



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:38 PM UTC

PDB ID : 4N5Z / pdb_00004n5z
Title : Crystal structure of aerosol transmissible influenza H5 hemagglutinin mutant (N158D, N224K, Q226L and T318I) from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-10-10
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

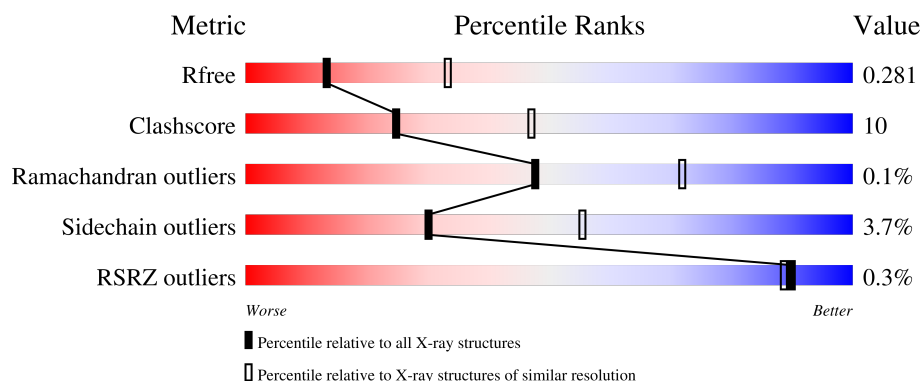
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	 71% 24% . .
1	C	334	 71% 24% . .
1	E	334	 71% 24% . .
1	G	334	 74% 21% . .
1	I	334	 67% 26% . .

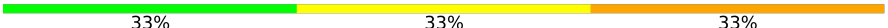
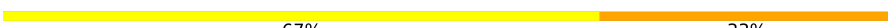
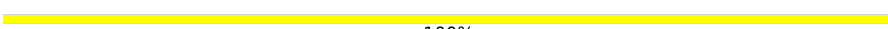
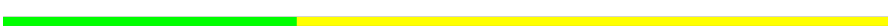
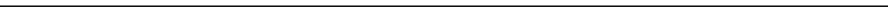
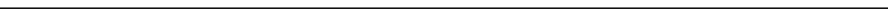
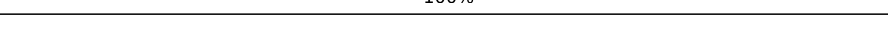
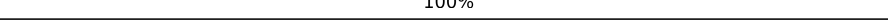
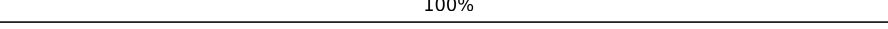
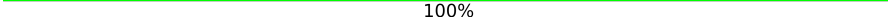
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Mol	Chain	Length	Quality of chain
1	K	334	 71%24%..
1	M	334	 69%25%..
1	O	334	 73%22%..
1	Q	334	 70%24%..
1	S	334	 71%24%..
1	U	334	 73%21%..
1	W	334	 69%26%..
1	Y	334	 75%20%..
1	a	334	 70%24%..
1	c	334	 75%20%..
2	B	181	 76%22%.
2	D	181	 76%22%.
2	F	181	 78%19%..
2	H	181	 67%29%..
2	J	181	 71%26%..
2	L	181	 76%22%..
2	N	181	 71%26%..
2	P	181	 75%23%.
2	R	181	 79%18%..
2	T	181	 73%25%.
2	V	181	 77%20%..
2	X	181	 74%24%.
2	Z	181	 5%66%31%..
2	b	181	 2%66%30%..
2	d	181	 3%71%26%..

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Mol	Chain	Length	Quality of chain
3	e	3	
3	g	3	
3	h	3	
3	j	3	
3	l	3	
3	n	3	
3	o	3	
3	p	3	
3	r	3	
3	t	3	
3	v	3	
3	x	3	
4	0	2	
4	f	2	
4	i	2	
4	k	2	
4	m	2	
4	q	2	
4	s	2	
4	u	2	
4	w	2	
4	y	2	
4	z	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60979 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	C	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	E	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	G	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	I	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	K	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	M	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	O	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	S	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	U	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	W	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	a	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	c	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q6DQ33
A	8	ASP	-	expression tag	UNP Q6DQ33
A	9	PRO	-	expression tag	UNP Q6DQ33
A	10	GLY	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	318	ILE	THR	engineered mutation	UNP Q6DQ33
C	7	ALA	-	expression tag	UNP Q6DQ33
C	8	ASP	-	expression tag	UNP Q6DQ33
C	9	PRO	-	expression tag	UNP Q6DQ33
C	10	GLY	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	318	ILE	THR	engineered mutation	UNP Q6DQ33
E	7	ALA	-	expression tag	UNP Q6DQ33
E	8	ASP	-	expression tag	UNP Q6DQ33
E	9	PRO	-	expression tag	UNP Q6DQ33
E	10	GLY	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	318	ILE	THR	engineered mutation	UNP Q6DQ33
G	7	ALA	-	expression tag	UNP Q6DQ33
G	8	ASP	-	expression tag	UNP Q6DQ33
G	9	PRO	-	expression tag	UNP Q6DQ33
G	10	GLY	-	expression tag	UNP Q6DQ33
G	158	ASP	ASN	engineered mutation	UNP Q6DQ33
G	224	LYS	ASN	engineered mutation	UNP Q6DQ33
G	226	LEU	GLN	engineered mutation	UNP Q6DQ33
G	318	ILE	THR	engineered mutation	UNP Q6DQ33
I	7	ALA	-	expression tag	UNP Q6DQ33
I	8	ASP	-	expression tag	UNP Q6DQ33
I	9	PRO	-	expression tag	UNP Q6DQ33
I	10	GLY	-	expression tag	UNP Q6DQ33
I	158	ASP	ASN	engineered mutation	UNP Q6DQ33
I	224	LYS	ASN	engineered mutation	UNP Q6DQ33
I	226	LEU	GLN	engineered mutation	UNP Q6DQ33
I	318	ILE	THR	engineered mutation	UNP Q6DQ33
K	7	ALA	-	expression tag	UNP Q6DQ33
K	8	ASP	-	expression tag	UNP Q6DQ33
K	9	PRO	-	expression tag	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
K	10	GLY	-	expression tag	UNP Q6DQ33
K	158	ASP	ASN	engineered mutation	UNP Q6DQ33
K	224	LYS	ASN	engineered mutation	UNP Q6DQ33
K	226	LEU	GLN	engineered mutation	UNP Q6DQ33
K	318	ILE	THR	engineered mutation	UNP Q6DQ33
M	7	ALA	-	expression tag	UNP Q6DQ33
M	8	ASP	-	expression tag	UNP Q6DQ33
M	9	PRO	-	expression tag	UNP Q6DQ33
M	10	GLY	-	expression tag	UNP Q6DQ33
M	158	ASP	ASN	engineered mutation	UNP Q6DQ33
M	224	LYS	ASN	engineered mutation	UNP Q6DQ33
M	226	LEU	GLN	engineered mutation	UNP Q6DQ33
M	318	ILE	THR	engineered mutation	UNP Q6DQ33
O	7	ALA	-	expression tag	UNP Q6DQ33
O	8	ASP	-	expression tag	UNP Q6DQ33
O	9	PRO	-	expression tag	UNP Q6DQ33
O	10	GLY	-	expression tag	UNP Q6DQ33
O	158	ASP	ASN	engineered mutation	UNP Q6DQ33
O	224	LYS	ASN	engineered mutation	UNP Q6DQ33
O	226	LEU	GLN	engineered mutation	UNP Q6DQ33
O	318	ILE	THR	engineered mutation	UNP Q6DQ33
Q	7	ALA	-	expression tag	UNP Q6DQ33
Q	8	ASP	-	expression tag	UNP Q6DQ33
Q	9	PRO	-	expression tag	UNP Q6DQ33
Q	10	GLY	-	expression tag	UNP Q6DQ33
Q	158	ASP	ASN	engineered mutation	UNP Q6DQ33
Q	224	LYS	ASN	engineered mutation	UNP Q6DQ33
Q	226	LEU	GLN	engineered mutation	UNP Q6DQ33
Q	318	ILE	THR	engineered mutation	UNP Q6DQ33
S	7	ALA	-	expression tag	UNP Q6DQ33
S	8	ASP	-	expression tag	UNP Q6DQ33
S	9	PRO	-	expression tag	UNP Q6DQ33
S	10	GLY	-	expression tag	UNP Q6DQ33
S	158	ASP	ASN	engineered mutation	UNP Q6DQ33
S	224	LYS	ASN	engineered mutation	UNP Q6DQ33
S	226	LEU	GLN	engineered mutation	UNP Q6DQ33
S	318	ILE	THR	engineered mutation	UNP Q6DQ33
U	7	ALA	-	expression tag	UNP Q6DQ33
U	8	ASP	-	expression tag	UNP Q6DQ33
U	9	PRO	-	expression tag	UNP Q6DQ33
U	10	GLY	-	expression tag	UNP Q6DQ33
U	158	ASP	ASN	engineered mutation	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
U	224	LYS	ASN	engineered mutation	UNP Q6DQ33
U	226	LEU	GLN	engineered mutation	UNP Q6DQ33
U	318	ILE	THR	engineered mutation	UNP Q6DQ33
W	7	ALA	-	expression tag	UNP Q6DQ33
W	8	ASP	-	expression tag	UNP Q6DQ33
W	9	PRO	-	expression tag	UNP Q6DQ33
W	10	GLY	-	expression tag	UNP Q6DQ33
W	158	ASP	ASN	engineered mutation	UNP Q6DQ33
W	224	LYS	ASN	engineered mutation	UNP Q6DQ33
W	226	LEU	GLN	engineered mutation	UNP Q6DQ33
W	318	ILE	THR	engineered mutation	UNP Q6DQ33
Y	7	ALA	-	expression tag	UNP Q6DQ33
Y	8	ASP	-	expression tag	UNP Q6DQ33
Y	9	PRO	-	expression tag	UNP Q6DQ33
Y	10	GLY	-	expression tag	UNP Q6DQ33
Y	158	ASP	ASN	engineered mutation	UNP Q6DQ33
Y	224	LYS	ASN	engineered mutation	UNP Q6DQ33
Y	226	LEU	GLN	engineered mutation	UNP Q6DQ33
Y	318	ILE	THR	engineered mutation	UNP Q6DQ33
a	7	ALA	-	expression tag	UNP Q6DQ33
a	8	ASP	-	expression tag	UNP Q6DQ33
a	9	PRO	-	expression tag	UNP Q6DQ33
a	10	GLY	-	expression tag	UNP Q6DQ33
a	158	ASP	ASN	engineered mutation	UNP Q6DQ33
a	224	LYS	ASN	engineered mutation	UNP Q6DQ33
a	226	LEU	GLN	engineered mutation	UNP Q6DQ33
a	318	ILE	THR	engineered mutation	UNP Q6DQ33
c	7	ALA	-	expression tag	UNP Q6DQ33
c	8	ASP	-	expression tag	UNP Q6DQ33
c	9	PRO	-	expression tag	UNP Q6DQ33
c	10	GLY	-	expression tag	UNP Q6DQ33
c	158	ASP	ASN	engineered mutation	UNP Q6DQ33
c	224	LYS	ASN	engineered mutation	UNP Q6DQ33
c	226	LEU	GLN	engineered mutation	UNP Q6DQ33
c	318	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	D	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	H	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	J	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	L	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	N	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	P	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	R	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	T	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	V	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	X	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	Z	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	b	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	d	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6DQ33
B	176	GLY	-	expression tag	UNP Q6DQ33
B	177	ARG	-	expression tag	UNP Q6DQ33
B	178	LEU	-	expression tag	UNP Q6DQ33
B	179	VAL	-	expression tag	UNP Q6DQ33
B	180	PRO	-	expression tag	UNP Q6DQ33
B	181	ARG	-	expression tag	UNP Q6DQ33
D	175	SER	-	expression tag	UNP Q6DQ33
D	176	GLY	-	expression tag	UNP Q6DQ33
D	177	ARG	-	expression tag	UNP Q6DQ33
D	178	LEU	-	expression tag	UNP Q6DQ33
D	179	VAL	-	expression tag	UNP Q6DQ33
D	180	PRO	-	expression tag	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	181	ARG	-	expression tag	UNP Q6DQ33
F	175	SER	-	expression tag	UNP Q6DQ33
F	176	GLY	-	expression tag	UNP Q6DQ33
F	177	ARG	-	expression tag	UNP Q6DQ33
F	178	LEU	-	expression tag	UNP Q6DQ33
F	179	VAL	-	expression tag	UNP Q6DQ33
F	180	PRO	-	expression tag	UNP Q6DQ33
F	181	ARG	-	expression tag	UNP Q6DQ33
H	175	SER	-	expression tag	UNP Q6DQ33
H	176	GLY	-	expression tag	UNP Q6DQ33
H	177	ARG	-	expression tag	UNP Q6DQ33
H	178	LEU	-	expression tag	UNP Q6DQ33
H	179	VAL	-	expression tag	UNP Q6DQ33
H	180	PRO	-	expression tag	UNP Q6DQ33
H	181	ARG	-	expression tag	UNP Q6DQ33
J	175	SER	-	expression tag	UNP Q6DQ33
J	176	GLY	-	expression tag	UNP Q6DQ33
J	177	ARG	-	expression tag	UNP Q6DQ33
J	178	LEU	-	expression tag	UNP Q6DQ33
J	179	VAL	-	expression tag	UNP Q6DQ33
J	180	PRO	-	expression tag	UNP Q6DQ33
J	181	ARG	-	expression tag	UNP Q6DQ33
L	175	SER	-	expression tag	UNP Q6DQ33
L	176	GLY	-	expression tag	UNP Q6DQ33
L	177	ARG	-	expression tag	UNP Q6DQ33
L	178	LEU	-	expression tag	UNP Q6DQ33
L	179	VAL	-	expression tag	UNP Q6DQ33
L	180	PRO	-	expression tag	UNP Q6DQ33
L	181	ARG	-	expression tag	UNP Q6DQ33
N	175	SER	-	expression tag	UNP Q6DQ33
N	176	GLY	-	expression tag	UNP Q6DQ33
N	177	ARG	-	expression tag	UNP Q6DQ33
N	178	LEU	-	expression tag	UNP Q6DQ33
N	179	VAL	-	expression tag	UNP Q6DQ33
N	180	PRO	-	expression tag	UNP Q6DQ33
N	181	ARG	-	expression tag	UNP Q6DQ33
P	175	SER	-	expression tag	UNP Q6DQ33
P	176	GLY	-	expression tag	UNP Q6DQ33
P	177	ARG	-	expression tag	UNP Q6DQ33
P	178	LEU	-	expression tag	UNP Q6DQ33
P	179	VAL	-	expression tag	UNP Q6DQ33
P	180	PRO	-	expression tag	UNP Q6DQ33

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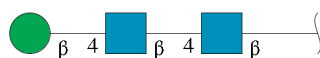
Chain	Residue	Modelled	Actual	Comment	Reference
P	181	ARG	-	expression tag	UNP Q6DQ33
R	175	SER	-	expression tag	UNP Q6DQ33
R	176	GLY	-	expression tag	UNP Q6DQ33
R	177	ARG	-	expression tag	UNP Q6DQ33
R	178	LEU	-	expression tag	UNP Q6DQ33
R	179	VAL	-	expression tag	UNP Q6DQ33
R	180	PRO	-	expression tag	UNP Q6DQ33
R	181	ARG	-	expression tag	UNP Q6DQ33
T	175	SER	-	expression tag	UNP Q6DQ33
T	176	GLY	-	expression tag	UNP Q6DQ33
T	177	ARG	-	expression tag	UNP Q6DQ33
T	178	LEU	-	expression tag	UNP Q6DQ33
T	179	VAL	-	expression tag	UNP Q6DQ33
T	180	PRO	-	expression tag	UNP Q6DQ33
T	181	ARG	-	expression tag	UNP Q6DQ33
V	175	SER	-	expression tag	UNP Q6DQ33
V	176	GLY	-	expression tag	UNP Q6DQ33
V	177	ARG	-	expression tag	UNP Q6DQ33
V	178	LEU	-	expression tag	UNP Q6DQ33
V	179	VAL	-	expression tag	UNP Q6DQ33
V	180	PRO	-	expression tag	UNP Q6DQ33
V	181	ARG	-	expression tag	UNP Q6DQ33
X	175	SER	-	expression tag	UNP Q6DQ33
X	176	GLY	-	expression tag	UNP Q6DQ33
X	177	ARG	-	expression tag	UNP Q6DQ33
X	178	LEU	-	expression tag	UNP Q6DQ33
X	179	VAL	-	expression tag	UNP Q6DQ33
X	180	PRO	-	expression tag	UNP Q6DQ33
X	181	ARG	-	expression tag	UNP Q6DQ33
Z	175	SER	-	expression tag	UNP Q6DQ33
Z	176	GLY	-	expression tag	UNP Q6DQ33
Z	177	ARG	-	expression tag	UNP Q6DQ33
Z	178	LEU	-	expression tag	UNP Q6DQ33
Z	179	VAL	-	expression tag	UNP Q6DQ33
Z	180	PRO	-	expression tag	UNP Q6DQ33
Z	181	ARG	-	expression tag	UNP Q6DQ33
b	175	SER	-	expression tag	UNP Q6DQ33
b	176	GLY	-	expression tag	UNP Q6DQ33
b	177	ARG	-	expression tag	UNP Q6DQ33
b	178	LEU	-	expression tag	UNP Q6DQ33
b	179	VAL	-	expression tag	UNP Q6DQ33
b	180	PRO	-	expression tag	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
b	181	ARG	-	expression tag	UNP Q6DQ33
d	175	SER	-	expression tag	UNP Q6DQ33
d	176	GLY	-	expression tag	UNP Q6DQ33
d	177	ARG	-	expression tag	UNP Q6DQ33
d	178	LEU	-	expression tag	UNP Q6DQ33
d	179	VAL	-	expression tag	UNP Q6DQ33
d	180	PRO	-	expression tag	UNP Q6DQ33
d	181	ARG	-	expression tag	UNP Q6DQ33

