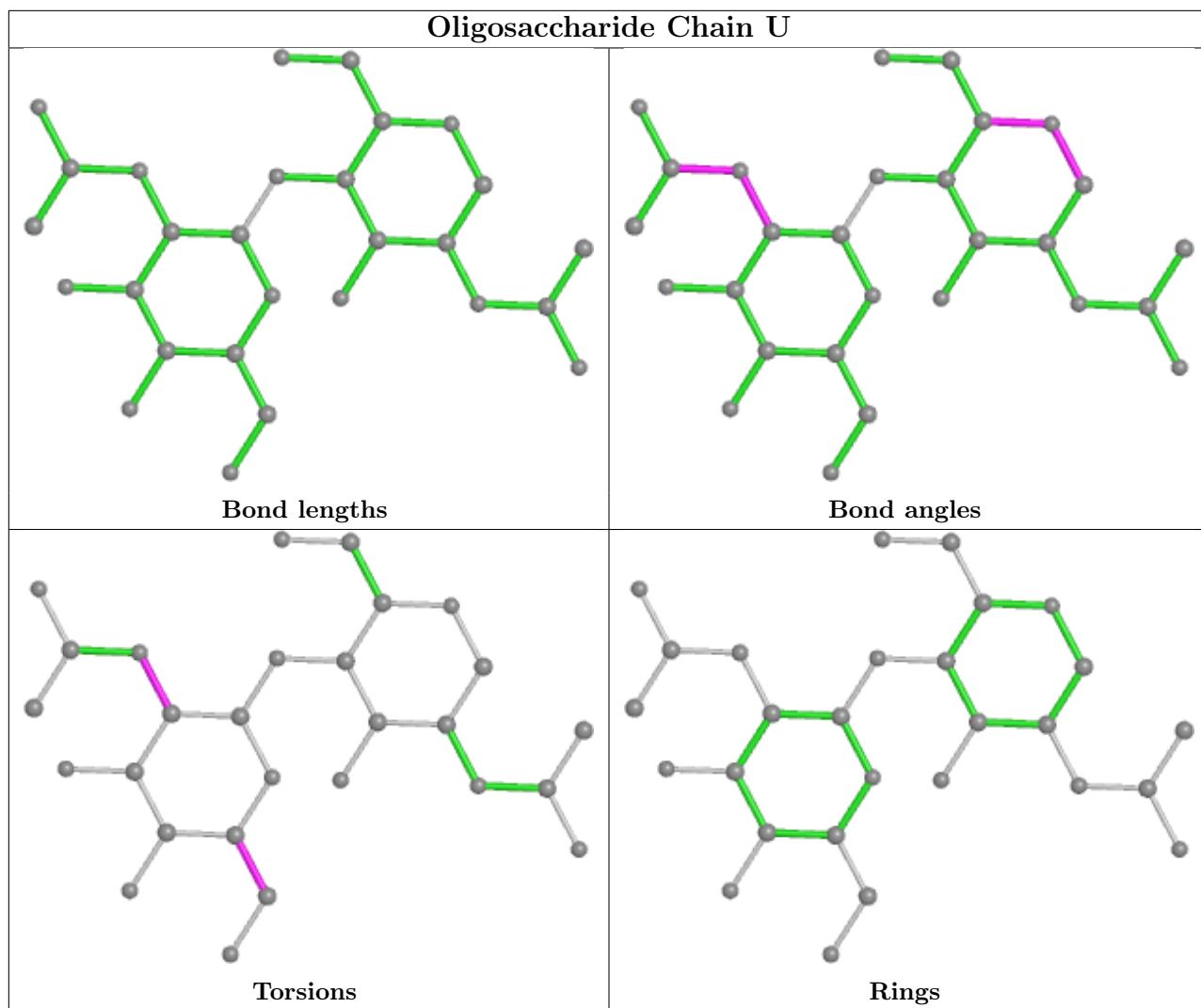
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