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



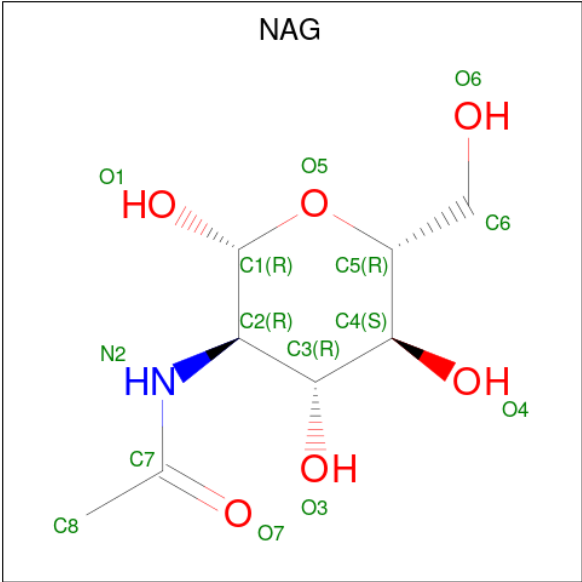
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	e	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	g	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	j	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	l	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	n	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	o	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	p	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	t	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	v	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	x	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	i	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	k	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	m	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	s	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	u	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	w	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	y	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	z	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	0	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

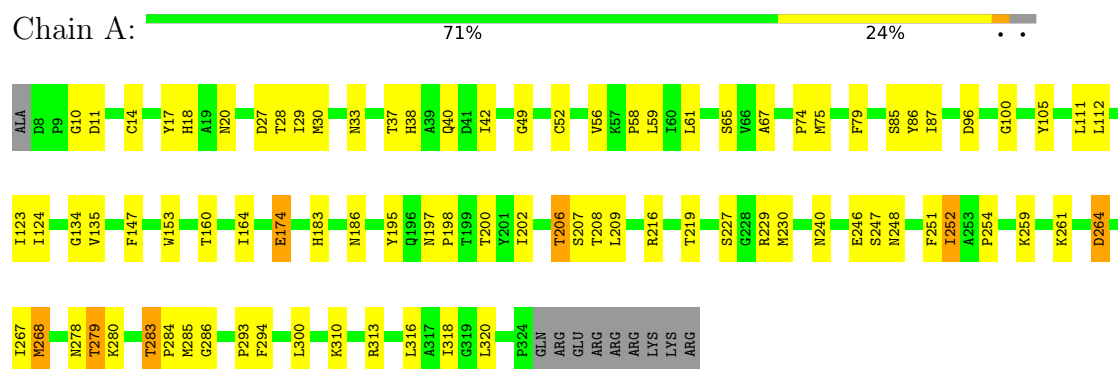


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	a	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		

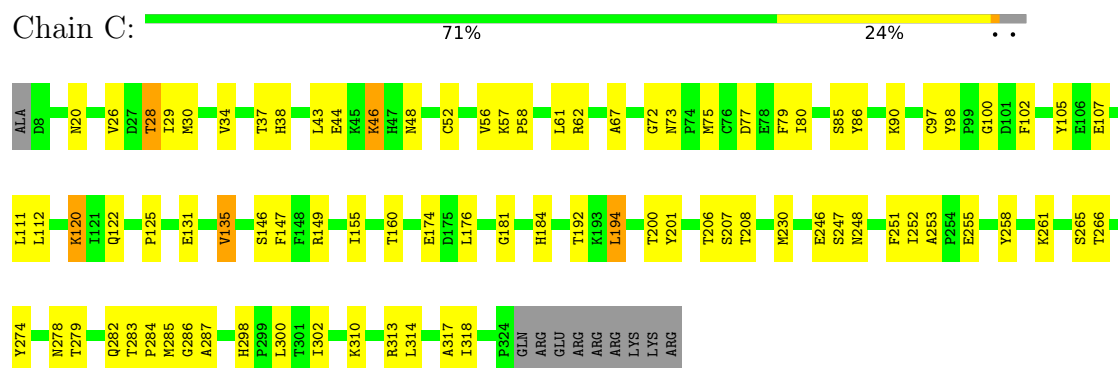
3 Residue-property plots

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

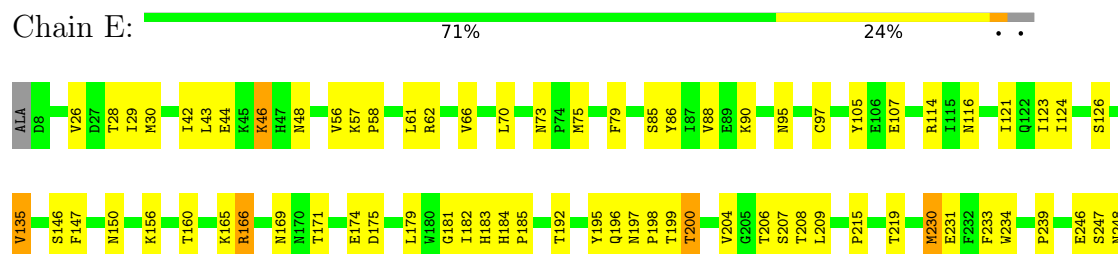
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain



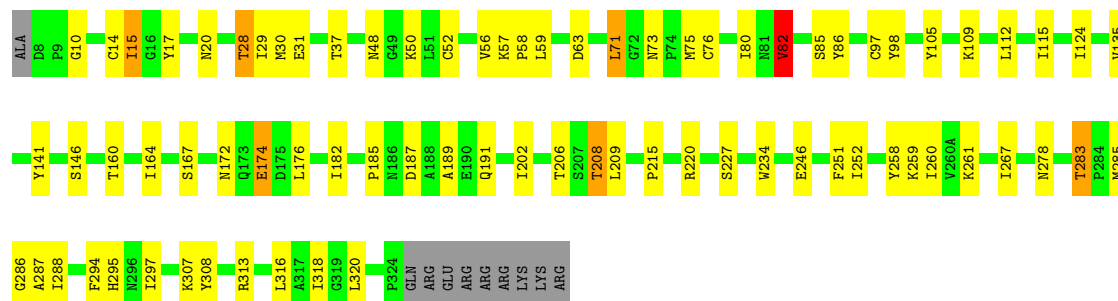
• Molecule 1: Hemagglutinin HA1 chain





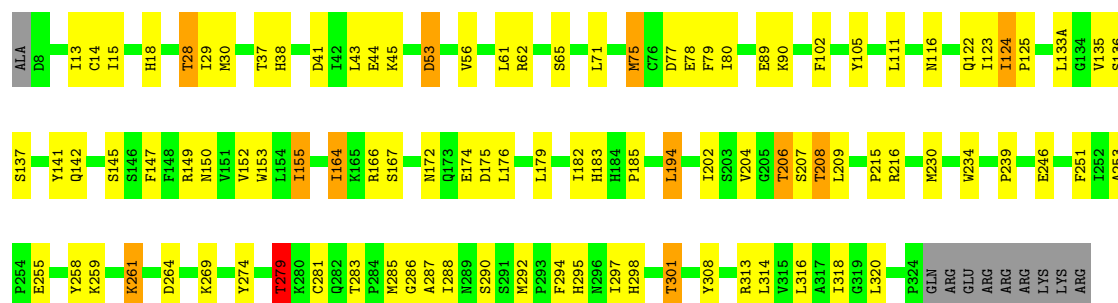
• Molecule 1: Hemagglutinin HA1 chain

Chain G: 74% 21%



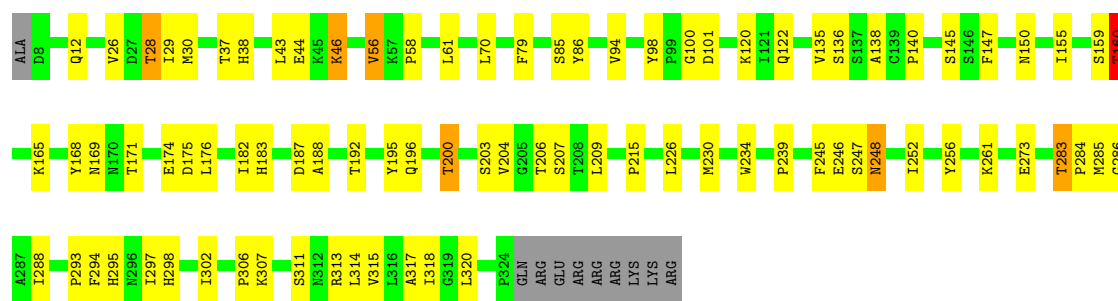
• Molecule 1: Hemagglutinin HA1 chain

Chain I: 67% 26%



• Molecule 1: Hemagglutinin HA1 chain

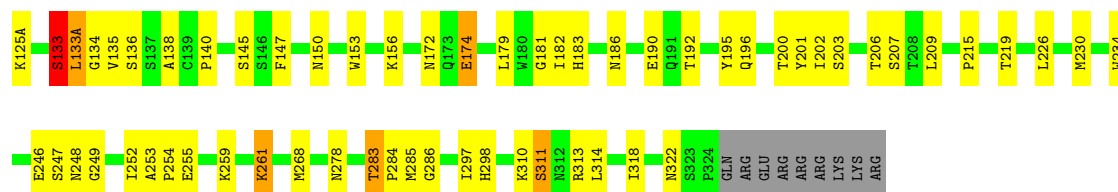
Chain K: 71% 24%



• Molecule 1: Hemagglutinin HA1 chain

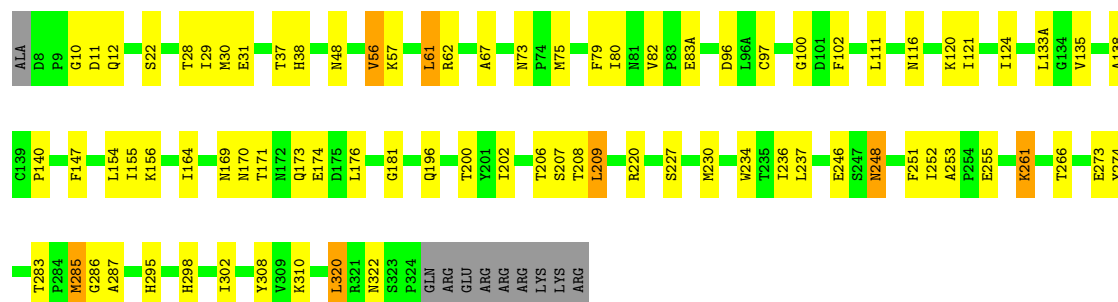
Chain M: 69% 25%





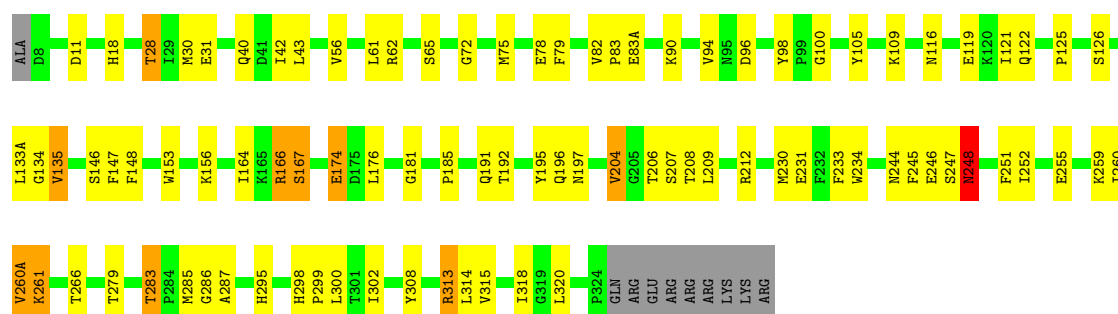
• Molecule 1: Hemagglutinin HA1 chain

Chain O: 73% 22%



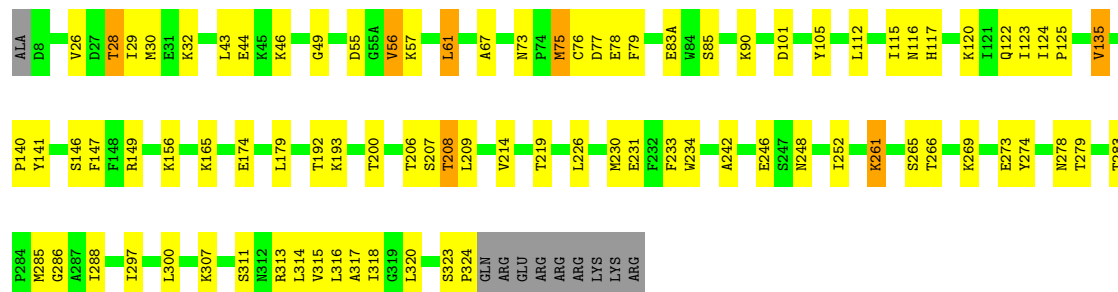
• Molecule 1: Hemagglutinin HA1 chain

Chain Q: 70% 24%



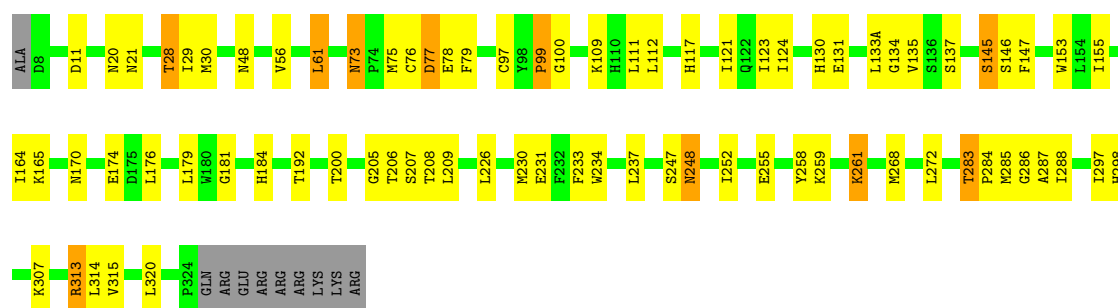
• Molecule 1: Hemagglutinin HA1 chain

Chain S: 71% 24%



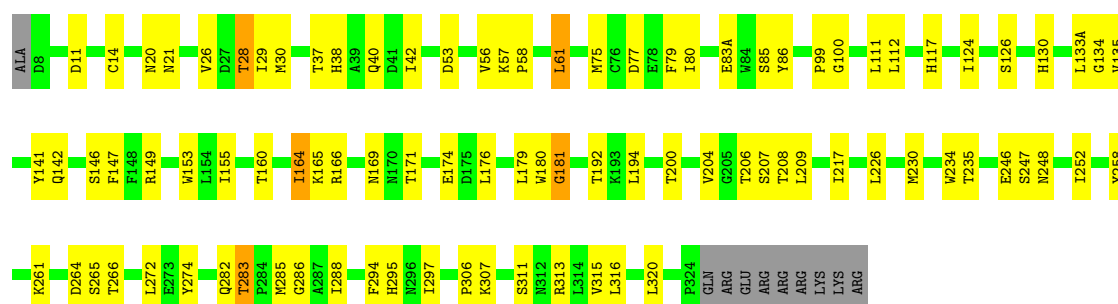
• Molecule 1: Hemagglutinin HA1 chain

Chain U:  73% 21%



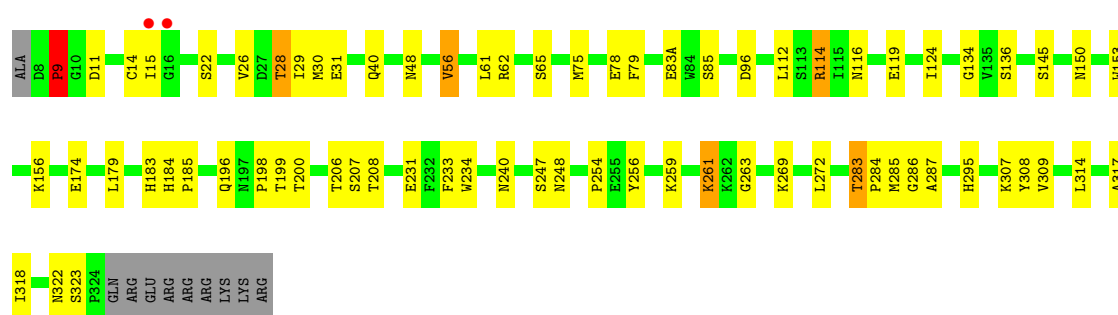
• Molecule 1: Hemagglutinin HA1 chain

Chain W:  69% 26%



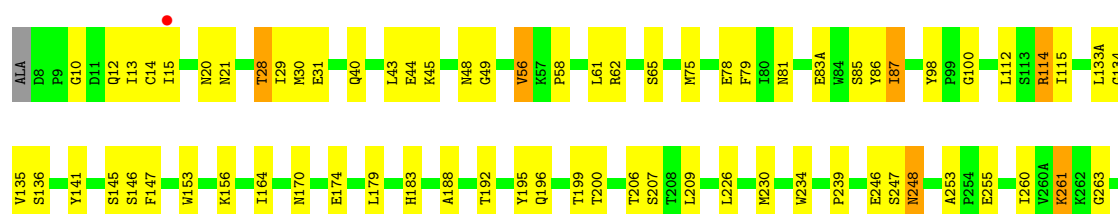
• Molecule 1: Hemagglutinin HA1 chain

Chain Y:  75% 20%



• Molecule 1: Hemagglutinin HA1 chain

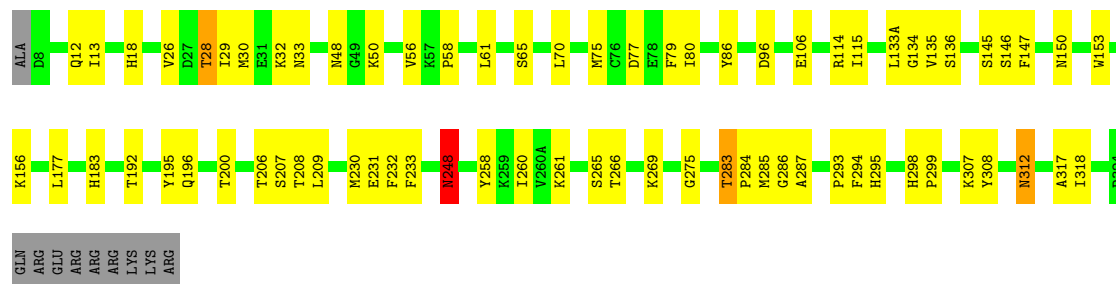
Chain a:  70% 24%





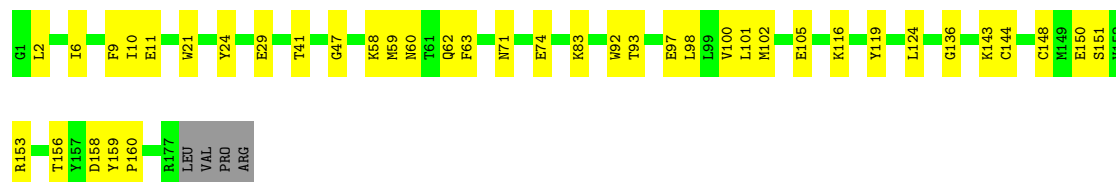
• Molecule 1: Hemagglutinin HA1 chain

Chain c: 75% 20% ..



• Molecule 2: Hemagglutinin

Chain B: 76% 22% .



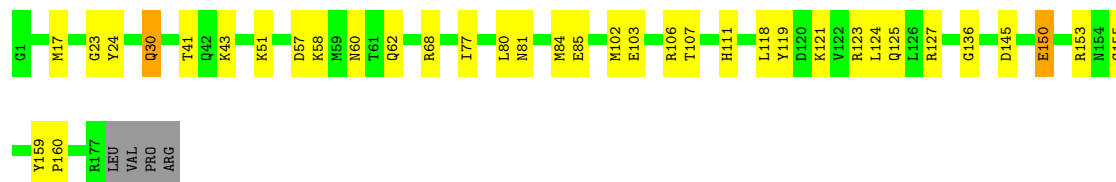
• Molecule 2: Hemagglutinin

Chain D: 76% 22% .



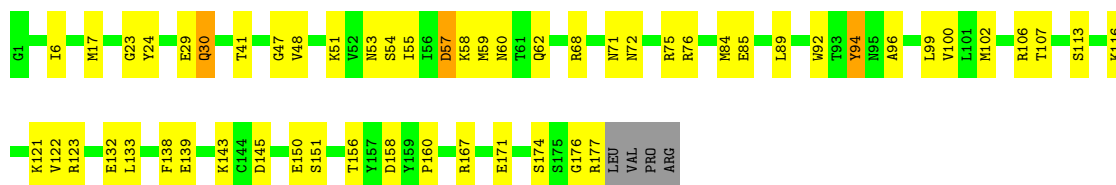
• Molecule 2: Hemagglutinin

Chain F: 78% 19% ..



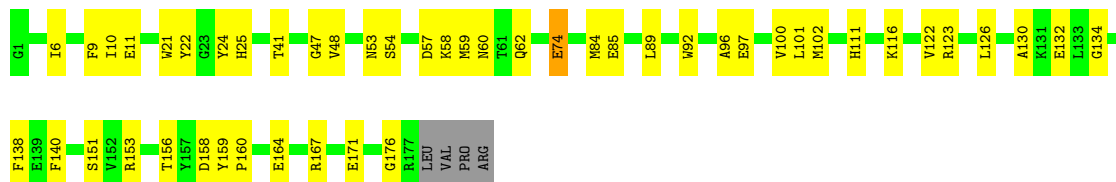
• Molecule 2: Hemagglutinin

Chain H: 67% 29% ..



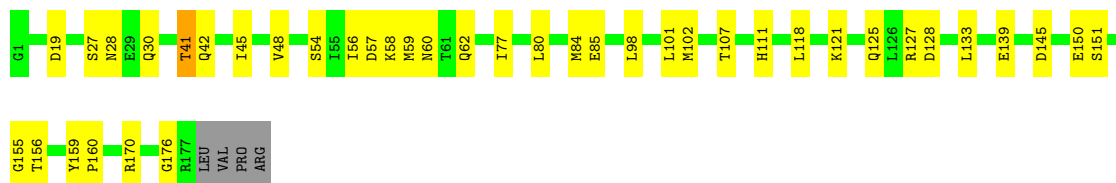
- Molecule 2: Hemagglutinin

Chain J: 71% 26% ..



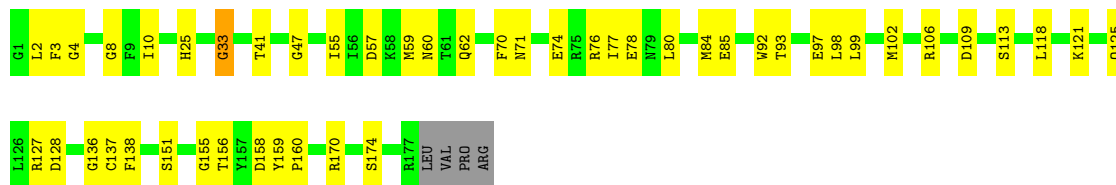
- Molecule 2: Hemagglutinin

Chain L: 76% 22% ..



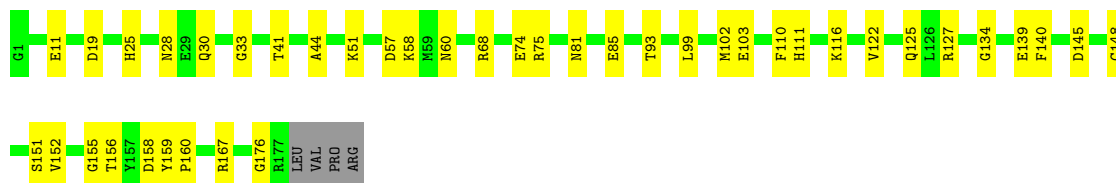
- Molecule 2: Hemagglutinin

Chain N: 71% 26% ..



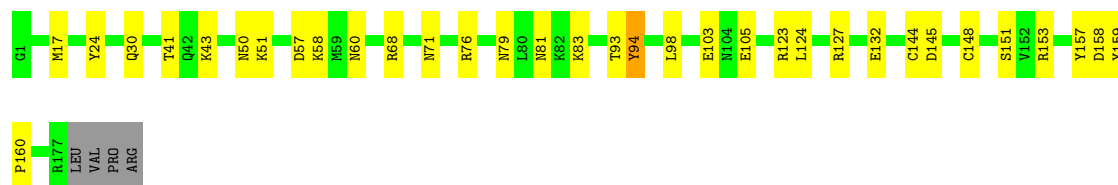
- Molecule 2: Hemagglutinin

Chain P: 75% 23% .



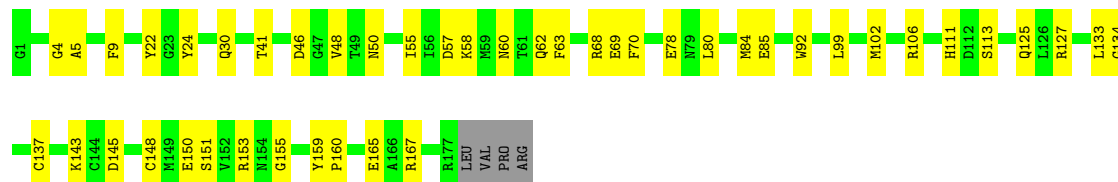
- Molecule 2: Hemagglutinin

Chain R: 79% 18% ..



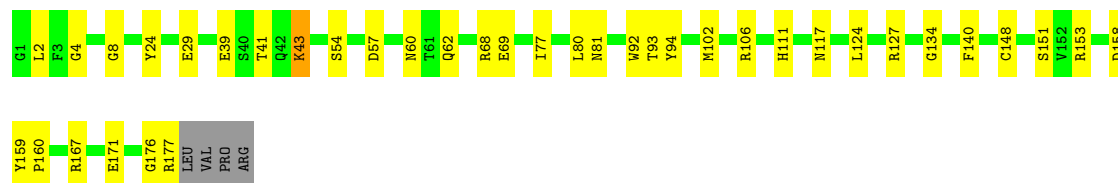
- Molecule 2: Hemagglutinin

Chain T: 73% 25% .



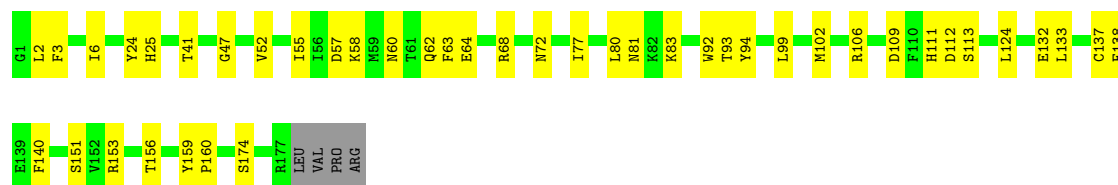
- Molecule 2: Hemagglutinin

Chain V: 77% 20% ..



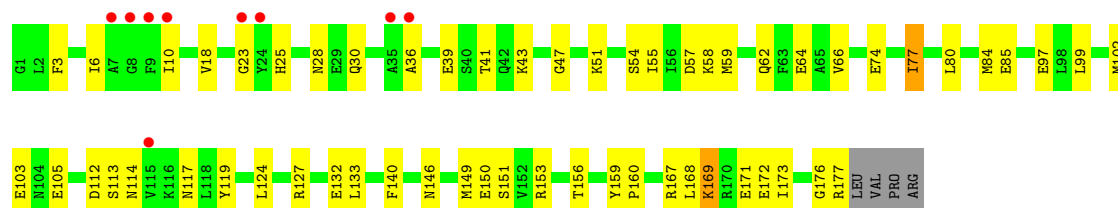
- Molecule 2: Hemagglutinin

Chain X: 74% 24% .

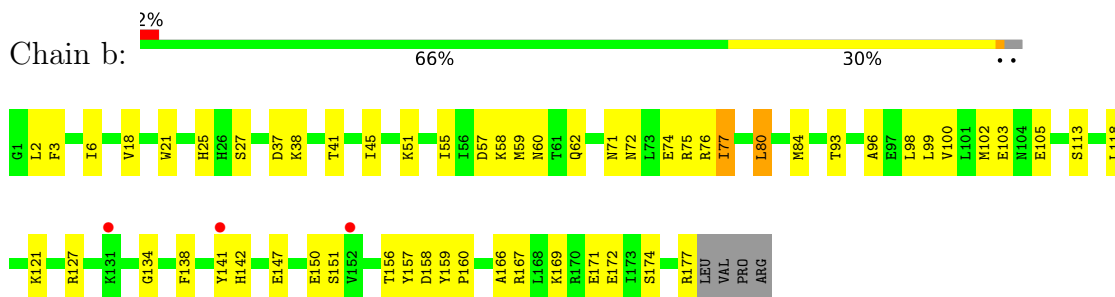


- Molecule 2: Hemagglutinin

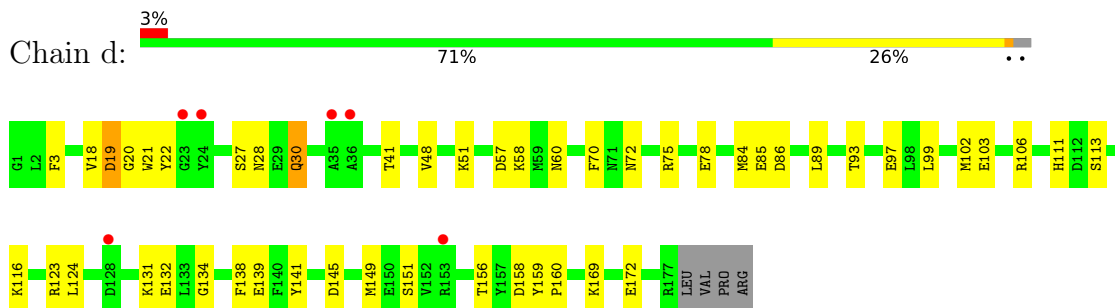
Chain Z: 5% 66% 31% ..



- Molecule 2: Hemagglutinin



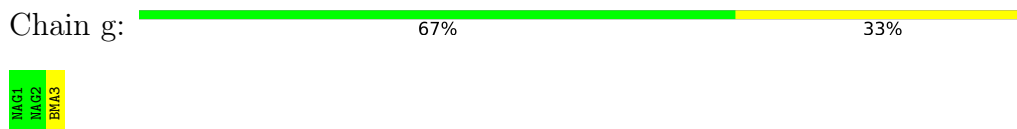
- Molecule 2: Hemagglutinin



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



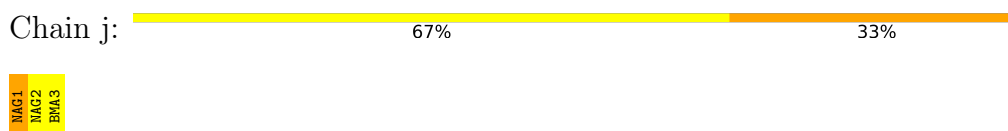
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain l:  100%

MAG1
MAG2
BMA3

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

Chain n:  33% 67%

MAG1
MAG2
BMA3

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

Chain o:  33% 67%

MAG1
MAG2
BMA3

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

Chain p:  33% 67%

MAG1
MAG2
BMA3

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

Chain r:  33% 67%

MAG1
MAG2
BMA3

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

Chain t:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain v:  33% 67%



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

Chain x:



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

Chain f:



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

Chain i:



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

Chain k:



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

Chain m:



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

Chain q:



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

Chain s:  50% 50%

MAG1
MAG2

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

Chain u:  50% 50%

MAG1
MAG2

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

Chain w:  100%

MAG1
MAG2

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

Chain y:  100%

MAG1
MAG2

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

Chain z:  100%

MAG1
MAG2

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

Chain 0:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.24Å 118.94Å 273.41Å 88.43° 89.68° 60.26°	Depositor
Resolution (Å)	47.75 – 2.95 47.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.75-2.95) 87.9 (47.75-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.281 0.235 , 0.281	Depositor DCC
R_{free} test set	11870 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.013 for k,-h+k,l 0.013 for h-k,h,l 0.055 for -h+k,-h,l 0.055 for -k,h-k,l 0.067 for h,h-k,-l 0.027 for -k,-h,-l 0.012 for -h,-k,l 0.026 for -h+k,k,-l 0.017 for h-k,-k,-l 0.011 for -h,-h+k,-l 0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60979	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.82	0/2640	1.14	4/3585 (0.1%)
1	C	0.72	0/2640	1.08	8/3585 (0.2%)
1	E	0.75	0/2640	1.10	6/3585 (0.2%)
1	G	0.83	0/2640	1.21	17/3585 (0.5%)
1	I	0.87	2/2640 (0.1%)	1.23	12/3585 (0.3%)
1	K	0.74	0/2640	1.07	5/3585 (0.1%)
1	M	0.81	0/2640	1.16	6/3585 (0.2%)
1	O	0.78	0/2640	1.11	13/3585 (0.4%)
1	Q	0.79	0/2640	1.12	6/3585 (0.2%)
1	S	0.72	0/2640	1.08	4/3585 (0.1%)
1	U	0.71	0/2640	1.07	12/3585 (0.3%)
1	W	0.71	0/2640	1.06	7/3585 (0.2%)
1	Y	0.58	0/2640	0.95	2/3585 (0.1%)
1	a	0.55	0/2640	0.94	7/3585 (0.2%)
1	c	0.57	0/2640	0.93	1/3585 (0.0%)
2	B	0.59	0/1460	0.97	1/1961 (0.1%)
2	D	0.49	0/1460	0.87	1/1961 (0.1%)
2	F	0.51	0/1460	0.87	1/1961 (0.1%)
2	H	0.59	0/1460	0.91	1/1961 (0.1%)
2	J	0.58	0/1460	0.96	3/1961 (0.2%)
2	L	0.51	0/1460	0.86	1/1961 (0.1%)
2	N	0.50	0/1460	0.93	2/1961 (0.1%)
2	P	0.52	0/1460	0.91	3/1961 (0.2%)
2	R	0.55	0/1460	0.88	1/1961 (0.1%)
2	T	0.49	0/1460	0.86	1/1961 (0.1%)
2	V	0.49	0/1460	0.91	1/1961 (0.1%)
2	X	0.49	0/1460	0.89	1/1961 (0.1%)
2	Z	0.44	0/1460	0.94	3/1961 (0.2%)
2	b	0.44	0/1460	0.90	2/1961 (0.1%)
2	d	0.45	0/1460	0.89	1/1961 (0.1%)
All	All	0.67	2/61500 (0.0%)	1.03	133/83190 (0.2%)