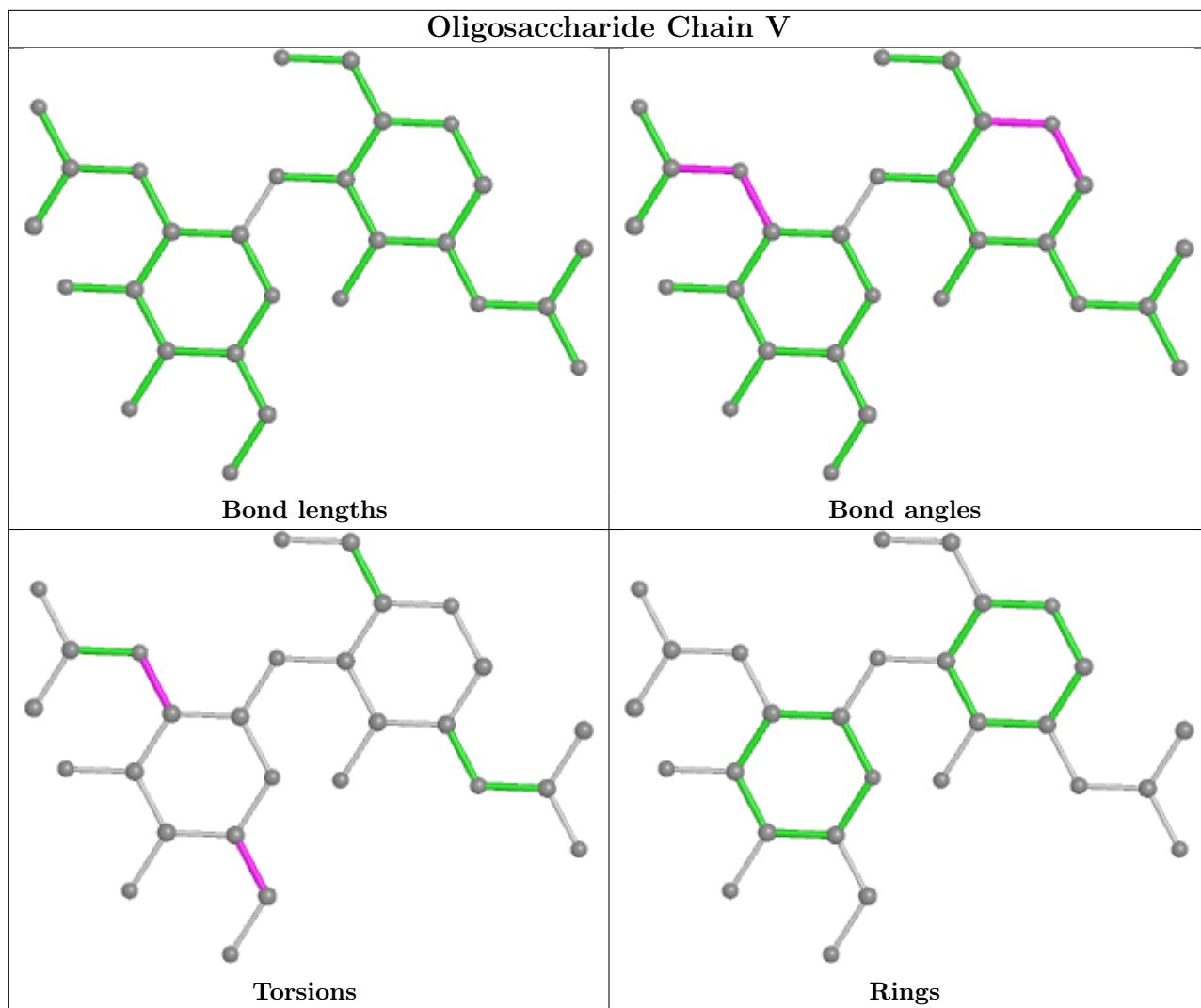


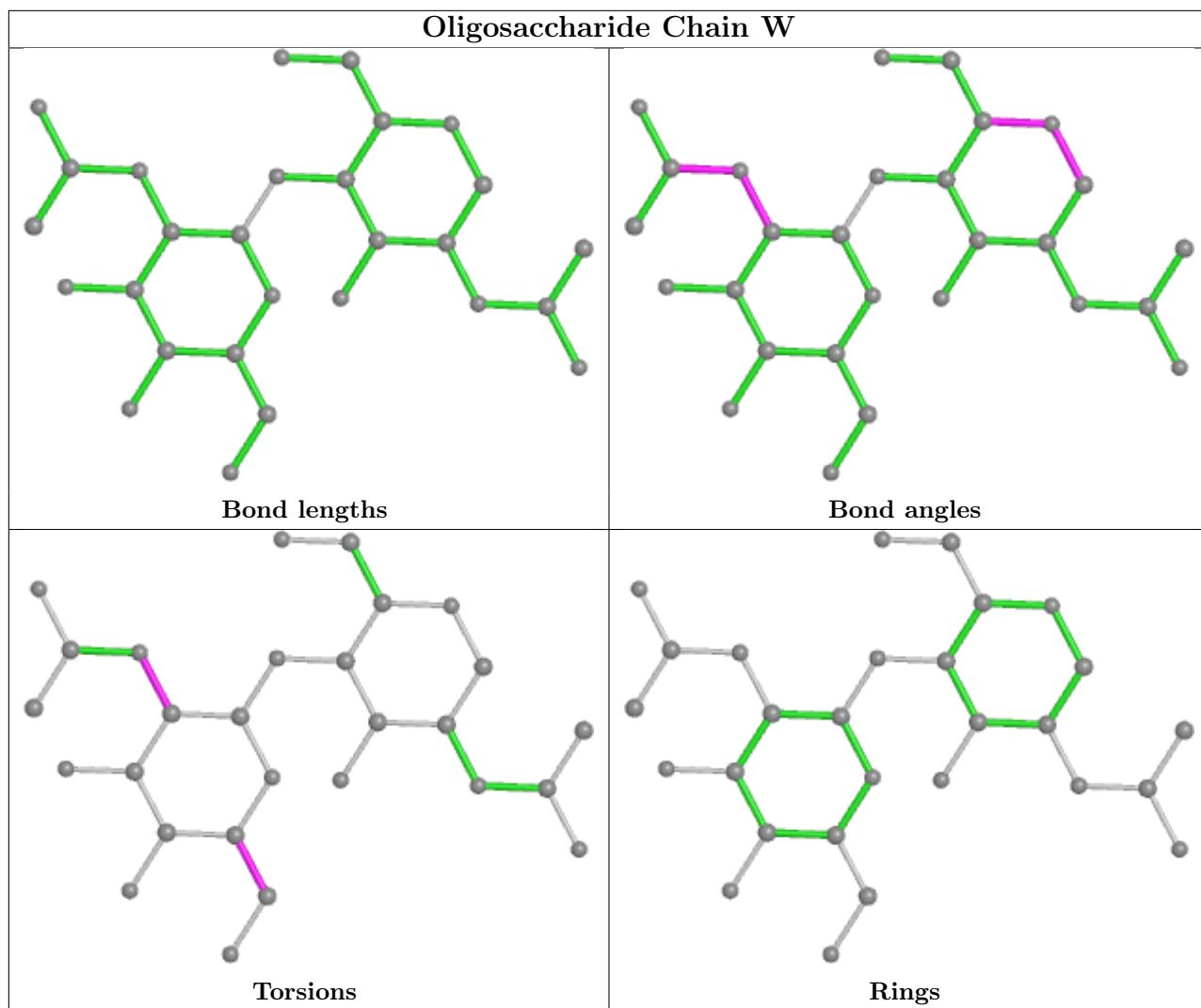


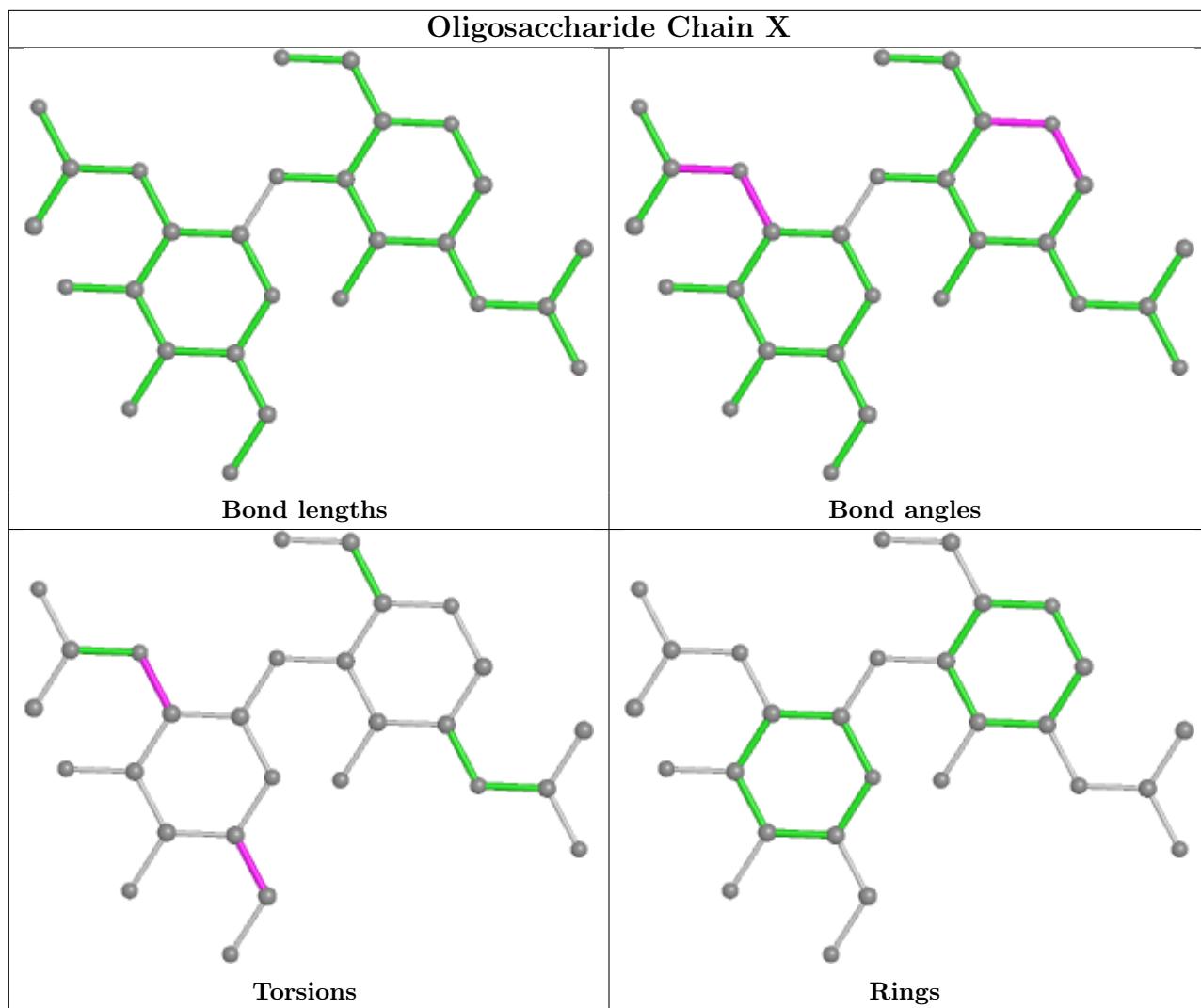


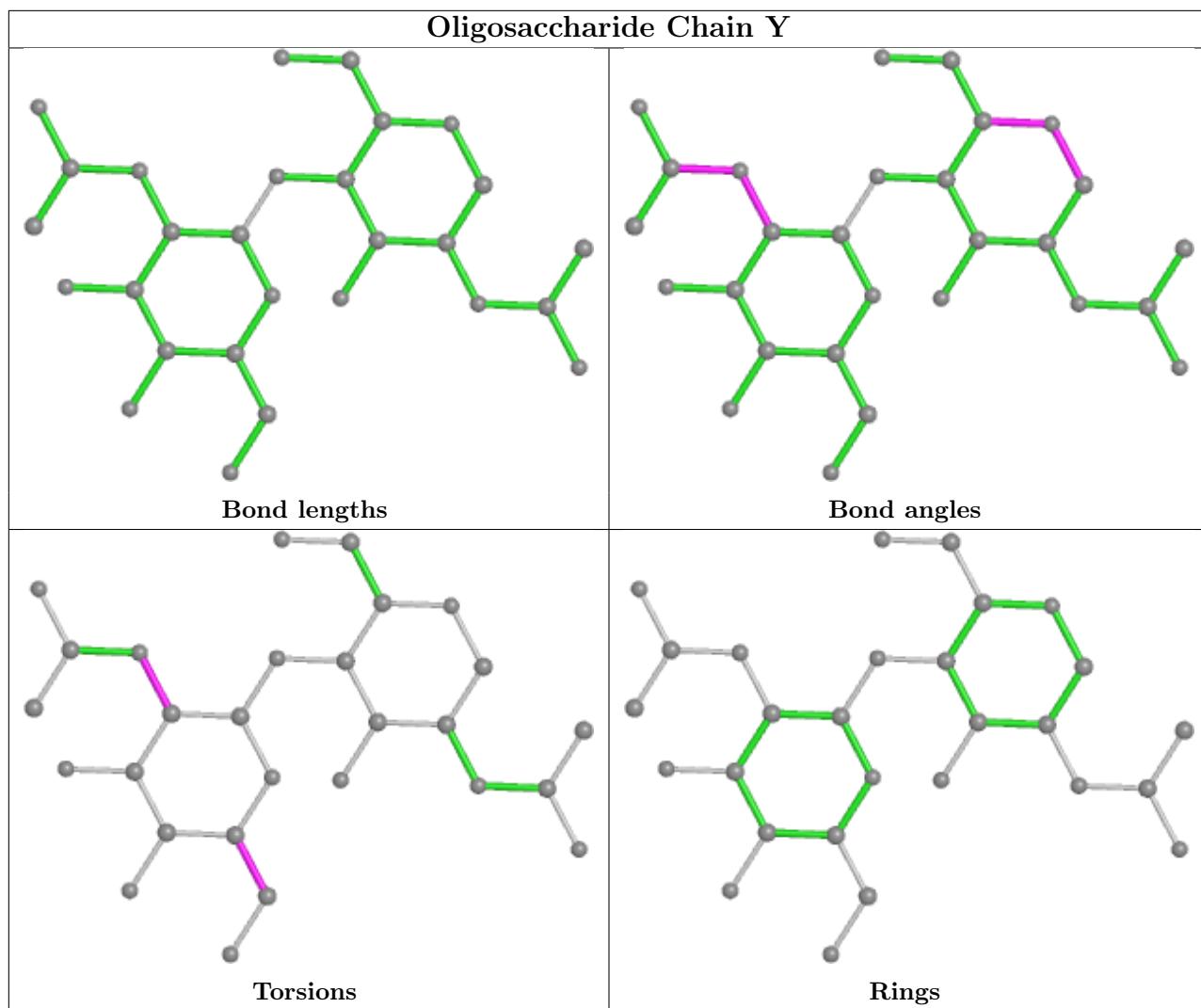


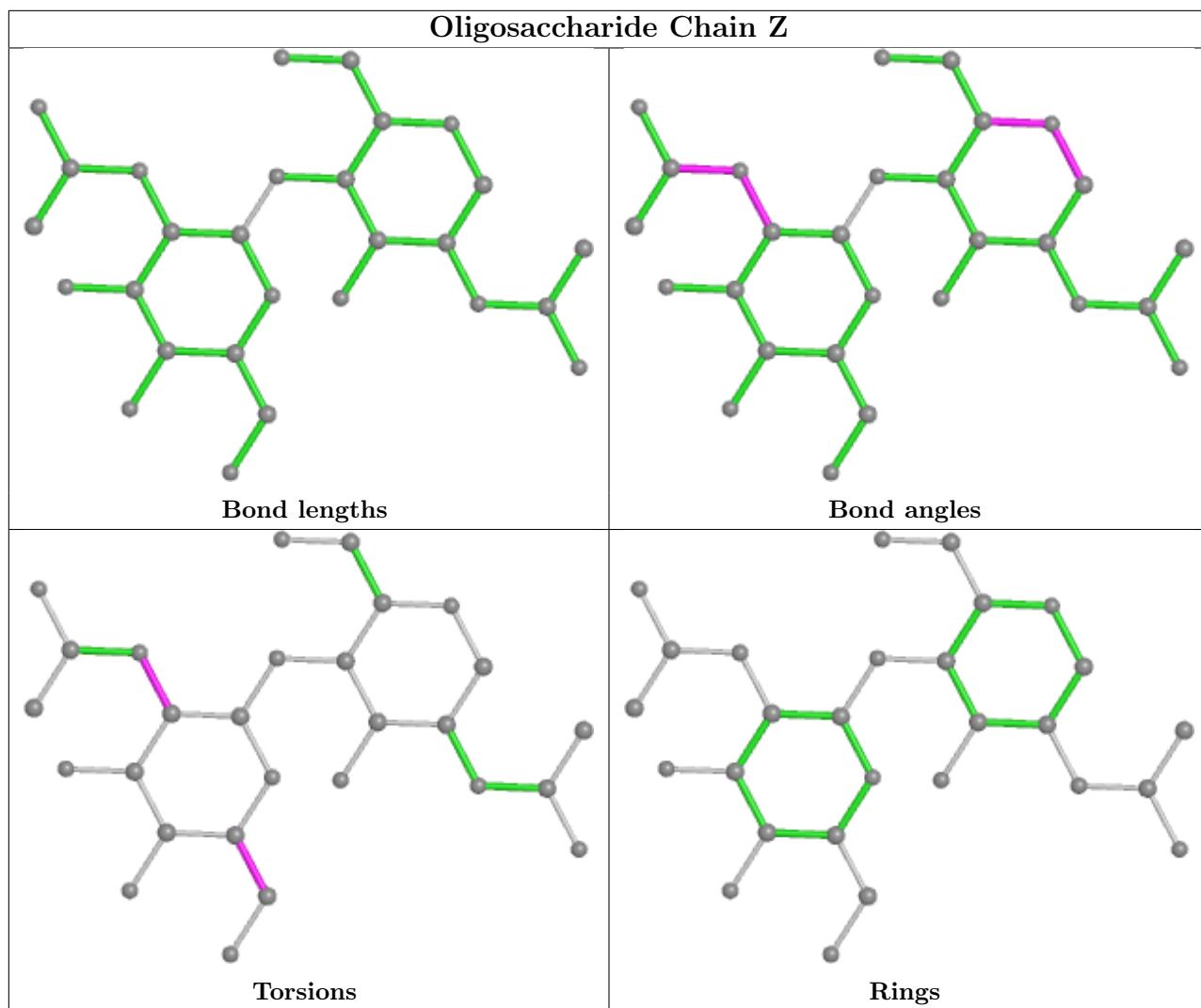


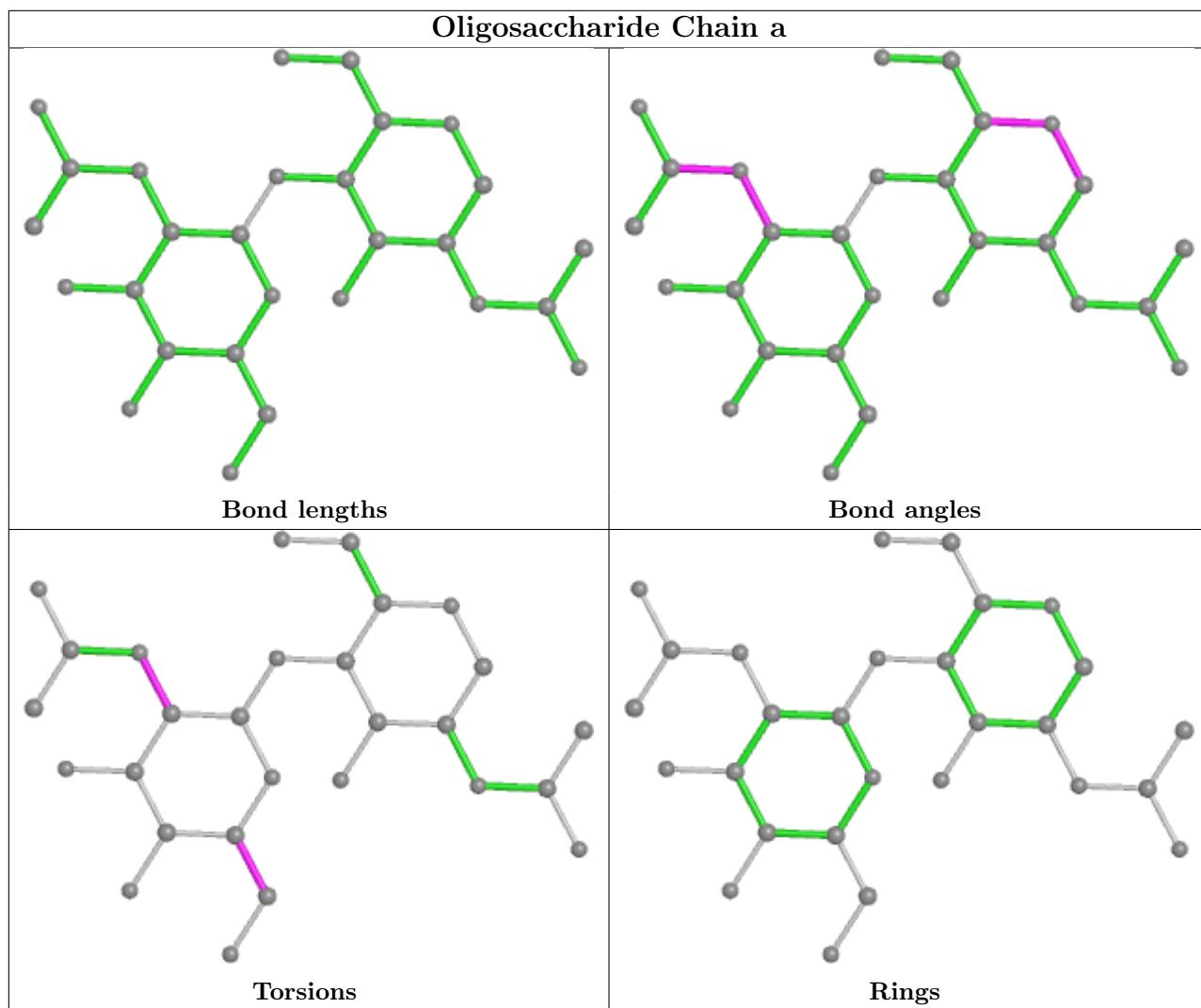


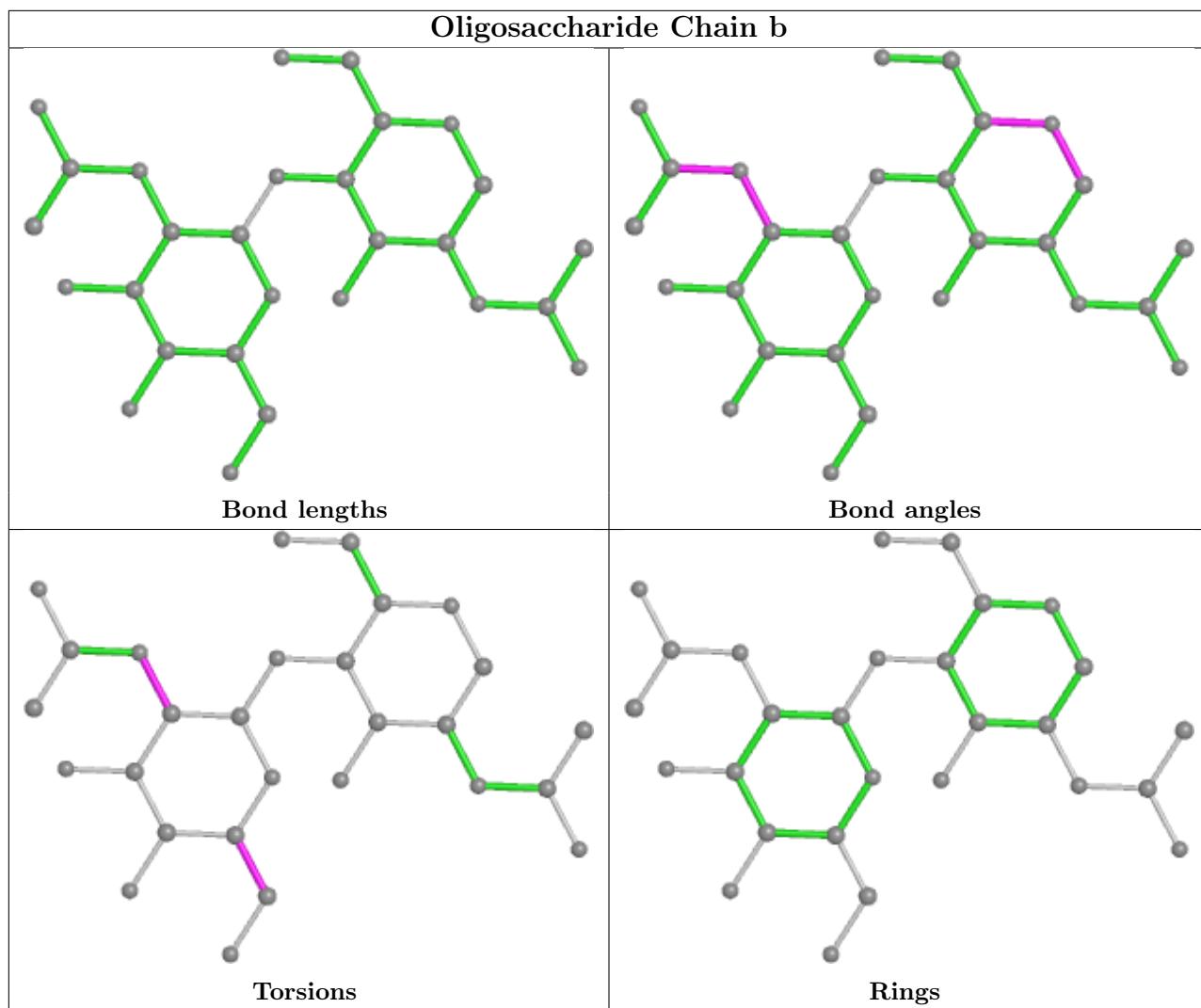


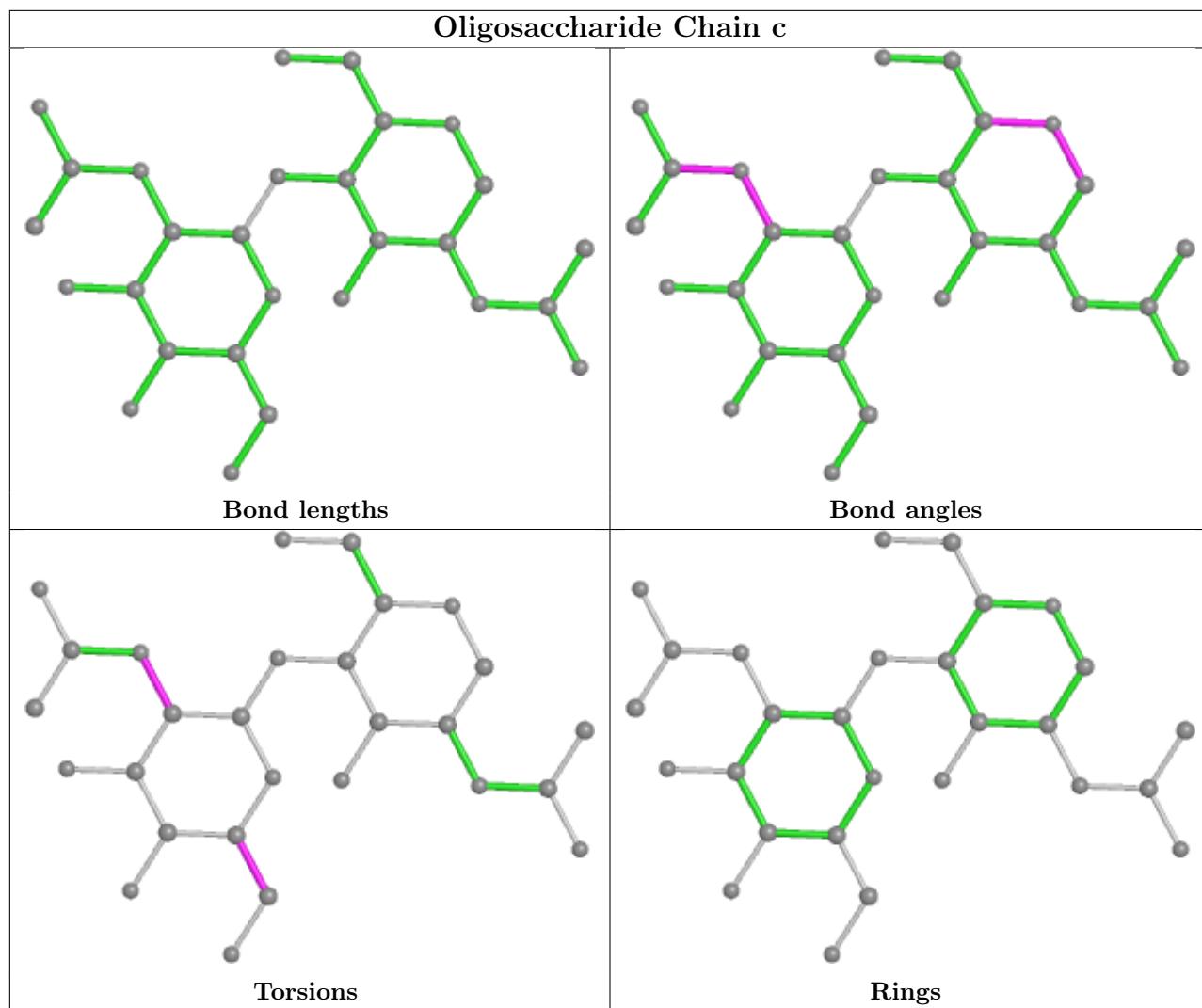


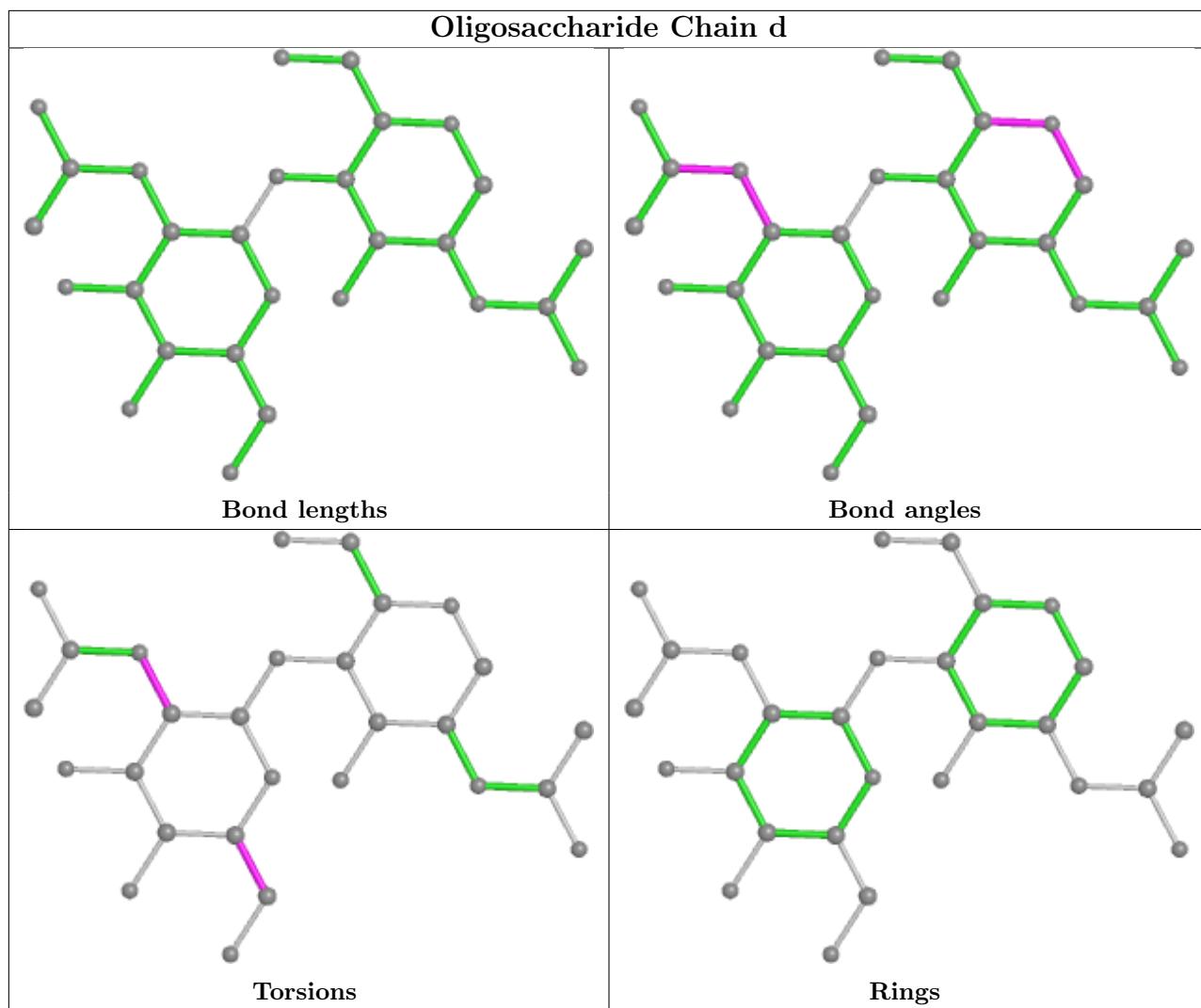


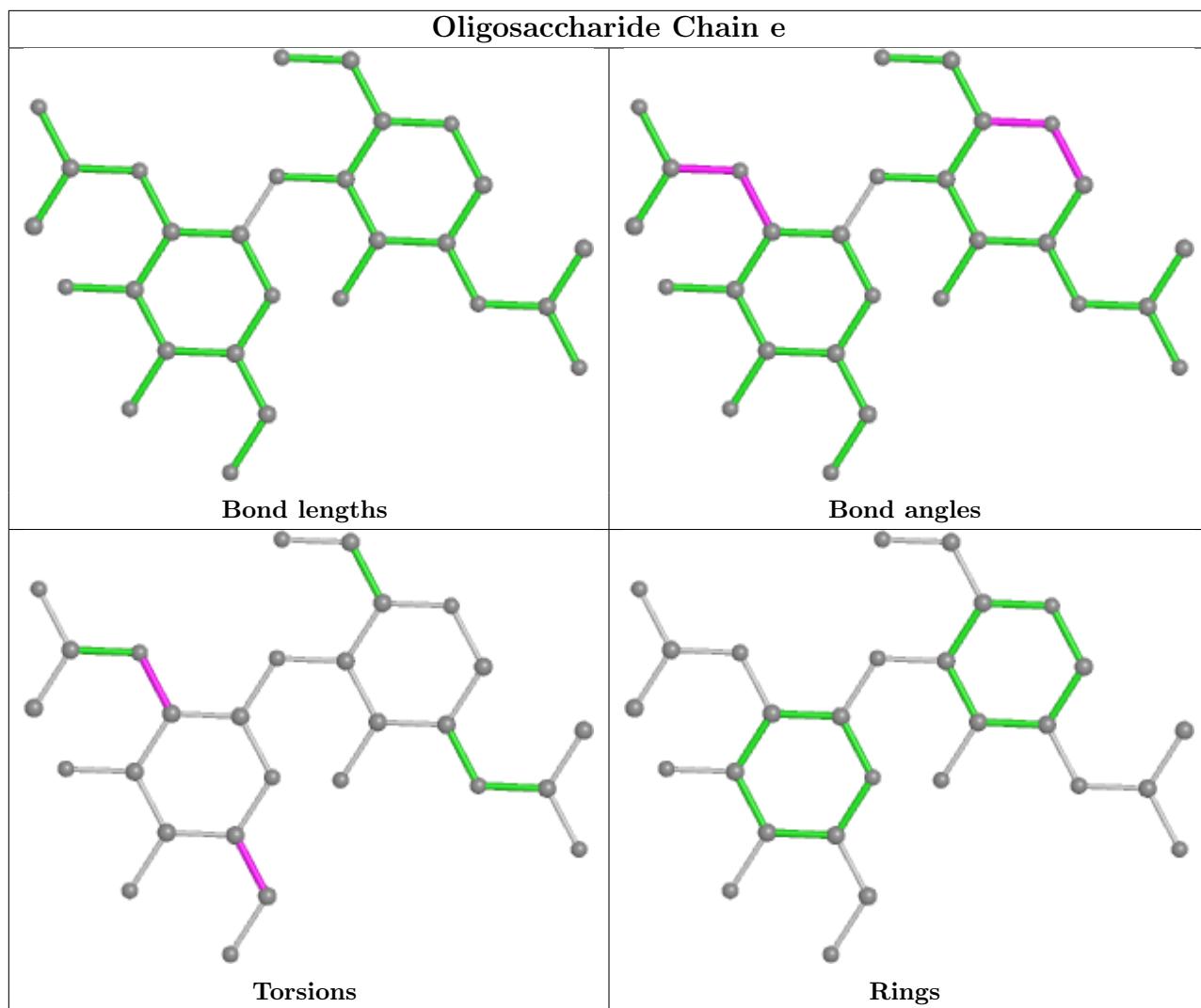


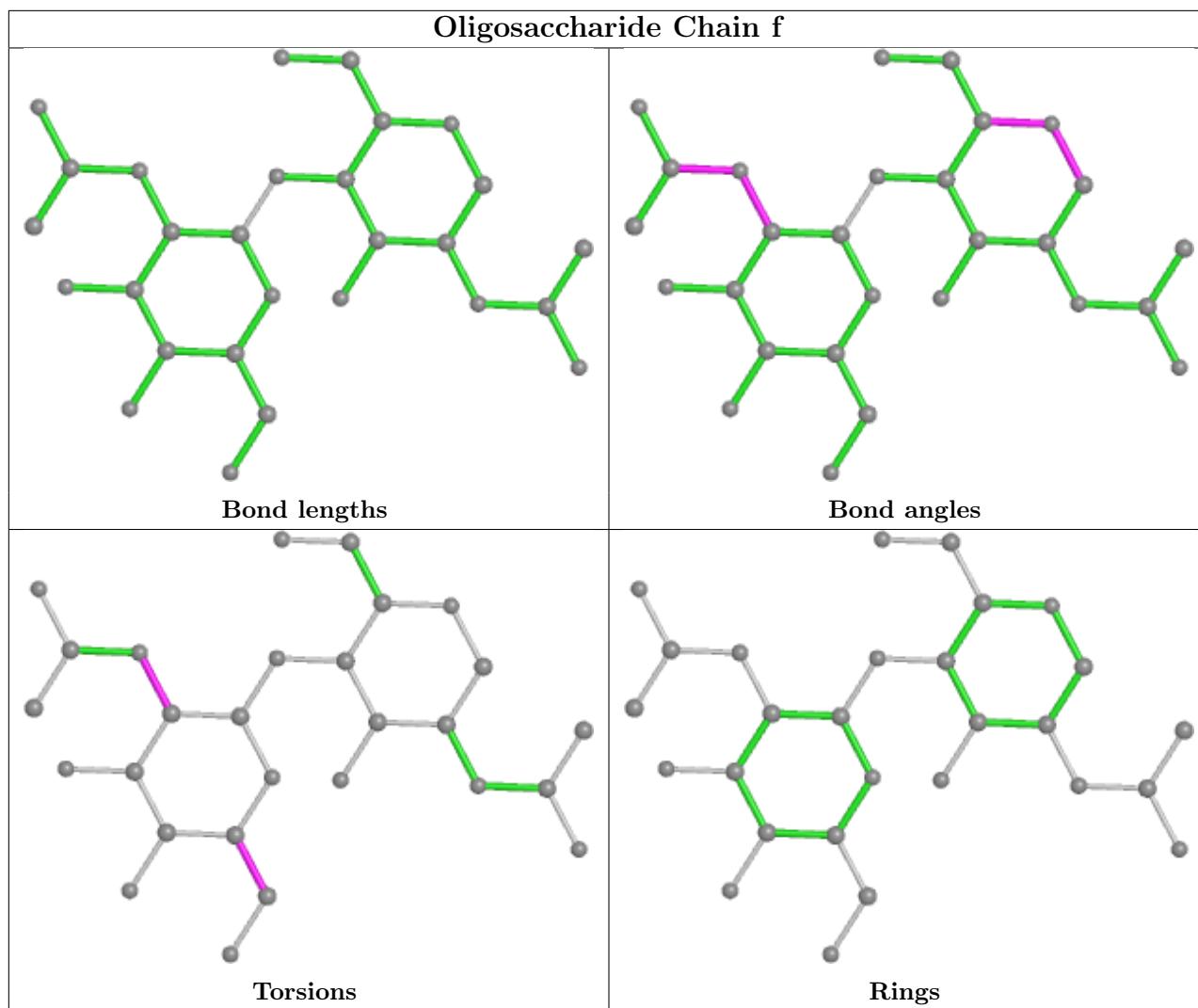