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	Y	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	152	VAL	CA-CB	5.57	1.61	1.54
1	I	279	THR	CA-C	-5.40	1.45	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	ALA	CA-C-N	-10.50	110.02	120.31
1	M	253	ALA	C-N-CA	-10.50	110.02	120.31
1	G	56	VAL	N-CA-C	8.57	121.48	108.71
1	G	82	VAL	N-CA-C	8.30	116.74	109.02
1	Y	9	PRO	CA-N-CD	-8.15	100.59	112.00
1	I	124	ILE	CA-C-N	7.72	128.17	119.83
1	I	124	ILE	C-N-CA	7.72	128.17	119.83
1	C	98	TYR	CA-C-N	7.65	128.09	119.83
1	C	98	TYR	C-N-CA	7.65	128.09	119.83
1	M	98	TYR	CA-C-N	7.44	127.43	119.76
1	M	98	TYR	C-N-CA	7.44	127.43	119.76
1	E	234	TRP	N-CA-C	7.21	120.04	109.07
1	G	124	ILE	CA-C-N	7.20	127.61	119.83
1	G	124	ILE	C-N-CA	7.20	127.61	119.83
1	I	255	GLU	N-CA-C	-7.19	102.49	112.12
1	O	56	VAL	N-CA-C	7.16	119.38	108.71
1	U	145	SER	N-CA-C	-7.06	100.03	110.48
1	G	10	GLY	N-CA-C	-7.05	103.52	112.54
1	A	279	THR	N-CA-C	6.99	117.25	108.45
1	O	124	ILE	CA-C-N	6.88	127.26	119.83
1	O	124	ILE	C-N-CA	6.88	127.26	119.83
1	Q	255	GLU	N-CA-C	-6.88	103.92	112.72
1	K	311	SER	N-CA-C	6.83	119.77	110.55
1	Q	56	VAL	N-CA-C	6.78	118.05	108.36
1	I	56	VAL	N-CA-C	6.73	118.73	108.71
1	W	164	ILE	N-CA-C	6.69	117.72	108.89
1	A	10	GLY	N-CA-C	-6.64	103.65	112.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	SER	N-CA-C	-6.64	104.82	113.12
1	W	160	THR	N-CA-C	6.64	119.81	109.52
1	C	255	GLU	N-CA-C	-6.63	104.23	112.72
1	S	56	VAL	N-CA-C	6.59	117.78	108.36
1	U	117	HIS	N-CA-C	6.58	119.21	108.55
1	M	56	VAL	N-CA-C	6.50	118.39	108.71
1	G	82	VAL	CB-CA-C	-6.46	104.67	111.00
1	a	10	GLY	N-CA-C	-6.38	104.38	112.54
2	H	121	LYS	N-CA-C	-6.34	104.24	112.23
2	b	18	VAL	N-CA-C	6.30	118.21	112.29
1	W	61	LEU	N-CA-C	-6.27	100.76	110.10
1	U	56	VAL	N-CA-C	6.22	117.25	108.36
1	G	63	ASP	N-CA-C	-6.18	105.68	112.72
1	U	255	GLU	N-CA-C	-6.14	104.86	112.72
1	C	181	GLY	N-CA-C	6.07	120.63	110.56
1	S	61	LEU	N-CA-C	-6.06	100.87	109.96
1	U	61	LEU	N-CA-C	-6.00	100.96	109.96
1	I	176	LEU	N-CA-C	5.98	118.16	108.41
2	L	127	ARG	CB-CA-C	-5.98	109.10	117.23
1	K	200	THR	N-CA-C	5.96	118.46	109.41
1	O	285	MET	N-CA-C	-5.96	106.17	113.50
2	b	174	SER	N-CA-C	-5.95	104.88	111.36
1	Y	56	VAL	N-CA-C	5.93	116.84	108.36
1	I	164	ILE	N-CA-C	5.88	116.65	108.89
1	U	181	GLY	N-CA-C	5.87	120.30	110.56
1	a	253	ALA	CA-C-N	-5.83	114.60	120.31
1	a	253	ALA	C-N-CA	-5.83	114.60	120.31
1	O	82	VAL	CA-C-N	5.83	125.80	120.21
1	O	82	VAL	C-N-CA	5.83	125.80	120.21
1	c	56	VAL	N-CA-C	5.82	116.69	108.36
1	Q	181	GLY	N-CA-C	5.75	120.10	110.56
2	J	84	MET	N-CA-C	5.72	117.32	111.14
2	N	33	GLY	N-CA-C	5.72	118.92	110.63
1	I	279	THR	CB-CA-C	-5.70	99.14	111.11
1	G	57	LYS	CA-C-N	5.70	125.60	119.85
1	G	57	LYS	C-N-CA	5.70	125.60	119.85
2	Z	169	LYS	N-CA-C	-5.68	105.85	112.89
1	O	181	GLY	N-CA-C	5.68	119.98	110.56
2	J	176	GLY	N-CA-C	-5.67	107.51	113.58
1	O	255	GLU	N-CA-C	-5.67	105.47	112.72
1	U	184	HIS	CA-C-N	5.66	126.91	119.84
1	U	184	HIS	C-N-CA	5.66	126.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	THR	CB-CA-C	-5.65	100.07	113.02
1	O	121	ILE	N-CA-C	5.62	116.83	108.46
1	Q	204	VAL	CA-C-N	-5.62	118.23	122.33
1	Q	204	VAL	C-N-CA	-5.62	118.23	122.33
1	E	184	HIS	CA-C-N	5.61	126.86	119.84
1	E	184	HIS	C-N-CA	5.61	126.86	119.84
2	T	127	ARG	CB-CA-C	-5.59	109.63	117.23
1	W	117	HIS	N-CA-C	5.59	118.54	108.48
1	K	234	TRP	N-CA-C	5.58	117.88	109.23
1	S	214	VAL	CA-C-N	5.58	125.53	119.78
1	S	214	VAL	C-N-CA	5.58	125.53	119.78
2	d	18	VAL	N-CA-C	5.56	117.52	112.29
1	A	160	THR	N-CA-C	5.55	118.12	109.52
1	a	255	GLU	N-CA-C	-5.54	105.63	112.72
1	O	10	GLY	N-CA-C	-5.52	105.48	112.54
2	F	127	ARG	CB-CA-C	-5.50	109.75	117.23
2	V	127	ARG	CB-CA-C	-5.49	109.77	117.23
2	B	62	GLN	N-CA-C	-5.48	100.73	109.07
1	Q	234	TRP	N-CA-C	5.47	117.39	109.07
2	D	127	ARG	CB-CA-C	-5.46	109.81	117.23
2	N	127	ARG	CB-CA-C	-5.46	109.81	117.23
1	I	53	ASP	N-CA-C	-5.46	103.33	110.53
1	W	181	GLY	N-CA-C	5.44	119.59	110.56
1	U	77	ASP	N-CA-C	5.43	122.36	110.80
1	K	101	ASP	N-CA-C	5.41	117.49	108.99
1	I	71	LEU	N-CA-C	-5.41	106.18	112.89
1	E	95	ASN	N-CA-C	5.40	118.02	108.24
1	K	160	THR	N-CA-C	5.39	117.87	109.52
1	I	290	SER	N-CA-C	5.34	117.19	109.07
2	J	74	GLU	N-CA-C	-5.34	104.34	111.87
1	U	73	ASN	CA-C-N	5.30	125.61	119.47
1	U	73	ASN	C-N-CA	5.30	125.61	119.47
1	a	56	VAL	N-CA-C	5.25	115.87	108.36
1	G	98	TYR	CA-C-N	5.24	125.49	119.83
1	G	98	TYR	C-N-CA	5.24	125.49	119.83
1	G	160	THR	N-CA-C	5.24	118.13	109.85
1	C	184	HIS	CA-C-N	5.24	126.39	119.84
1	C	184	HIS	C-N-CA	5.24	126.39	119.84
1	C	131	GLU	N-CA-C	5.24	117.49	107.75
1	W	124	ILE	CA-C-N	5.21	125.46	119.83
1	W	124	ILE	C-N-CA	5.21	125.46	119.83
1	E	181	GLY	N-CA-C	5.21	119.20	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	TRP	N-CA-C	5.20	117.09	109.24
1	G	71	LEU	N-CA-C	-5.18	106.11	112.90
1	I	133(A)	LEU	N-CA-C	-5.18	106.36	113.30
1	E	200	THR	N-CA-C	5.15	117.24	109.41
1	C	194	LEU	N-CA-C	5.15	118.02	111.69
1	O	298	HIS	CA-C-N	-5.13	114.38	119.56
1	O	298	HIS	C-N-CA	-5.13	114.38	119.56
1	a	298	HIS	CA-C-N	5.12	124.73	119.56
1	a	298	HIS	C-N-CA	5.12	124.73	119.56
2	P	127	ARG	CB-CA-C	-5.11	110.28	117.23
1	I	279	THR	N-CA-C	5.11	116.43	109.18
1	M	133	SER	N-CA-C	5.10	118.53	112.72
1	O	200	THR	N-CA-C	5.09	117.15	109.41
2	X	72	ASN	N-CA-C	5.08	118.74	112.54
2	P	176	GLY	CA-C-N	5.06	130.81	121.70
2	P	176	GLY	C-N-CA	5.06	130.81	121.70
2	R	127	ARG	CB-CA-C	-5.05	110.36	117.23
1	G	141	TYR	CA-C-N	-5.04	114.54	122.76
1	G	141	TYR	C-N-CA	-5.04	114.54	122.76
1	U	99	PRO	N-CA-C	5.04	118.78	111.03
2	Z	127	ARG	CB-CA-C	-5.01	110.41	117.23
2	Z	18	VAL	N-CA-C	5.01	119.39	113.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	9	PRO	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	2574	0	2525	58	0
1	C	2574	0	2525	59	0
1	E	2574	0	2525	58	0
1	G	2574	0	2525	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2574	0	2525	62	0
1	K	2574	0	2525	60	0
1	M	2574	0	2525	59	0
1	O	2574	0	2524	47	0
1	Q	2574	0	2525	61	0
1	S	2574	0	2525	65	0
1	U	2574	0	2525	55	0
1	W	2574	0	2525	59	0
1	Y	2574	0	2525	48	0
1	a	2574	0	2526	60	0
1	c	2574	0	2525	49	0
2	B	1433	0	1340	32	0
2	D	1433	0	1340	26	0
2	F	1433	0	1340	24	0
2	H	1433	0	1340	43	0
2	J	1433	0	1340	41	0
2	L	1433	0	1340	30	0
2	N	1433	0	1340	36	0
2	P	1433	0	1340	26	0
2	R	1433	0	1340	23	0
2	T	1433	0	1340	34	0
2	V	1433	0	1340	28	0
2	X	1433	0	1340	30	0
2	Z	1433	0	1340	42	0
2	b	1433	0	1340	46	0
2	d	1433	0	1340	43	0
3	e	39	0	34	1	0
3	g	39	0	34	0	0
3	h	39	0	34	1	0
3	j	39	0	34	1	0
3	l	39	0	34	0	0
3	n	39	0	34	0	0
3	o	39	0	34	0	0
3	p	39	0	34	0	0
3	r	39	0	34	0	0
3	t	39	0	34	1	0
3	v	39	0	34	0	0
3	x	39	0	34	0	0
4	o	28	0	25	1	0
4	f	28	0	25	0	0
4	i	28	0	25	0	0
4	k	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	m	28	0	25	1	0
4	q	28	0	25	0	0
4	s	28	0	25	1	0
4	u	28	0	25	1	0
4	w	28	0	25	0	0
4	y	28	0	25	1	0
4	z	28	0	25	1	0
5	C	14	0	13	0	0
5	K	14	0	13	0	0
5	M	14	0	13	0	0
5	O	14	0	13	0	0
5	Y	14	0	13	1	0
5	a	14	0	13	0	0
5	c	14	0	13	0	0
All	All	60979	0	58749	1168	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 10.

All (1168) 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:K:192:THR:HG21	1:S:192:THR:HG21	1.34	1.08
1:I:283:THR:HG22	1:I:285:MET:H	1.26	1.00
1:Q:283:THR:HG22	1:Q:285:MET:H	1.25	1.00
1:G:283:THR:HG22	1:G:285:MET:H	1.27	0.99
1:U:206:THR:HG22	1:U:208:THR:H	1.25	0.98
1:O:283:THR:HG22	1:O:285:MET:H	1.29	0.97
1:S:283:THR:HG22	1:S:285:MET:H	1.35	0.90
1:U:283:THR:HG22	1:U:285:MET:H	1.38	0.89
1:A:206:THR:HG22	1:A:208:THR:H	1.37	0.87
1:A:283:THR:HG22	1:A:285:MET:H	1.41	0.85
1:Q:166:ARG:HG3	1:Q:166:ARG:HH11	1.41	0.85
1:E:166:ARG:HG3	1:E:166:ARG:HH11	1.43	0.84
1:G:206:THR:HG22	1:G:208:THR:H	1.41	0.84
1:Y:283:THR:HG22	1:Y:285:MET:H	1.41	0.84
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.83
1:M:283:THR:HG22	1:M:285:MET:H	1.42	0.83
1:W:283:THR:HG22	1:W:285:MET:H	1.44	0.83
1:W:206:THR:HG22	1:W:208:THR:H	1.43	0.82
1:c:283:THR:HG22	1:c:285:MET:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:THR:HG22	1:I:208:THR:H	1.44	0.80
1:W:134:GLY:HA3	1:W:153:TRP:HB3	1.64	0.79
1:a:29:ILE:HD11	2:b:102:MET:HG2	1.65	0.78
1:W:206:THR:HB	1:W:209:LEU:H	1.48	0.77
1:K:283:THR:HG22	1:K:285:MET:H	1.50	0.77
1:a:12:GLN:HB2	2:b:27:SER:HB3	1.65	0.76
1:a:61:LEU:HA	1:a:79:PHE:CZ	2.21	0.76
1:S:29:ILE:HD11	2:T:102:MET:HG2	1.67	0.75
1:C:283:THR:HG22	1:C:285:MET:H	1.52	0.75
1:c:12:GLN:HB2	2:d:27:SER:HB3	1.69	0.75
1:S:206:THR:HB	1:S:209:LEU:H	1.51	0.75
1:K:192:THR:CG2	1:S:192:THR:HG21	2.16	0.74
1:S:43:LEU:HB2	1:S:314:LEU:HB2	1.69	0.74
1:I:29:ILE:HD11	2:J:102:MET:HG2	1.70	0.74
1:K:70:LEU:O	1:K:150:ASN:ND2	2.21	0.74
1:K:29:ILE:HD11	2:L:102:MET:HA	1.70	0.74
1:U:131:GLU:HB3	1:U:133(A):LEU:HD23	1.69	0.74
1:C:192:THR:HG21	1:W:192:THR:HG21	1.70	0.74
1:S:61:LEU:HA	1:S:79:PHE:CZ	2.23	0.73
1:a:134:GLY:HA3	1:a:153:TRP:HB3	1.68	0.73
1:E:70:LEU:O	1:E:150:ASN:ND2	2.20	0.73
1:I:279:THR:HB	1:I:281:CYS:H	1.54	0.73
1:c:312:ASN:N	1:c:312:ASN:OD1	2.21	0.73
2:N:174:SER:O	2:P:167:ARG:NH1	2.21	0.73
1:I:283:THR:HB	1:I:286:GLY:O	1.89	0.73
2:b:134:GLY:HA2	2:d:124:LEU:HD22	1.70	0.73
2:b:141:TYR:O	2:b:169:LYS:HG2	1.89	0.72
1:K:44:GLU:OE1	1:K:46:LYS:HG3	1.90	0.72
2:T:30:GLN:HE22	2:T:145:ASP:HB2	1.53	0.71
2:X:62:GLN:HG3	2:X:92:TRP:CG	2.25	0.71
1:I:61:LEU:HA	1:I:79:PHE:CZ	2.26	0.71
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.73	0.71
1:C:57:LYS:HE2	1:C:274:TYR:CZ	2.25	0.71
1:Y:134:GLY:HA3	1:Y:153:TRP:HB3	1.70	0.71
1:a:283:THR:HG22	1:a:285:MET:H	1.53	0.71
1:U:76:CYS:O	1:U:78:GLU:N	2.21	0.71
1:c:156:LYS:HD2	1:c:196:GLN:HB2	1.70	0.71
1:E:192:THR:HG21	1:U:192:THR:HG21	1.72	0.71
2:N:106:ARG:HH22	2:R:105:GLU:HG2	1.56	0.71
1:M:83(A):GLU:OE1	1:M:261:LYS:NZ	2.24	0.71
1:c:134:GLY:HA3	1:c:153:TRP:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:MET:HE2	2:D:85:GLU:HG2	1.71	0.71
1:A:30:MET:HG2	2:H:47:GLY:O	1.90	0.70
1:K:12:GLN:HB2	2:L:27:SER:HB3	1.73	0.70
1:C:80:ILE:O	1:C:120:LYS:NZ	2.25	0.70
2:Z:173:ILE:HG23	2:Z:177:ARG:HE	1.57	0.70
2:Z:124:LEU:HD22	2:d:134:GLY:HA2	1.74	0.69
1:U:61:LEU:HA	1:U:79:PHE:CZ	2.28	0.69
1:S:32:LYS:NZ	2:V:54:SER:OG	2.27	0.68
1:Q:283:THR:HB	1:Q:286:GLY:O	1.93	0.68
1:Y:62:ARG:NH1	1:Y:78:GLU:OE2	2.26	0.68
2:H:84:MET:HE2	2:H:85:GLU:HG2	1.76	0.68
1:Y:307:LYS:NZ	2:Z:64:GLU:OE2	2.26	0.68
2:L:57:ASP:O	2:L:60:ASN:HB2	1.94	0.68
2:T:55:ILE:HG12	2:T:99:LEU:HD21	1.75	0.67
1:S:206:THR:HG22	1:S:208:THR:H	1.57	0.67
1:I:62:ARG:O	1:I:90:LYS:HD2	1.95	0.67
1:U:206:THR:HB	1:U:209:LEU:H	1.59	0.67
1:Y:61:LEU:HA	1:Y:79:PHE:CZ	2.29	0.67
2:d:19:ASP:OD1	2:d:19:ASP:N	2.28	0.67
2:B:29:GLU:OE1	2:B:143:LYS:NZ	2.24	0.66
1:Y:26:VAL:HG21	1:Y:317:ALA:HB2	1.76	0.66
1:G:182:ILE:HD11	1:G:215:PRO:HD3	1.78	0.66
2:D:106:ARG:HG2	2:F:106:ARG:HH22	1.61	0.66
1:Y:314:LEU:HD21	2:Z:97:GLU:HG2	1.77	0.66
2:R:30:GLN:HE22	2:R:145:ASP:HB2	1.59	0.66
2:D:57:ASP:O	2:D:60:ASN:HB2	1.96	0.66
1:G:29:ILE:HD11	2:H:102:MET:HG2	1.78	0.66
1:G:288:ILE:HD11	1:G:297:ILE:HG13	1.78	0.66
2:J:54:SER:O	2:J:58:LYS:HG2	1.96	0.65
1:S:135:VAL:HG22	1:S:146:SER:HA	1.78	0.65
1:U:28:THR:HG23	1:U:30:MET:H	1.61	0.65
2:J:126:LEU:HD13	2:J:140:PHE:HE1	1.61	0.65
2:L:84:MET:HE2	2:L:85:GLU:HG2	1.79	0.65
1:I:13:ILE:HG22	2:J:138:PHE:HB2	1.79	0.65
1:M:100:GLY:HA3	1:M:230:MET:O	1.97	0.65
1:I:77:ASP:OD2	1:I:149:ARG:NH2	2.29	0.65
1:K:183:HIS:ND1	1:K:195:TYR:OH	2.30	0.64
1:S:165:LYS:HE2	1:S:246:GLU:OE2	1.97	0.64
1:I:30:MET:HG2	2:B:47:GLY:O	1.96	0.64
1:O:22:SER:O	1:O:322:ASN:ND2	2.31	0.64
1:a:43:LEU:HD23	1:a:45:LYS:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:MET:SD	1:S:252:ILE:HD11	2.38	0.64
2:F:30:GLN:HE22	2:F:145:ASP:HA	1.60	0.64
1:G:307:LYS:HE3	2:H:60:ASN:O	1.97	0.64
1:M:12:GLN:HG3	2:N:138:PHE:O	1.98	0.64
2:P:28:ASN:ND2	2:P:30:GLN:OE1	2.31	0.64
1:G:318:ILE:HG23	2:H:48:VAL:HG11	1.79	0.64
1:c:307:LYS:NZ	2:d:60:ASN:O	2.31	0.64
1:K:100:GLY:HA3	1:K:230:MET:O	1.97	0.64
1:O:28:THR:HG23	1:O:30:MET:H	1.63	0.64
2:L:133:LEU:HD21	2:L:139:GLU:HB2	1.80	0.64
1:E:44:GLU:OE1	1:E:46:LYS:HG3	1.99	0.63
1:Y:9:PRO:HD2	1:Y:9:PRO:O	1.96	0.63
2:H:29:GLU:OE1	2:H:143:LYS:NZ	2.28	0.63
1:Q:283:THR:HG22	1:Q:285:MET:N	2.08	0.63
1:O:156:LYS:HD2	1:O:196:GLN:HB2	1.80	0.63
1:Q:18:HIS:ND1	2:R:17:MET:O	2.27	0.63
1:W:29:ILE:HD11	2:X:102:MET:HG2	1.80	0.63
2:J:151:SER:O	2:J:156:THR:N	2.32	0.63
1:M:283:THR:HB	1:M:286:GLY:O	1.99	0.62
1:M:268:MET:HE3	1:M:284:PRO:HA	1.82	0.62
1:G:59:LEU:HD13	1:G:82:VAL:HG11	1.81	0.62
1:W:126:SER:HB2	1:W:166:ARG:HH22	1.62	0.62
1:Y:150:ASN:HA	1:Y:256:TYR:HD2	1.63	0.62
1:M:12:GLN:HE21	2:N:137:CYS:HB3	1.63	0.62
2:F:84:MET:HE2	2:F:85:GLU:HG2	1.79	0.62
2:J:57:ASP:O	2:J:60:ASN:HB2	1.98	0.62
2:T:4:GLY:HA3	2:V:117:ASN:ND2	2.15	0.62
2:b:3:PHE:CE2	2:b:113:SER:HB2	2.35	0.62
1:W:200:THR:HA	1:W:248:ASN:OD1	2.00	0.62
1:E:56:VAL:HB	1:E:85:SER:HB3	1.82	0.62
1:O:116:ASN:HB2	1:O:261:LYS:HG2	1.82	0.61
1:Y:200:THR:HA	1:Y:248:ASN:OD1	2.00	0.61
2:Z:149:MET:O	2:Z:153:ARG:HG3	1.99	0.61
1:C:26:VAL:HA	1:C:313:ARG:NH2	2.14	0.61
1:K:283:THR:HB	1:K:286:GLY:O	2.01	0.61
1:a:135:VAL:HG23	1:a:146:SER:HA	1.83	0.61
2:T:68:ARG:NH2	2:X:83:LYS:HG3	2.14	0.61
1:Q:65:SER:OG	1:Q:96:ASP:HA	2.00	0.61
2:N:99:LEU:HD13	2:R:98:LEU:HD21	1.82	0.61
2:b:72:ASN:OD1	2:b:75:ARG:NH2	2.33	0.61
1:M:192:THR:HG21	1:c:196:GLN:HE22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:PHE:H	2:B:92:TRP:NE1	1.99	0.61
1:c:26:VAL:HG21	1:c:317:ALA:HB2	1.83	0.61
1:O:29:ILE:HD11	2:P:102:MET:HG2	1.83	0.61
2:F:57:ASP:O	2:F:60:ASN:HB2	2.00	0.61
2:d:72:ASN:OD1	2:d:75:ARG:NH1	2.33	0.61
1:M:29:ILE:HD11	2:N:102:MET:HA	1.82	0.61
1:W:265:SER:OG	1:W:266:THR:N	2.34	0.61
2:T:84:MET:HE2	2:T:85:GLU:HG2	1.83	0.61
1:E:192:THR:CG2	1:U:192:THR:HG21	2.31	0.60
1:O:283:THR:HB	1:O:286:GLY:O	2.00	0.60
2:D:151:SER:O	2:D:156:THR:N	2.34	0.60
1:K:294:PHE:HZ	2:L:59:MET:HE2	1.66	0.60
1:a:13:ILE:HG22	2:b:138:PHE:HB2	1.82	0.60
2:V:24:TYR:CD2	2:V:153:ARG:HG2	2.36	0.60
1:W:288:ILE:HD11	1:W:297:ILE:HG13	1.82	0.60
2:H:151:SER:O	2:H:156:THR:N	2.34	0.60
1:C:100:GLY:HA3	1:C:230:MET:O	2.02	0.60
2:N:57:ASP:O	2:N:60:ASN:HB2	2.02	0.60
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.37	0.60
1:Q:28:THR:HG23	1:Q:30:MET:H	1.67	0.60
1:a:183:HIS:ND1	1:a:195:TYR:OH	2.25	0.60
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.84	0.60
1:M:55:ASP:O	1:M:278:ASN:ND2	2.34	0.60
1:M:174:GLU:HG3	1:M:259:LYS:HB3	1.82	0.60
1:Y:322:ASN:OD1	1:Y:323:SER:N	2.35	0.60
2:Z:55:ILE:HG12	2:Z:99:LEU:HD21	1.84	0.59
1:I:316:LEU:HD23	2:J:100:VAL:HG13	1.82	0.59
1:K:284:PRO:HG2	1:K:298:HIS:CE1	2.37	0.59
1:E:204:VAL:HG12	1:E:209:LEU:HD23	1.85	0.59
1:S:283:THR:HB	1:S:286:GLY:O	2.03	0.59
1:W:14:CYS:HB2	2:X:25:HIS:HB3	1.85	0.59
1:a:48:ASN:HD21	1:a:287:ALA:HB3	1.68	0.59
2:N:84:MET:HE2	2:N:85:GLU:HG2	1.85	0.59
2:b:167:ARG:NH1	2:b:171:GLU:OE2	2.36	0.59
1:A:61:LEU:HA	1:A:79:PHE:CZ	2.38	0.59
1:C:318:ILE:HG23	2:D:48:VAL:HG11	1.84	0.59
1:E:200:THR:HA	1:E:248:ASN:OD1	2.03	0.59
1:S:147:PHE:CE1	1:S:230:MET:HE3	2.38	0.59
1:a:179:LEU:HD23	1:a:234:TRP:HB3	1.85	0.59
2:b:55:ILE:HG12	2:b:99:LEU:HD21	1.84	0.59
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:288:ILE:HD11	1:U:297:ILE:HG13	1.83	0.58
1:Q:166:ARG:HG3	1:Q:166:ARG:NH1	2.16	0.58
2:b:2:LEU:HG	2:d:3:PHE:HZ	1.68	0.58
1:S:49:GLY:HA2	1:S:285:MET:O	2.03	0.58
1:E:126:SER:OG	1:E:166:ARG:NH2	2.35	0.58
1:S:90:LYS:NZ	1:S:273:GLU:OE2	2.35	0.58
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.83	0.58
1:S:28:THR:HG23	1:S:30:MET:H	1.68	0.58
2:B:124:LEU:HD22	2:J:134:GLY:HA2	1.85	0.58
1:Y:156:LYS:HD2	1:Y:196:GLN:HB2	1.86	0.58
2:b:169:LYS:HG3	2:b:177:ARG:NH2	2.19	0.58
2:B:2:LEU:O	2:H:113:SER:OG	2.21	0.57
1:A:268:MET:HE3	1:A:284:PRO:HA	1.85	0.57
1:K:61:LEU:HA	1:K:79:PHE:CZ	2.39	0.57
1:Q:147:PHE:CZ	1:Q:230:MET:HE3	2.39	0.57
1:U:147:PHE:CZ	1:U:230:MET:HE3	2.39	0.57
1:C:28:THR:HG22	1:C:30:MET:H	1.69	0.57
1:G:187:ASP:OD2	1:G:189:ALA:HB3	2.05	0.57
1:Q:40:GLN:HB2	1:Q:318:ILE:HD11	1.85	0.57
2:R:57:ASP:O	2:R:60:ASN:HB2	2.05	0.57
1:W:28:THR:HG23	1:W:30:MET:H	1.68	0.57
1:c:48:ASN:HD21	1:c:287:ALA:HB3	1.69	0.57
1:O:320:LEU:HD23	2:P:111:HIS:HB3	1.85	0.57
1:S:147:PHE:CZ	1:S:230:MET:HE3	2.39	0.57
1:W:56:VAL:HB	1:W:85:SER:HB3	1.86	0.57
1:W:180:TRP:HZ3	1:W:235:THR:HG22	1.69	0.57
2:T:24:TYR:CD2	2:T:153:ARG:HG2	2.39	0.57
1:I:14:CYS:HB2	2:J:25:HIS:HB3	1.85	0.57
1:I:37:THR:HG22	1:I:38:HIS:CD2	2.39	0.57
1:U:231:GLU:HG2	1:U:233:PHE:CE1	2.39	0.57
1:W:61:LEU:HA	1:W:79:PHE:CZ	2.39	0.57
1:E:179:LEU:O	1:E:254:PRO:HB3	2.05	0.57
2:Z:167:ARG:O	2:Z:171:GLU:HG2	2.05	0.57
1:Y:28:THR:HG22	1:Y:30:MET:H	1.70	0.57
1:K:318:ILE:HG23	2:L:48:VAL:HG11	1.87	0.56
2:N:10:ILE:HG12	2:N:136:GLY:HA3	1.86	0.56
2:T:106:ARG:HG3	2:V:106:ARG:HH22	1.70	0.56
2:Z:84:MET:HE2	2:Z:85:GLU:HG2	1.87	0.56
1:E:166:ARG:HG3	1:E:166:ARG:NH1	2.12	0.56
1:U:231:GLU:HG2	1:U:233:PHE:HE1	1.70	0.56
1:U:261:LYS:HD2	1:a:141:TYR:OH	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HD2	1:E:196:GLN:HB2	1.86	0.56
1:S:123:ILE:HG13	1:S:124:ILE:HG13	1.86	0.56
1:a:147:PHE:CZ	1:a:230:MET:HE3	2.41	0.56
1:c:61:LEU:HA	1:c:79:PHE:CZ	2.39	0.56
2:H:53:ASN:O	2:H:57:ASP:HB2	2.05	0.56
4:m:1:NAG:H4	4:m:2:NAG:H4	1.86	0.56
1:U:100:GLY:HA3	1:U:230:MET:O	2.05	0.56
2:B:151:SER:O	2:B:156:THR:N	2.37	0.56
1:M:70:LEU:O	1:M:150:ASN:ND2	2.39	0.56
1:M:311:SER:HB3	2:N:97:GLU:OE2	2.05	0.56
1:S:26:VAL:HG21	1:S:317:ALA:HB2	1.88	0.56
1:S:318:ILE:HG23	2:T:48:VAL:HG11	1.88	0.56
1:O:100:GLY:HA3	1:O:230:MET:O	2.06	0.56
1:S:269:LYS:HE3	2:T:69:GLU:OE1	2.06	0.56
1:W:83(A):GLU:OE1	1:W:261:LYS:NZ	2.38	0.56
1:W:307:LYS:NZ	2:X:64:GLU:OE2	2.38	0.56
1:A:206:THR:HB	1:A:209:LEU:HB3	1.88	0.56
1:W:135:VAL:HG23	1:W:146:SER:HA	1.88	0.56
1:I:202:ILE:HD11	1:I:251:PHE:HA	1.88	0.56
1:M:73:ASN:ND2	1:M:97:CYS:HB3	2.21	0.56
1:Q:166:ARG:HH11	1:Q:166:ARG:CG	2.15	0.56
2:P:122:VAL:HA	2:P:125:GLN:HE21	1.70	0.56
2:Z:133:LEU:O	2:b:127:ARG:NH1	2.38	0.55
1:G:283:THR:HB	1:G:286:GLY:O	2.06	0.55
1:c:115:ILE:HD13	1:c:260:ILE:HG12	1.88	0.55
1:U:130:HIS:CE1	1:U:164:ILE:HG12	2.41	0.55
1:c:318:ILE:HG23	2:d:48:VAL:HG11	1.88	0.55
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.88	0.55
1:K:294:PHE:CZ	2:L:59:MET:HE2	2.41	0.55
2:P:28:ASN:HD22	2:P:145:ASP:HA	1.71	0.55
2:Z:51:LYS:HD3	2:Z:103:GLU:HB3	1.88	0.55
1:W:180:TRP:CZ3	1:W:235:THR:HG22	2.41	0.55
1:K:183:HIS:HB2	1:K:252:ILE:HD11	1.89	0.55
1:Y:48:ASN:ND2	1:Y:287:ALA:HB3	2.22	0.55
2:N:76:ARG:NH1	2:P:74:GLU:OE1	2.39	0.55
2:Z:169:LYS:HD2	2:Z:172:GLU:OE1	2.06	0.55
1:U:123:ILE:HG13	1:U:124:ILE:HG13	1.88	0.55