## 5.6 Ligand geometry (i)

16 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	F	701	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	I	701	1	14,14,15	0.31	0	17,19,21	0.56	0
3	NAG	M	701	1	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	O	701	1	14,14,15	0.31	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	P	701	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	E	701	1	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	N	701	1	14,14,15	0.30	0	17,19,21	0.55	0
3	NAG	D	701	1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	L	701	1	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	G	701	1	14,14,15	0.31	0	17,19,21	0.56	0
3	NAG	H	701	1	14,14,15	0.31	0	17,19,21	0.56	0
3	NAG	J	701	1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	K	701	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	C	701	1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	A	701	1	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	B	701	1	14,14,15	0.31	0	17,19,21	0.55	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	F	701	1	-	2/6/23/26	0/1/1/1
3	NAG	I	701	1	-	2/6/23/26	0/1/1/1
3	NAG	M	701	1	-	2/6/23/26	0/1/1/1
3	NAG	O	701	1	-	2/6/23/26	0/1/1/1
3	NAG	P	701	1	-	2/6/23/26	0/1/1/1
3	NAG	E	701	1	-	2/6/23/26	0/1/1/1
3	NAG	N	701	1	-	2/6/23/26	0/1/1/1
3	NAG	D	701	1	-	2/6/23/26	0/1/1/1
3	NAG	L	701	1	-	2/6/23/26	0/1/1/1
3	NAG	G	701	1	-	2/6/23/26	0/1/1/1
3	NAG	H	701	1	-	2/6/23/26	0/1/1/1