2:X:55:ILE:HG12	2:X:99:LEU:HD21	1.88	0.55
1:U:73:ASN:HD21	1:U:97:CYS:HB3	1.72	0.55
2:J:53:ASN:O	2:J:57:ASP:HB2	2.06	0.55
2:P:125:GLN:OE1	2:P:155:GLY:HA2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.70	0.55
1:K:26:VAL:HG12	1:K:315:VAL:HG12	1.89	0.55
1:A:56:VAL:HB	1:A:85:SER:HB3	1.89	0.55
2:X:68:ARG:NH1	2:X:81:ASN:OD1	2.40	0.55
1:C:192:THR:CG2	1:W:192:THR:HG21	2.35	0.54
1:I:62:ARG:NH1	1:I:78:GLU:OE2	2.39	0.54
1:I:283:THR:HG22	1:I:285:MET:N	2.10	0.54
1:U:48:ASN:HD21	1:U:287:ALA:HB3	1.73	0.54
1:S:75:MET:HE1	1:S:140:PRO:HG2	1.87	0.54
2:T:62:GLN:HG3	2:T:92:TRP:CG	2.42	0.54
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.54
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.88	0.54
2:d:70:PHE:CD2	2:d:78:GLU:HA	2.42	0.54
1:M:182:ILE:HD11	1:M:215:PRO:HD3	1.89	0.54
1:Q:61:LEU:HA	1:Q:79:PHE:CZ	2.42	0.54
2:D:106:ARG:CG	2:F:106:ARG:HH22	2.19	0.54
1:K:188:ALA:O	1:K:192:THR:HG22	2.07	0.54
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.41	0.54
3:h:1:NAG:O3	3:h:2:NAG:O5	2.24	0.54
1:W:133(A):LEU:O	1:W:135:VAL:HG12	2.06	0.54
2:F:77:ILE:HA	2:F:80:LEU:HB3	1.88	0.54
1:A:29:ILE:HD11	2:B:102:MET:HA	1.90	0.54
1:c:28:THR:O	1:c:32:LYS:NZ	2.34	0.54
1:C:265:SER:OG	1:C:266:THR:N	2.40	0.54
1:K:204:VAL:HG22	1:K:245:PHE:HD1	1.72	0.54
1:O:251:PHE:CE2	1:O:253:ALA:HB2	2.43	0.54
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.72	0.54
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.43	0.54
1:E:247:SER:OG	1:E:248:ASN:N	2.41	0.54
1:Y:116:ASN:HB2	1:Y:261:LYS:HG2	1.90	0.54
1:Y:283:THR:HB	1:Y:286:GLY:O	2.08	0.54
2:Z:102:MET:HE2	2:d:102:MET:HE1	1.89	0.54
4:y:1:NAG:H3	4:y:2:NAG:O7	2.08	0.54
1:M:73:ASN:HB3	1:M:76:CYS:SG	2.48	0.53
1:M:179:LEU:HD23	1:M:234:TRP:HB3	1.89	0.53
2:X:3:PHE:CE2	2:X:113:SER:HB2	2.43	0.53
1:E:57:LYS:HE2	1:E:274:TYR:CZ	2.43	0.53
1:U:29:ILE:HD11	2:V:102:MET:HG2	1.90	0.53
1:W:283:THR:HB	1:W:286:GLY:O	2.08	0.53
2:Z:54:SER:O	2:Z:58:LYS:HG2	2.08	0.53
1:C:73:ASN:ND2	1:C:97:CYS:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:135:VAL:HG22	1:Q:146:SER:HA	1.89	0.53
1:c:206:THR:HB	1:c:209:LEU:H	1.74	0.53
2:d:30:GLN:HE21	2:d:30:GLN:N	2.07	0.53
1:O:295:HIS:CE1	1:O:308:TYR:HD1	2.27	0.53
1:Q:204:VAL:HG12	1:Q:209:LEU:HD23	1.91	0.53
1:c:13:ILE:HG22	2:d:138:PHE:HB2	1.89	0.53
2:V:134:GLY:HA2	2:X:124:LEU:HD22	1.90	0.53
1:W:247:SER:OG	1:W:248:ASN:N	2.40	0.53
2:J:22:TYR:OH	2:J:111:HIS:ND1	2.24	0.53
1:a:48:ASN:ND2	1:a:287:ALA:HB3	2.24	0.53
2:D:51:LYS:HD3	2:D:103:GLU:HB3	1.91	0.53
1:C:75:MET:HE2	1:C:75:MET:HA	1.90	0.53
1:K:200:THR:HA	1:K:248:ASN:OD1	2.08	0.53
1:O:62:ARG:HD3	1:O:273:GLU:OE1	2.08	0.53
1:c:18:HIS:HB2	2:d:21:TRP:HA	1.90	0.53
2:b:169:LYS:HG3	2:b:177:ARG:HH22	1.71	0.53
1:E:206:THR:HG22	1:E:208:THR:H	1.73	0.53
1:K:288:ILE:HD11	1:K:297:ILE:HG13	1.91	0.53
1:O:11:ASP:C	2:P:140:PHE:HD2	2.17	0.53
1:Y:15:ILE:O	2:Z:10:ILE:HD13	2.09	0.53
1:c:29:ILE:HD11	2:d:102:MET:HG2	1.91	0.53
2:Z:159:TYR:HB3	2:Z:160:PRO:HD3	1.90	0.53
2:d:30:GLN:HE22	2:d:145:ASP:HA	1.73	0.53
1:C:52:CYS:HB3	1:C:278:ASN:HA	1.91	0.53
2:T:134:GLY:HA2	2:V:124:LEU:HD22	1.91	0.53
2:Z:150:GLU:OE2	2:Z:153:ARG:HD2	2.08	0.53
1:K:206:THR:HG22	1:K:207:SER:N	2.24	0.52
1:M:43:LEU:HB2	1:M:314:LEU:HB2	1.91	0.52
1:U:99:PRO:HD2	1:U:226:LEU:HD12	1.91	0.52
1:S:288:ILE:HD11	1:S:297:ILE:HG13	1.89	0.52
2:L:118:LEU:HD12	2:L:121:LYS:HD3	1.89	0.52
2:T:143:LYS:HG3	2:T:165:GLU:OE2	2.10	0.52
1:C:57:LYS:HE2	1:C:274:TYR:CE2	2.43	0.52
1:K:136:SER:C	1:K:145:SER:HB2	2.34	0.52
1:M:202:ILE:HA	1:M:247:SER:HB3	1.91	0.52
2:N:70:PHE:HD1	2:R:76:ARG:NH1	2.08	0.52
2:Z:168:LEU:O	2:Z:172:GLU:HG3	2.08	0.52
1:M:200:THR:HG21	1:M:249:GLY:HA3	1.92	0.52
1:Q:147:PHE:CE1	1:Q:230:MET:HE3	2.45	0.52
2:Z:58:LYS:NZ	2:d:97:GLU:OE1	2.34	0.52
1:E:57:LYS:HE2	1:E:274:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:LEU:HA	1:E:79:PHE:CZ	2.45	0.52
1:I:41:ASP:OD2	1:I:45:LYS:NZ	2.42	0.52
1:W:206:THR:HG22	1:W:207:SER:N	2.25	0.52
1:Y:48:ASN:HD21	1:Y:287:ALA:HB3	1.73	0.52
1:c:70:LEU:O	1:c:150:ASN:ND2	2.41	0.52
2:J:62:GLN:HG3	2:J:92:TRP:CG	2.45	0.52
1:S:57:LYS:HE2	1:S:274:TYR:CE2	2.45	0.52
1:a:62:ARG:NH1	1:a:78:GLU:OE2	2.39	0.52
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.75	0.52
1:Y:9:PRO:O	1:Y:9:PRO:CD	2.57	0.52
1:a:266:THR:HG22	1:a:302:ILE:HD12	1.91	0.52
2:P:57:ASP:O	2:P:60:ASN:HB2	2.10	0.52
1:K:147:PHE:CZ	1:K:230:MET:HE3	2.44	0.52
1:C:176:LEU:HD23	1:C:258:TYR:O	2.10	0.52
1:Q:231:GLU:HG2	1:Q:233:PHE:CE1	2.45	0.52
1:U:283:THR:HB	1:U:286:GLY:O	2.10	0.52
2:J:130:ALA:HB2	2:J:140:PHE:HD1	1.74	0.52
1:C:43:LEU:HB2	1:C:314:LEU:HB2	1.92	0.52
1:O:169:ASN:O	1:O:171:THR:HG23	2.10	0.52
1:U:30:MET:HG2	2:X:47:GLY:O	2.10	0.52
2:d:169:LYS:O	2:d:172:GLU:HB3	2.10	0.52
1:Q:279:THR:HG21	1:Q:287:ALA:HB1	1.91	0.51
1:Y:231:GLU:HG2	1:Y:233:PHE:CE1	2.44	0.51
1:a:56:VAL:HB	1:a:85:SER:HB3	1.92	0.51
2:H:85:GLU:O	2:H:89:LEU:HG	2.09	0.51
1:Q:83(A):GLU:OE1	1:Q:261:LYS:NZ	2.43	0.51
1:K:136:SER:O	1:K:145:SER:HB2	2.10	0.51
1:c:48:ASN:ND2	1:c:287:ALA:HB3	2.26	0.51
2:R:24:TYR:CD2	2:R:153:ARG:HG2	2.45	0.51
2:V:57:ASP:O	2:V:60:ASN:HB2	2.10	0.51
1:M:136:SER:C	1:M:145:SER:HB2	2.36	0.51
1:Y:40:GLN:HB2	1:Y:318:ILE:HD11	1.92	0.51
2:T:133:LEU:HD12	2:T:137:CYS:HB2	1.92	0.51
1:Q:313:ARG:NH2	1:Q:315:VAL:HG21	2.24	0.51
2:H:59:MET:HE2	2:H:96:ALA:HB2	1.92	0.51
1:A:65:SER:OG	1:A:96:ASP:OD1	2.25	0.51
1:G:164:ILE:O	1:G:246:GLU:HA	2.10	0.51
1:O:61:LEU:HA	1:O:79:PHE:CZ	2.45	0.51
2:T:57:ASP:O	2:T:60:ASN:HB2	2.11	0.51
1:G:320:LEU:HD23	1:G:320:LEU:H	1.75	0.51
2:T:4:GLY:HA3	2:V:117:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:158:ASP:OD1	2:b:160:PRO:HD2	2.11	0.51
2:H:132:GLU:HG3	2:H:138:PHE:CE1	2.45	0.51
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.41	0.51
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.93	0.51
1:a:136:SER:O	1:a:145:SER:HB2	2.11	0.51
1:c:65:SER:OG	1:c:96:ASP:OD1	2.20	0.51
2:P:51:LYS:HD3	2:P:103:GLU:HB3	1.93	0.51
2:R:24:TYR:CE2	2:R:153:ARG:HG2	2.45	0.51
1:I:147:PHE:CZ	1:I:230:MET:HE3	2.46	0.51
1:K:120:LYS:HG2	1:K:256:TYR:HB3	1.93	0.51
1:Y:29:ILE:HD11	2:Z:102:MET:HG2	1.93	0.51
2:R:123:ARG:HD2	2:R:132:GLU:OE2	2.11	0.51
2:T:22:TYR:OH	2:T:111:HIS:ND1	2.36	0.51
1:C:283:THR:HB	1:C:286:GLY:O	2.10	0.50
1:O:206:THR:HG22	1:O:207:SER:N	2.25	0.50
1:Q:28:THR:HG22	1:Q:31:GLU:H	1.74	0.50
2:V:176:GLY:O	2:V:177:ARG:HG3	2.11	0.50
1:A:268:MET:HG2	1:A:284:PRO:HG3	1.93	0.50
1:A:49:GLY:HA2	1:A:285:MET:O	2.11	0.50
1:G:316:LEU:HD23	2:H:100:VAL:HG13	1.92	0.50
1:I:136:SER:O	1:I:145:SER:HB2	2.10	0.50
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.46	0.50
1:S:231:GLU:HG2	1:S:233:PHE:CE1	2.46	0.50
1:W:100:GLY:HA3	1:W:230:MET:O	2.11	0.50
2:L:151:SER:O	2:L:156:THR:N	2.43	0.50
2:d:84:MET:HE2	2:d:85:GLU:HG2	1.93	0.50
1:A:147:PHE:CZ	1:A:230:MET:HE3	2.47	0.50
1:M:179:LEU:O	1:M:254:PRO:HB3	2.11	0.50
1:S:55:ASP:O	1:S:278:ASN:ND2	2.43	0.50
2:T:159:TYR:HB3	2:T:160:PRO:HD3	1.93	0.50
1:Y:206:THR:HG22	1:Y:208:THR:H	1.76	0.50
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.47	0.50
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.12	0.50
1:Q:245:PHE:CD2	1:Q:251:PHE:HZ	2.30	0.50
1:a:83(A):GLU:OE1	1:a:261:LYS:NZ	2.45	0.50
2:L:54:SER:O	2:L:58:LYS:HG2	2.12	0.50
2:b:151:SER:HA	2:b:156:THR:HB	1.92	0.50
1:K:43:LEU:HB2	1:K:314:LEU:HB2	1.94	0.50
1:Q:100:GLY:HA3	1:Q:230:MET:O	2.11	0.50
1:a:28:THR:OG1	2:b:105:GLU:HB2	2.12	0.50
2:N:71:ASN:OD1	2:N:74:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:158:ASP:OD1	2:N:160:PRO:HD2	2.12	0.50
2:d:3:PHE:CE2	2:d:113:SER:HB2	2.47	0.50
1:E:206:THR:HG22	1:E:207:SER:N	2.27	0.50
1:K:147:PHE:CE1	1:K:230:MET:HE3	2.47	0.50
1:U:135:VAL:HG23	1:U:146:SER:HA	1.94	0.50
2:H:176:GLY:O	2:H:177:ARG:HG3	2.10	0.50
2:Z:3:PHE:CE1	2:Z:113:SER:HB2	2.47	0.50
2:b:118:LEU:HD12	2:b:121:LYS:HD3	1.94	0.50
2:b:105:GLU:HB3	2:d:106:ARG:HH22	1.77	0.50
1:I:53:ASP:OD1	1:I:274:TYR:OH	2.20	0.49
1:I:183:HIS:O	1:I:185:PRO:HD3	2.11	0.49
1:S:77:ASP:OD2	1:S:141:TYR:HE1	1.95	0.49
1:U:284:PRO:HG2	1:U:298:HIS:CE1	2.46	0.49
1:W:130:HIS:CE1	1:W:164:ILE:HG12	2.47	0.49
1:Y:119:GLU:HB3	1:Y:259:LYS:HB2	1.92	0.49
1:a:87:ILE:HD12	1:a:267:ILE:HG12	1.94	0.49
1:a:156:LYS:HD2	1:a:196:GLN:HB2	1.93	0.49
1:c:28:THR:HG22	1:c:30:MET:H	1.77	0.49
2:F:103:GLU:O	2:F:107:THR:OG1	2.24	0.49
2:J:159:TYR:HB3	2:J:160:PRO:HD3	1.94	0.49
2:P:68:ARG:NH1	2:P:81:ASN:OD1	2.45	0.49
2:X:62:GLN:HG3	2:X:92:TRP:CD2	2.47	0.49
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.27	0.49
1:O:170:ASN:HB2	1:O:237:LEU:HD23	1.93	0.49
1:W:204:VAL:HG12	1:W:209:LEU:HD23	1.94	0.49
2:V:167:ARG:O	2:V:171:GLU:HG2	2.12	0.49
1:A:240:ASN:O	3:e:1:NAG:H82	2.12	0.49
1:E:165:LYS:HE2	1:E:246:GLU:OE2	2.12	0.49
1:G:206:THR:HB	1:G:209:LEU:H	1.76	0.49
1:M:105:TYR:CE2	1:M:109:LYS:HE3	2.48	0.49
1:c:295:HIS:CE1	1:c:308:TYR:HD1	2.30	0.49
2:L:41:THR:O	2:L:45:ILE:HG13	2.12	0.49
1:G:48:ASN:O	1:G:50:LYS:HG3	2.13	0.49
1:Q:266:THR:HG22	1:Q:302:ILE:HD12	1.94	0.49
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.95	0.49
2:H:116:LYS:HZ1	2:J:116:LYS:NZ	2.10	0.49
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.13	0.49
1:E:26:VAL:HG12	1:E:315:VAL:HG12	1.94	0.49
1:a:283:THR:HB	1:a:286:GLY:O	2.12	0.49
1:c:200:THR:HA	1:c:248:ASN:OD1	2.12	0.49
2:B:105:GLU:HB3	2:H:106:ARG:HH22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:SER:OG	1:K:246:GLU:HB3	2.13	0.49
1:Q:206:THR:HG22	1:Q:208:THR:H	1.77	0.49
1:A:202:ILE:HD11	1:A:251:PHE:HA	1.94	0.49
1:A:206:THR:CG2	1:A:207:SER:N	2.75	0.49
1:M:22:SER:O	1:M:322:ASN:ND2	2.45	0.49
1:O:37:THR:HG22	1:O:38:HIS:CE1	2.48	0.49
1:U:135:VAL:HG23	1:U:146:SER:CA	2.43	0.49
2:V:159:TYR:HB3	2:V:160:PRO:HD3	1.94	0.49
2:Z:58:LYS:NZ	2:d:97:GLU:HB3	2.28	0.49
4:z:1:NAG:O3	4:z:2:NAG:H2	2.13	0.49
1:O:73:ASN:HD21	1:O:97:CYS:HB3	1.76	0.49
1:S:61:LEU:HA	1:S:79:PHE:HZ	1.73	0.49
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.12	0.49
2:V:39:GLU:O	2:V:43:LYS:HB2	2.13	0.49
1:I:182:ILE:HD11	1:I:215:PRO:HD3	1.94	0.49
1:S:206:THR:HG22	1:S:207:SER:N	2.28	0.49
1:W:135:VAL:HG23	1:W:146:SER:CA	2.43	0.49
1:W:176:LEU:HD23	1:W:258:TYR:O	2.12	0.49
1:a:100:GLY:HA3	1:a:230:MET:O	2.12	0.49
1:c:30:MET:HG2	2:Z:47:GLY:O	2.13	0.49
2:T:46:ASP:O	2:T:50:ASN:ND2	2.46	0.49
1:C:251:PHE:CE2	1:C:253:ALA:HB2	2.48	0.48
1:K:30:MET:HG2	2:D:47:GLY:O	2.13	0.48
1:O:102:PHE:HE1	1:O:234:TRP:CD1	2.31	0.48
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.53	0.48
2:N:159:TYR:HB3	2:N:160:PRO:HD3	1.95	0.48
1:A:264:ASP:OD1	1:A:264:ASP:N	2.45	0.48
1:C:160:THR:HG22	1:S:165:LYS:NZ	2.28	0.48
2:H:30:GLN:HE22	2:H:145:ASP:HA	1.78	0.48
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.78	0.48
2:b:71:ASN:OD1	2:b:74:GLU:HG3	2.14	0.48
1:Q:43:LEU:HB2	1:Q:314:LEU:HB2	1.95	0.48
1:W:57:LYS:HE2	1:W:274:TYR:CE2	2.49	0.48
1:c:231:GLU:HG2	1:c:233:PHE:HE1	1.78	0.48
2:T:113:SER:OG	2:X:2:LEU:O	2.21	0.48
1:A:17:TYR:CE2	2:B:6:ILE:HA	2.48	0.48
1:K:295:HIS:CD2	1:K:306:PRO:HG2	2.48	0.48
1:Q:98:TYR:CG	1:Q:230:MET:HE2	2.49	0.48
1:S:206:THR:HB	1:S:209:LEU:CB	2.43	0.48
2:B:58:LYS:NZ	2:J:97:GLU:OE1	2.46	0.48
2:P:159:TYR:HB3	2:P:160:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG22	1:A:207:SER:N	2.28	0.48
1:G:172:ASN:CG	1:G:259:LYS:HD3	2.38	0.48
1:M:183:HIS:ND1	1:M:195:TYR:OH	2.24	0.48
1:a:200:THR:HA	1:a:248:ASN:OD1	2.14	0.48
1:c:206:THR:HG22	1:c:207:SER:N	2.28	0.48
2:L:77:ILE:HA	2:L:80:LEU:HB3	1.96	0.48
2:V:62:GLN:HG3	2:V:92:TRP:CD2	2.49	0.48