3	NAG	J	701	1	-	2/6/23/26	0/1/1/1
3	NAG	K	701	1	-	2/6/23/26	0/1/1/1
3	NAG	C	701	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	B	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	O5-C5-C6-O6
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	F	701	NAG	C4-C5-C6-O6
3	I	701	NAG	C4-C5-C6-O6
3	K	701	NAG	C4-C5-C6-O6
3	G	701	NAG	C4-C5-C6-O6
3	C	701	NAG	C4-C5-C6-O6
3	J	701	NAG	C4-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	L	701	NAG	C4-C5-C6-O6
3	D	701	NAG	C4-C5-C6-O6
3	E	701	NAG	C4-C5-C6-O6
3	H	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	A	701	NAG	C4-C5-C6-O6

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-20620. 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 [\(i\)](#)

This section was not generated.

### 6.2 Central slices [\(i\)](#)

This section was not generated.

### 6.3 Largest variance slices [\(i\)](#)

This section was not generated.

### 6.4 Orthogonal surface views [\(i\)](#)

This section was not generated.

### 6.5 Mask visualisation [\(i\)](#)

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

## 7 Map analysis [\(i\)](#)

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

### 7.1 Map-value distribution [\(i\)](#)

This section was not generated.

### 7.2 Volume estimate versus contour level [\(i\)](#)

This section was not generated.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit [\(i\)](#)

This section was not generated.