2:b:98:LEU:HD21	2:d:99:LEU:HD13	1.94	0.48
1:I:172:ASN:CG	1:I:259:LYS:HD3	2.39	0.48
1:O:196:GLN:HE22	1:a:192:THR:HG21	1.79	0.48
2:H:167:ARG:O	2:H:171:GLU:HG3	2.14	0.48
4:k:1:NAG:H4	4:k:2:NAG:O3	2.14	0.48
1:M:186:ASN:HB2	1:M:190:GLU:OE2	2.13	0.48
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.96	0.48
1:C:37:THR:HG22	1:C:38:HIS:CD2	2.49	0.48
1:K:204:VAL:HG22	1:K:245:PHE:CD1	2.48	0.48
1:Q:195:TYR:O	1:Q:197:ASN:N	2.46	0.48
1:U:11:ASP:HB2	2:V:140:PHE:HD2	1.79	0.48
1:U:134:GLY:HA3	1:U:153:TRP:HB3	1.94	0.48
1:W:42:ILE:O	1:W:294:PHE:HB2	2.13	0.48
2:D:134:GLY:HA2	2:F:124:LEU:HD22	1.96	0.48
2:N:128:ASP:O	2:N:170:ARG:NH1	2.47	0.48
1:A:124:ILE:HD12	1:A:254:PRO:HG2	1.96	0.47
1:E:116:ASN:HB2	1:E:261:LYS:HG2	1.96	0.47
1:I:28:THR:HG23	1:I:30:MET:H	1.79	0.47
2:F:68:ARG:NH1	2:F:81:ASN:OD1	2.46	0.47
1:E:62:ARG:O	1:E:90:LYS:HD2	2.14	0.47
1:O:206:THR:HB	1:O:209:LEU:HB2	1.96	0.47
2:F:118:LEU:HD12	2:F:121:LYS:HD3	1.96	0.47
2:H:94:TYR:CD1	2:H:94:TYR:C	2.92	0.47
2:Z:149:MET:HB2	2:Z:153:ARG:HH21	1.79	0.47
2:Z:173:ILE:CG2	2:Z:177:ARG:HE	2.26	0.47
1:A:202:ILE:HG12	1:A:247:SER:OG	2.15	0.47
1:E:42:ILE:HG13	1:E:314:LEU:HB3	1.96	0.47
1:G:135:VAL:HG23	1:G:146:SER:HA	1.96	0.47
1:I:44:GLU:HB2	1:I:292:MET:HG3	1.97	0.47
2:D:131:LYS:HB3	2:D:139:GLU:HB3	1.96	0.47
2:R:159:TYR:HB3	2:R:160:PRO:HD3	1.97	0.47
2:V:68:ARG:NH1	2:V:81:ASN:OD1	2.47	0.47
1:A:100:GLY:HA3	1:A:230:MET:O	2.14	0.47
1:C:298:HIS:CE1	1:C:300:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:ASN:ND2	1:G:97:CYS:HB3	2.29	0.47
1:K:98:TYR:CG	1:K:230:MET:HE2	2.49	0.47
1:c:308:TYR:HD2	2:d:89:LEU:HD22	1.79	0.47
4:s:1:NAG:O3	4:s:2:NAG:H2	2.14	0.47
1:U:109:LYS:HD3	2:V:69:GLU:OE2	2.15	0.47
2:D:171:GLU:HA	2:D:174:SER:HB2	1.96	0.47
2:J:164:GLU:OE2	2:J:167:ARG:NE	2.46	0.47
2:N:98:LEU:HD21	2:P:99:LEU:HD13	1.96	0.47
2:T:80:LEU:HD13	2:V:81:ASN:OD1	2.15	0.47
2:V:2:LEU:O	2:X:113:SER:OG	2.31	0.47
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.30	0.47
1:I:251:PHE:CE2	1:I:253:ALA:HB2	2.49	0.47
1:K:247:SER:OG	1:K:248:ASN:N	2.45	0.47
1:Q:105:TYR:CE2	1:Q:109:LYS:HE3	2.50	0.47
1:Q:295:HIS:CE1	1:Q:308:TYR:HD1	2.32	0.47
2:D:62:GLN:HG3	2:D:92:TRP:CG	2.50	0.47
2:L:84:MET:CE	2:L:85:GLU:HG2	2.44	0.47
2:P:25:HIS:HA	2:P:33:GLY:O	2.14	0.47
2:X:6:ILE:HG13	2:X:112:ASP:HA	1.97	0.47
1:A:206:THR:HB	1:A:209:LEU:H	1.78	0.47
1:E:28:THR:HG23	1:E:30:MET:H	1.80	0.47
1:K:169:ASN:O	1:K:171:THR:HG23	2.14	0.47
1:M:172:ASN:HB3	1:M:174:GLU:OE2	2.14	0.47
1:O:73:ASN:ND2	1:O:97:CYS:HB3	2.29	0.47
1:O:266:THR:HG22	1:O:302:ILE:HD12	1.96	0.47
1:Q:116:ASN:HB2	1:Q:261:LYS:HG2	1.97	0.47
1:Q:247:SER:OG	1:Q:248:ASN:N	2.47	0.47
1:W:77:ASP:OD2	1:W:141:TYR:HE1	1.98	0.47
1:W:147:PHE:CZ	1:W:230:MET:HE3	2.49	0.47
2:B:83:LYS:HG3	2:H:68:ARG:HH21	1.79	0.47
2:D:55:ILE:HG12	2:D:99:LEU:HD21	1.96	0.47
2:F:150:GLU:OE2	2:F:153:ARG:HD2	2.15	0.47
1:S:116:ASN:HB2	1:S:261:LYS:HG2	1.96	0.47
1:W:179:LEU:HD23	1:W:234:TRP:HB3	1.96	0.47
1:Y:14:CYS:HB2	2:Z:25:HIS:HB3	1.97	0.47
2:d:159:TYR:HB3	2:d:160:PRO:HD3	1.96	0.47
1:A:29:ILE:HD11	2:B:102:MET:HG2	1.97	0.47
1:a:44:GLU:HB2	1:a:292:MET:HG3	1.97	0.47
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.95	0.47
1:M:28:THR:HG23	1:M:30:MET:H	1.79	0.47
1:Q:62:ARG:NH2	1:Q:78:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:307:LYS:NZ	2:V:60:ASN:O	2.47	0.47
1:c:50:LYS:HD3	1:c:275:GLY:HA3	1.97	0.47
2:d:30:GLN:HE21	2:d:30:GLN:H	1.61	0.47
1:E:307:LYS:HD2	2:F:62:GLN:HB3	1.97	0.46
1:O:196:GLN:NE2	1:a:192:THR:HG21	2.30	0.46
1:S:56:VAL:HB	1:S:85:SER:HB3	1.97	0.46
1:a:133(A):LEU:O	1:a:135:VAL:HG12	2.15	0.46
1:a:314:LEU:HD22	2:b:100:VAL:HG21	1.97	0.46
2:b:37:ASP:OD1	2:b:38:LYS:N	2.48	0.46
1:C:282:GLN:NE2	1:C:283:THR:H	2.13	0.46
2:b:57:ASP:O	2:b:60:ASN:HB2	2.14	0.46
1:A:14:CYS:O	2:B:24:TYR:HA	2.15	0.46
1:M:29:ILE:HD11	2:N:102:MET:HG2	1.96	0.46
2:D:54:SER:O	2:D:58:LYS:HG2	2.16	0.46
2:Z:28:ASN:ND2	2:Z:146:ASN:OD1	2.44	0.46
2:Z:51:LYS:NZ	2:Z:103:GLU:O	2.46	0.46
2:b:159:TYR:HB3	2:b:160:PRO:HD3	1.98	0.46
1:A:197:ASN:HA	1:A:198:PRO:HD3	1.87	0.46
1:K:165:LYS:HE2	1:K:246:GLU:OE2	2.15	0.46
2:F:51:LYS:HD3	2:F:103:GLU:HB3	1.97	0.46
2:Z:151:SER:O	2:Z:156:THR:N	2.48	0.46
2:d:141:TYR:O	2:d:169:LYS:HG2	2.15	0.46
1:C:206:THR:HG22	1:C:207:SER:N	2.30	0.46
1:E:160:THR:HG21	1:W:165:LYS:HE3	1.97	0.46
1:I:150:ASN:ND2	1:I:258:TYR:OH	2.48	0.46
1:K:182:ILE:HD11	1:K:215:PRO:HD3	1.96	0.46
1:a:206:THR:HG22	1:a:207:SER:N	2.30	0.46
2:J:59:MET:HE1	2:J:96:ALA:HB2	1.96	0.46
2:Z:119:TYR:OH	2:Z:132:GLU:OE1	2.28	0.46
1:C:61:LEU:HA	1:C:79:PHE:CZ	2.50	0.46
1:I:43:LEU:HB2	1:I:314:LEU:HB2	1.97	0.46
1:I:153:TRP:O	1:I:155:ILE:HD12	2.15	0.46
1:M:133:SER:O	1:M:133(A):LEU:HD23	2.16	0.46
1:M:138:ALA:C	1:M:140:PRO:HD3	2.40	0.46
1:a:49:GLY:HA2	1:a:285:MET:O	2.16	0.46
2:b:21:TRP:HZ3	2:b:45:ILE:HG13	1.79	0.46
1:A:18:HIS:HB2	2:B:21:TRP:HA	1.97	0.46
1:K:320:LEU:HB3	2:L:111:HIS:CD2	2.50	0.46
1:M:40:GLN:HB2	1:M:318:ILE:CD1	2.46	0.46
1:U:170:ASN:HB2	1:U:237:LEU:HD23	1.98	0.46
1:W:164:ILE:O	1:W:246:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:43:LEU:HD21	1:a:296:ASN:ND2	2.30	0.46
2:H:62:GLN:HG3	2:H:92:TRP:CG	2.51	0.46
1:E:283:THR:HB	1:E:286:GLY:O	2.15	0.46
1:K:320:LEU:HB3	2:L:111:HIS:CG	2.49	0.46
1:S:67:ALA:HB2	1:S:105:TYR:CE1	2.51	0.46
1:S:101:ASP:O	1:S:231:GLU:HA	2.16	0.46
1:c:33:ASN:ND2	4:0:1:NAG:O7	2.49	0.46
2:N:62:GLN:HG3	2:N:92:TRP:CG	2.51	0.46
2:b:147:GLU:HA	2:b:150:GLU:HB2	1.98	0.46
1:M:40:GLN:HB2	1:M:318:ILE:HD11	1.98	0.46
1:O:236:ILE:HD12	1:O:236:ILE:HG23	1.72	0.46
1:Q:192:THR:HG21	1:Y:196:GLN:HE22	1.81	0.46
1:S:122:GLN:NE2	1:S:125:PRO:HA	2.31	0.46
1:Y:11:ASP:HB2	2:Z:140:PHE:HB2	1.98	0.46
2:L:128:ASP:O	2:L:170:ARG:NH1	2.49	0.46
2:b:151:SER:O	2:b:156:THR:N	2.48	0.46
2:b:151:SER:O	2:b:157:TYR:N	2.49	0.46
1:C:230:MET:SD	1:C:252:ILE:HD11	2.55	0.46
1:E:206:THR:HB	1:E:209:LEU:H	1.81	0.46
1:G:73:ASN:O	1:G:76:CYS:HB2	2.15	0.46
1:G:176:LEU:HD23	1:G:258:TYR:O	2.16	0.46
1:W:53:ASP:OD1	1:W:57:LYS:HA	2.15	0.46
2:D:99:LEU:HD13	2:L:98:LEU:HD21	1.97	0.46
1:C:160:THR:HG22	1:S:165:LYS:HZ1	1.82	0.45
1:Q:245:PHE:CD2	1:Q:251:PHE:CZ	3.04	0.45
1:W:40:GLN:HB3	1:W:316:LEU:HB2	1.98	0.45
2:J:151:SER:HA	2:J:156:THR:HB	1.98	0.45
1:C:201:TYR:OH	1:C:246:GLU:OE1	2.28	0.45
1:G:135:VAL:HG23	1:G:146:SER:CA	2.46	0.45
1:Y:30:MET:HE3	2:Z:105:GLU:OE1	2.15	0.45
1:Y:65:SER:OG	1:Y:96:ASP:HA	2.16	0.45
1:c:177:LEU:HB3	1:c:258:TYR:HB2	1.97	0.45
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.16	0.45
2:B:97:GLU:OE1	2:H:58:LYS:NZ	2.49	0.45
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.99	0.45
2:d:123:ARG:HD2	2:d:132:GLU:OE2	2.16	0.45
1:A:40:GLN:OE1	1:A:318:ILE:HD11	2.16	0.45
1:A:183:HIS:HD2	1:A:229:ARG:O	1.99	0.45
1:G:182:ILE:HD11	1:G:215:PRO:CD	2.45	0.45
1:Q:206:THR:HB	1:Q:209:LEU:CB	2.47	0.45
2:D:58:LYS:HE2	2:L:101:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:LYS:HZ2	2:H:107:THR:HG1	1.56	0.45
2:Z:173:ILE:HG23	2:Z:177:ARG:NE	2.28	0.45
2:b:51:LYS:HD3	2:b:103:GLU:HB3	1.97	0.45
2:d:131:LYS:HB2	2:d:141:TYR:HE2	1.81	0.45
1:A:27:ASP:OD1	1:A:33:ASN:N	2.30	0.45
1:Q:62:ARG:O	1:Q:90:LYS:HD2	2.16	0.45
1:U:61:LEU:HA	1:U:79:PHE:HZ	1.81	0.45
1:c:133(A):LEU:O	1:c:135:VAL:HG12	2.16	0.45
1:K:56:VAL:HB	1:K:85:SER:HB3	1.98	0.45
2:H:54:SER:O	2:H:58:LYS:HG2	2.16	0.45
2:T:5:ALA:HA	2:T:9:PHE:CE1	2.52	0.45
2:T:68:ARG:HH22	2:X:83:LYS:HG3	1.79	0.45
1:M:102:PHE:HE1	1:M:234:TRP:CD1	2.35	0.45
1:Q:65:SER:OG	1:Q:96:ASP:OD1	2.25	0.45
1:S:156:LYS:NZ	1:S:193:LYS:O	2.44	0.45
1:Y:56:VAL:HB	1:Y:85:SER:HB3	1.99	0.45
2:H:17:MET:SD	2:H:23:GLY:HA3	2.57	0.45
2:L:42:GLN:HA	2:L:45:ILE:HD12	1.97	0.45
2:b:142:HIS:HD2	2:b:166:ALA:HB2	1.81	0.45
2:d:57:ASP:O	2:d:60:ASN:HB2	2.16	0.45
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.50	0.45
1:C:282:GLN:HE21	1:C:283:THR:H	1.64	0.45
1:G:28:THR:HG22	1:G:31:GLU:H	1.81	0.45
1:O:147:PHE:CZ	1:O:230:MET:HE3	2.51	0.45
1:W:77:ASP:O	1:W:80:ILE:HG13	2.16	0.45
1:Y:83(A):GLU:OE2	1:Y:261:LYS:NZ	2.49	0.45
1:a:320:LEU:HD13	2:b:6:ILE:HD13	1.98	0.45
2:N:125:GLN:OE1	2:N:155:GLY:HA2	2.16	0.45
2:R:71:ASN:C	2:R:71:ASN:OD1	2.60	0.45
1:C:317:ALA:O	2:D:107:THR:HG21	2.17	0.45
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.98	0.45
1:G:71:LEU:HD23	1:G:71:LEU:HA	1.82	0.45
1:Q:42:ILE:HG13	1:Q:314:LEU:HB3	1.98	0.45
1:S:179:LEU:HD23	1:S:234:TRP:HB3	1.99	0.45
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.51	0.45
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.16	0.45
1:U:179:LEU:HD23	1:U:234:TRP:HB3	1.99	0.45
1:W:316:LEU:HD13	2:X:52:VAL:HG22	1.98	0.45
1:Y:269:LYS:O	1:Y:284:PRO:HB3	2.17	0.45
2:V:77:ILE:HA	2:V:80:LEU:HB3	1.99	0.45
2:Z:23:GLY:HA3	2:Z:36:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:84:MET:HG3	2:b:84:MET:SD	2.56	0.45
1:A:37:THR:HG22	1:A:38:HIS:CD2	2.52	0.45
1:C:147:PHE:CZ	1:C:230:MET:HE3	2.52	0.45
1:C:155:ILE:CD1	1:C:194:LEU:HD22	2.47	0.45
1:M:200:THR:HG22	1:M:248:ASN:OD1	2.17	0.45
1:O:154:LEU:HA	1:O:154:LEU:HD23	1.75	0.45
1:W:37:THR:HG22	1:W:38:HIS:ND1	2.32	0.45
2:B:148:CYS:O	2:B:151:SER:OG	2.34	0.45
2:Z:58:LYS:HZ3	2:d:97:GLU:HB3	1.80	0.45
1:G:20:ASN:ND2	1:G:37:THR:HG23	2.32	0.44
1:O:83(A):GLU:OE1	1:O:261:LYS:NZ	2.49	0.44
1:Q:298:HIS:CE1	1:Q:300:LEU:HB2	2.52	0.44
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.44
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.52	0.44
2:L:28:ASN:ND2	2:L:30:GLN:OE1	2.50	0.44
2:N:3:PHE:CE2	2:N:113:SER:HB2	2.51	0.44
1:A:283:THR:HB	1:A:286:GLY:O	2.17	0.44
1:C:34:VAL:HG11	2:D:108:LEU:HD11	1.99	0.44
1:C:200:THR:HA	1:C:248:ASN:OD1	2.17	0.44
1:I:116:ASN:HB2	1:I:261:LYS:HG2	2.00	0.44
1:I:206:THR:HB	1:I:209:LEU:H	1.81	0.44
1:O:57:LYS:HE2	1:O:274:TYR:CE2	2.52	0.44
1:U:247:SER:OG	1:U:248:ASN:N	2.49	0.44
1:c:77:ASP:O	1:c:80:ILE:HG13	2.18	0.44
1:c:206:THR:HB	1:c:209:LEU:HB2	1.99	0.44
1:c:283:THR:HB	1:c:286:GLY:O	2.17	0.44
1:c:298:HIS:HA	1:c:299:PRO:HD3	1.77	0.44
2:H:167:ARG:NH1	2:H:171:GLU:OE2	2.50	0.44
2:N:55:ILE:HG12	2:N:99:LEU:CD2	2.48	0.44
1:A:195:TYR:O	1:A:197:ASN:N	2.47	0.44
1:K:37:THR:HG22	1:K:38:HIS:CD2	2.52	0.44
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.53	0.44
1:O:138:ALA:C	1:O:140:PRO:HD3	2.42	0.44
1:Y:206:THR:HG22	1:Y:207:SER:N	2.33	0.44
1:a:164:ILE:N	1:a:247:SER:O	2.50	0.44
1:c:58:PRO:HB3	1:c:86:TYR:CE1	2.53	0.44
2:H:76:ARG:HH12	2:J:74:GLU:CD	2.25	0.44
2:T:125:GLN:OE1	2:T:155:GLY:HA2	2.17	0.44
2:X:132:GLU:HG3	2:X:138:PHE:CE1	2.52	0.44
1:A:200:THR:HG22	1:A:248:ASN:OD1	2.17	0.44
1:E:66:VAL:HB	1:E:105:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:320:LEU:HB3	2:T:111:HIS:CG	2.52	0.44
1:W:26:VAL:HG12	1:W:315:VAL:HG12	2.00	0.44
1:Y:114:ARG:HH21	1:Y:263:GLY:C	2.24	0.44
1:a:135:VAL:HG23	1:a:146:SER:CA	2.47	0.44
2:P:19:ASP:OD1	2:P:19:ASP:N	2.51	0.44
2:T:70:PHE:CE2	2:T:78:GLU:HA	2.53	0.44
1:C:122:GLN:NE2	1:C:125:PRO:HA	2.33	0.44
1:C:247:SER:OG	1:C:248:ASN:N	2.41	0.44
1:K:122:GLN:HB2	1:K:256:TYR:CE1	2.52	0.44
1:K:283:THR:HG23	1:K:298:HIS:HB3	1.99	0.44
1:a:28:THR:HG22	1:a:31:GLU:O	2.18	0.44
1:c:147:PHE:CZ	1:c:230:MET:HE3	2.53	0.44
2:D:24:TYR:CD2	2:D:153:ARG:HG2	2.53	0.44
2:H:71:ASN:OD1	2:H:71:ASN:C	2.61	0.44
2:N:70:PHE:HD2	2:N:78:GLU:HG3	1.81	0.44
2:X:159:TYR:HB3	2:X:160:PRO:HD3	2.00	0.44
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.99	0.44
1:E:107:GLU:OE1	2:D:75:ARG:HB2	2.18	0.44
1:S:314:LEU:HD23	1:S:314:LEU:HA	1.89	0.44
1:a:307:LYS:HB3	2:b:62:GLN:NE2	2.32	0.44
1:E:88:VAL:HG22	1:E:268:MET:HE2	2.00	0.44
1:E:123:ILE:HG13	1:E:124:ILE:HG13	1.99	0.44
1:G:295:HIS:CE1	1:G:308:TYR:HD1	2.35	0.44
1:Q:82:VAL:HA	1:Q:83:PRO:HD3	1.82	0.44
1:U:206:THR:HG22	1:U:207:SER:N	2.33	0.44
1:Y:314:LEU:HD23	1:Y:314:LEU:HA	1.77	0.44
2:R:79:ASN:O	2:R:83:LYS:HG2	2.18	0.44
2:Z:6:ILE:HG13	2:Z:112:ASP:HA	2.00	0.44
1:A:42:ILE:HB	1:A:293:PRO:HG2	1.99	0.44
1:I:147:PHE:CE1	1:I:230:MET:HE3	2.52	0.44
1:I:288:ILE:HD11	1:I:297:ILE:CG1	2.48	0.44
1:O:236:ILE:HD13	1:O:236:ILE:HA	1.83	0.44
1:U:176:LEU:HD23	1:U:258:TYR:O	2.18	0.44
1:Y:28:THR:HG22	1:Y:31:GLU:H	1.83	0.44
2:F:17:MET:SD	2:F:23:GLY:HA3	2.58	0.44
2:H:76:ARG:NH2	2:J:74:GLU:OE2	2.51	0.44
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.18	0.44
1:E:73:ASN:ND2	1:E:97:CYS:HB3	2.33	0.44
1:M:61:LEU:HA	1:M:79:PHE:CZ	2.52	0.44
1:S:112:LEU:HD23	1:S:112:LEU:HA	1.68	0.44
1:S:112:LEU:HD23	1:S:115:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:295:HIS:ND1	1:W:297:ILE:HG12	2.33	0.44
2:F:24:TYR:CD2	2:F:153:ARG:HG2	2.53	0.44
2:T:167:ARG:NH2	2:X:174:SER:O	2.51	0.44
2:X:2:LEU:HD13	2:X:109:ASP:OD2	2.18	0.44
1:I:136:SER:C	1:I:145:SER:HB2	2.43	0.43
1:K:175:ASP:OD1	1:K:239:PRO:HD3	2.18	0.43
1:M:206:THR:HG22	1:M:207:SER:N	2.33	0.43
1:Q:156:LYS:HD2	1:Q:196:GLN:HB2	1.99	0.43
1:Q:259:LYS:NZ	3:j:1:NAG:H62	2.33	0.43
1:S:206:THR:HB	1:S:209:LEU:HB2	1.99	0.43
1:S:219:THR:O	1:U:205:GLY:HA3	2.18	0.43
1:a:30:MET:HB2	2:b:105:GLU:OE1	2.17	0.43
1:c:106:GLU:HB3	2:b:76:ARG:HD3	2.00	0.43
2:V:4:GLY:O	2:V:8:GLY:HA3	2.18	0.43
2:X:63:PHE:H	2:X:92:TRP:NE1	2.14	0.43
2:d:51:LYS:HD3	2:d:103:GLU:HB3	1.99	0.43
1:C:20:ASN:HD21	1:C:37:THR:HG23	1.81	0.43
1:C:283:THR:HG23	1:C:284:PRO:HD2	2.01	0.43
1:G:30:MET:HG2	2:J:47:GLY:O	2.18	0.43
1:S:226:LEU:HA	1:S:226:LEU:HD23	1.73	0.43
1:S:323:SER:HA	1:S:324:PRO:HD2	1.90	0.43
1:W:99:PRO:HD2	1:W:226:LEU:HD12	2.00	0.43
1:Y:231:GLU:HG2	1:Y:233:PHE:HE1	1.83	0.43
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.74	0.43
2:b:169:LYS:O	2:b:177:ARG:NH2	2.50	0.43
2:d:58:LYS:HA	2:d:58:LYS:HD3	1.81	0.43
1:C:73:ASN:HD21	1:C:97:CYS:HB3	1.82	0.43
1:E:147:PHE:HE1	1:E:230:MET:HE2	1.83	0.43
1:E:231:GLU:HG2	1:E:233:PHE:CE1	2.54	0.43
1:G:17:TYR:CE2	2:H:6:ILE:HA	2.54	0.43
1:G:58:PRO:HB3	1:G:86:TYR:CE1	2.52	0.43
1:I:89:GLU:O	1:I:269:LYS:HA	2.18	0.43
1:Q:298:HIS:HE1	1:Q:300:LEU:HD12	1.83	0.43
1:W:194:LEU:HA	1:W:194:LEU:HD23	1.79	0.43
1:a:98:TYR:CE2	1:a:226:LEU:HD13	2.53	0.43
1:a:112:LEU:HA	1:a:112:LEU:HD23	1.72	0.43
1:C:135:VAL:HG22	1:C:146:SER:C	2.43	0.43
1:E:26:VAL:HG12	1:E:315:VAL:CG1	2.47	0.43
1:E:314:LEU:HD23	1:E:314:LEU:HA	1.72	0.43
1:I:44:GLU:HB2	1:I:292:MET:HB2	1.99	0.43
1:K:206:THR:HB	1:K:209:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:GLN:HG2	2:P:139:GLU:HA	2.00	0.43
1:U:133(A):LEU:O	1:U:135:VAL:HG12	2.18	0.43
1:a:314:LEU:HD23	1:a:314:LEU:HA	1.72	0.43
2:N:55:ILE:HG12	2:N:99:LEU:HD21	1.99	0.43
2:Z:58:LYS:HA	2:Z:58:LYS:HD2	1.79	0.43
2:b:102:MET:HE1	2:d:102:MET:HE2	2.00	0.43
4:u:1:NAG:H3	4:u:2:NAG:H2	2.00	0.43
1:A:320:LEU:HD13	2:B:6:ILE:HD13	1.99	0.43
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.54	0.43
1:M:15:ILE:O	2:N:10:ILE:HD13	2.18	0.43
1:O:67:ALA:HB3	1:O:96:ASP:OD1	2.18	0.43
1:O:133(A):LEU:HD23	1:O:133(A):LEU:HA	1.69	0.43
1:O:206:THR:HG22	1:O:207:SER:H	1.83	0.43
1:S:200:THR:HG22	1:S:248:ASN:OD1	2.18	0.43
1:U:121:ILE:HG21	1:U:259:LYS:HE2	1.99	0.43
1:W:295:HIS:CD2	1:W:306:PRO:HG2	2.53	0.43
2:F:58:LYS:HA	2:F:58:LYS:HD3	1.74	0.43
2:H:123:ARG:HD2	2:H:132:GLU:OE2	2.19	0.43
2:Z:114:ASN:HA	2:Z:117:ASN:HB2	2.00	0.43
2:b:172:GLU:HG2	2:b:177:ARG:HG2	1.99	0.43
2:d:131:LYS:HB2	2:d:141:TYR:CE2	2.53	0.43
1:C:20:ASN:ND2	1:C:37:THR:HG23	2.34	0.43
1:C:67:ALA:HB2	1:C:105:TYR:CE1	2.54	0.43
1:E:73:ASN:HD21	1:E:97:CYS:HB3	1.83	0.43
1:E:206:THR:CG2	1:E:207:SER:N	2.82	0.43
1:U:147:PHE:HZ	1:U:230:MET:HE3	1.81	0.43
1:Y:136:SER:O	1:Y:145:SER:HB2	2.17	0.43
1:a:28:THR:HG23	1:a:30:MET:H	1.82	0.43
1:a:40:GLN:HB2	1:a:318:ILE:HD11	2.00	0.43
2:J:58:LYS:C	2:J:60:ASN:H	2.26	0.43
2:P:134:GLY:HA2	2:R:124:LEU:HD22	2.01	0.43
2:T:70:PHE:HD2	2:T:78:GLU:HG3	1.82	0.43
1:O:28:THR:HG22	1:O:31:GLU:H	1.83	0.43
1:O:206:THR:HB	1:O:209:LEU:CB	2.49	0.43
1:a:15:ILE:HG23	2:b:118:LEU:HD23	2.01	0.43
2:T:148:CYS:O	2:T:151:SER:OG	2.31	0.43
2:X:57:ASP:O	2:X:60:ASN:HB2	2.18	0.43
2:X:58:LYS:HD3	2:X:58:LYS:HA	1.78	0.43
1:C:102:PHE:O	1:C:105:TYR:HB2	2.18	0.43
1:G:283:THR:HG22	1:G:285:MET:N	2.11	0.43
1:O:48:ASN:ND2	1:O:287:ALA:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:188:ALA:O	1:a:192:THR:HG22	2.18	0.43
2:D:77:ILE:HA	2:D:80:LEU:HB3	1.99	0.43
2:H:133:LEU:HD11	2:H:139:GLU:HB2	2.00	0.43
2:P:151:SER:O	2:P:156:THR:N	2.52	0.43
2:X:133:LEU:HD12	2:X:137:CYS:HB2	1.99	0.43
2:X:151:SER:O	2:X:156:THR:N	2.52	0.43
2:d:158:ASP:OD1	2:d:160:PRO:HD2	2.17	0.43
1:I:295:HIS:HE2	1:I:301:THR:HG21	1.83	0.43
1:U:206:THR:CG2	1:U:207:SER:N	2.82	0.43
1:U:320:LEU:HB3	2:V:111:HIS:CG	2.54	0.43
1:W:126:SER:HB2	1:W:166:ARG:NH2	2.31	0.43
1:Y:198:PRO:HD2	1:Y:199:THR:H	1.84	0.43
1:a:14:CYS:HB2	2:b:25:HIS:HB3	2.00	0.43
2:H:55:ILE:HG12	2:H:99:LEU:HD21	2.01	0.43
2:J:24:TYR:CD2	2:J:153:ARG:HG2	2.54	0.43
2:d:123:ARG:HB2	2:d:138:PHE:CZ	2.54	0.43
1:E:147:PHE:CZ	1:E:230:MET:HE3	2.54	0.43
1:G:115:ILE:HD13	1:G:260:ILE:HG12	2.01	0.43
1:K:29:ILE:H	1:K:29:ILE:HG13	1.67	0.43
1:M:73:ASN:HD21	1:M:97:CYS:HB3	1.83	0.43
1:M:138:ALA:O	1:M:140:PRO:HD3	2.19	0.43
1:M:147:PHE:CZ	1:M:230:MET:HE3	2.54	0.43
1:M:156:LYS:HD2	1:M:196:GLN:HB2	2.01	0.43
1:U:133(A):LEU:C	1:U:155:ILE:HD12	2.44	0.43
1:U:137:SER:HA	1:U:145:SER:HB2	2.00	0.43
2:N:25:HIS:HA	2:N:33:GLY:O	2.18	0.43
2:Z:74:GLU:O	2:Z:77:ILE:HG13	2.19	0.43
2:b:74:GLU:O	2:b:77:ILE:HG13	2.19	0.43
1:E:197:ASN:HA	1:E:198:PRO:HD3	1.91	0.42
1:O:48:ASN:HD21	1:O:287:ALA:HB3	1.84	0.42
1:O:202:ILE:HD11	1:O:251:PHE:HA	2.01	0.42
1:Y:112:LEU:HD23	1:Y:112:LEU:HA	1.87	0.42
1:Y:183:HIS:O	1:Y:185:PRO:HD3	2.19	0.42
1:a:294:PHE:HZ	2:b:59:MET:HG3	1.84	0.42
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.54	0.42
1:C:279:THR:OG1	1:C:287:ALA:HB1	2.20	0.42
1:G:288:ILE:HD11	1:G:297:ILE:CG1	2.47	0.42
1:K:159:SER:O	1:K:196:GLN:NE2	2.52	0.42
1:M:62:ARG:NH2	1:M:78:GLU:OE1	2.53	0.42
1:M:82:VAL:HA	1:M:83:PRO:HD3	1.73	0.42
1:M:201:TYR:O	1:M:247:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:316:LEU:HA	1:S:316:LEU:HD23	1.86	0.42
1:U:112:LEU:HD23	1:U:112:LEU:HA	1.77	0.42
1:W:206:THR:CG2	1:W:207:SER:N	2.82	0.42
1:a:58:PRO:HB3	1:a:86:TYR:CE1	2.55	0.42
2:H:72:ASN:OD1	2:H:75:ARG:NH2	2.52	0.42
1:C:62:ARG:O	1:C:90:LYS:HD2	2.20	0.42
1:I:279:THR:HB	1:I:281:CYS:N	2.28	0.42
1:I:295:HIS:HE1	1:I:298:HIS:O	2.03	0.42
1:O:164:ILE:O	1:O:246:GLU:HA	2.20	0.42
1:O:173:GLN:HB2	1:O:174:GLU:OE1	2.19	0.42
2:B:116:LYS:O	2:B:116:LYS:HG2	2.19	0.42
2:B:151:SER:HA	2:B:156:THR:HB	2.01	0.42
2:N:118:LEU:HD12	2:N:121:LYS:HD3	2.01	0.42
2:b:102:MET:HE1	2:d:102:MET:CE	2.49	0.42
1:A:186:ASN:OD1	1:A:227:SER:HB3	2.19	0.42
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.19	0.42
1:I:318:ILE:HG23	2:J:48:VAL:HG11	2.01	0.42
1:Q:206:THR:HG22	1:Q:207:SER:N	2.33	0.42
1:Y:240:ASN:OD1	5:Y:2001:NAG:H5	2.19	0.42
1:Y:295:HIS:CE1	1:Y:308:TYR:HD1	2.37	0.42
1:c:269:LYS:O	1:c:284:PRO:HB3	2.19	0.42
2:N:55:ILE:O	2:N:59:MET:HG2	2.19	0.42
1:A:20:ASN:ND2	1:A:37:THR:HG23	2.34	0.42
1:G:14:CYS:O	2:H:24:TYR:HA	2.19	0.42
2:H:151:SER:HA	2:H:156:THR:HB	2.02	0.42
2:J:167:ARG:NH1	2:J:171:GLU:OE2	2.52	0.42
2:d:28:ASN:HB3	2:d:149:MET:CE	2.49	0.42
1:A:267:ILE:HD13	1:A:267:ILE:HG21	1.76	0.42
1:C:44:GLU:OE1	1:C:46:LYS:HG3	2.20	0.42
1:Q:11:ASP:OD2	2:R:144:CYS:N	2.50	0.42
1:Q:121:ILE:HD13	1:Q:121:ILE:HG21	1.71	0.42
1:Q:185:PRO:HG3	1:Q:191:GLN:OE1	2.20	0.42
1:Y:22:SER:O	1:Y:322:ASN:ND2	2.53	0.42
1:c:135:VAL:HG23	1:c:146:SER:HA	2.00	0.42
2:J:58:LYS:HD2	2:J:58:LYS:HA	1.85	0.42
2:V:158:ASP:OD1	2:V:160:PRO:HD2	2.18	0.42
1:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.42
1:I:75:MET:HE3	1:I:141:TYR:O	2.19	0.42
1:I:123:ILE:HG13	1:I:124:ILE:HG13	2.01	0.42
1:Q:30:MET:HG2	2:N:47:GLY:O	2.19	0.42
1:Q:298:HIS:HA	1:Q:299:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:51:LYS:HD3	2:R:103:GLU:HB3	2.02	0.42
2:R:68:ARG:NH1	2:R:81:ASN:OD1	2.53	0.42
2:R:158:ASP:OD1	2:R:160:PRO:HD2	2.20	0.42
1:A:147:PHE:CE1	1:A:230:MET:HE3	2.55	0.42
1:E:29:ILE:HD11	2:F:102:MET:HG2	2.02	0.42
1:G:52:CYS:HB3	1:G:278:ASN:HA	2.01	0.42
1:S:83(A):GLU:OE1	1:S:261:LYS:NZ	2.52	0.42
1:c:183:HIS:ND1	1:c:195:TYR:OH	2.42	0.42
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.19	0.42
2:R:148:CYS:O	2:R:151:SER:OG	2.24	0.42
2:V:148:CYS:O	2:V:151:SER:OG	2.34	0.42
1:A:29:ILE:H	1:A:29:ILE:HG13	1.72	0.42
1:K:293:PRO:HB3	2:L:56:ILE:HG12	2.01	0.42
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.20	0.42
1:S:307:LYS:NZ	2:T:60:ASN:O	2.53	0.42
1:a:209:LEU:HD12	1:a:209:LEU:HA	1.91	0.42
1:c:232:PHE:C	1:c:233:PHE:HD1	2.27	0.42
2:J:100:VAL:O	2:J:101:LEU:C	2.63	0.42
2:Z:59:MET:HB3	2:Z:62:GLN:OE1	2.19	0.42
1:A:285:MET:HE2	1:A:285:MET:HB3	1.81	0.42
1:K:226:LEU:HD23	1:K:226:LEU:HA	1.67	0.42
1:S:44:GLU:OE1	1:S:46:LYS:HE2	2.20	0.42
1:S:73:ASN:HB3	1:S:76:CYS:SG	2.59	0.42
1:W:181:GLY:O	1:W:252:ILE:HB	2.20	0.42
1:c:12:GLN:OE1	2:d:139:GLU:HG3	2.20	0.42
2:P:75:ARG:HA	2:P:75:ARG:HD3	1.90	0.42
2:P:158:ASP:OD1	2:P:160:PRO:HD2	2.18	0.42
2:Z:39:GLU:O	2:Z:43:LYS:HG3	2.19	0.42
1:I:18:HIS:N	2:J:21:TRP:O	2.47	0.41
1:a:170:ASN:ND2	1:a:239:PRO:HA	2.35	0.41
1:c:133(A):LEU:HA	1:c:133(A):LEU:HD23	1.82	0.41
1:C:77:ASP:OD1	1:C:149:ARG:NE	2.51	0.41
1:G:17:TYR:HB2	1:G:320:LEU:HD11	2.02	0.41
1:G:267:ILE:HG21	1:G:267:ILE:HD13	1.77	0.41
1:K:28:THR:HG23	1:K:30:MET:H	1.84	0.41
1:Q:126:SER:OG	1:Q:166:ARG:NH2	2.53	0.41
1:S:320:LEU:HB3	2:T:111:HIS:CD2	2.55	0.41
1:U:29:ILE:HD11	2:V:102:MET:HA	2.01	0.41
1:a:179:LEU:CD2	1:a:234:TRP:HB3	2.49	0.41
2:H:58:LYS:HD3	2:H:58:LYS:HA	1.70	0.41
2:d:3:PHE:HB3	2:d:116:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.81	0.41
1:E:121:ILE:HG21	1:E:121:ILE:HD13	1.82	0.41
1:I:206:THR:CG2	1:I:207:SER:N	2.82	0.41
1:U:20:ASN:HB2	1:U:21[A]:ASN:H	1.70	0.41
1:U:230:MET:SD	1:U:252:ILE:HD11	2.60	0.41
1:Y:247:SER:OG	1:Y:248:ASN:N	2.44	0.41
1:a:283:THR:HG23	1:a:298:HIS:HB3	2.02	0.41
2:B:98:LEU:HD21	2:H:99:LEU:HD13	2.02	0.41
2:P:148:CYS:O	2:P:152:VAL:HG23	2.19	0.41
1:A:174:GLU:OE2	1:A:259:LYS:NZ	2.51	0.41
1:G:105:TYR:CE2	1:G:109:LYS:HE3	2.55	0.41
1:I:308:TYR:HD2	2:J:89:LEU:HD22	1.86	0.41
1:K:307:LYS:HB3	2:L:62:GLN:NE2	2.36	0.41
1:U:313:ARG:NH2	1:U:315:VAL:HG21	2.35	0.41
1:W:141:TYR:CD2	1:W:142:GLN:HG2	2.56	0.41
1:Y:184:HIS:HA	1:Y:185:PRO:HD3	1.85	0.41
2:N:106:ARG:HH12	2:R:105:GLU:HB3	1.85	0.41
1:A:216:ARG:HH11	1:A:216:ARG:HD3	1.73	0.41
1:C:72:GLY:O	1:C:149:ARG:HG3	2.21	0.41
1:G:48:ASN:HD21	1:G:287:ALA:HB3	1.85	0.41
1:I:194:LEU:HD23	1:I:194:LEU:N	2.36	0.41
1:K:12:GLN:N	2:L:27:SER:O	2.49	0.41
1:K:192:THR:HG22	1:K:192:THR:H	1.65	0.41
1:M:181:GLY:O	1:M:252:ILE:HB	2.21	0.41
1:Q:72:GLY:O	1:Q:148:PHE:HA	2.19	0.41
1:U:314:LEU:HD23	1:U:314:LEU:HA	1.88	0.41
1:a:164:ILE:O	1:a:246:GLU:HA	2.20	0.41
1:a:279:THR:HG21	1:a:287:ALA:HB1	2.02	0.41
2:F:125:GLN:OE1	2:F:155:GLY:HA2	2.20	0.41
1:A:123:ILE:HG13	1:A:124:ILE:HG13	2.02	0.41
1:C:135:VAL:HG22	1:C:146:SER:O	2.21	0.41
1:a:114:ARG:HH21	1:a:263:GLY:C	2.28	0.41
2:T:84:MET:CE	2:T:85:GLU:HG2	2.49	0.41
2:V:62:GLN:HG3	2:V:92:TRP:CG	2.55	0.41
1:E:169:ASN:O	1:E:171:THR:HG23	2.20	0.41
1:E:200:THR:HG22	1:E:248:ASN:OD1	2.20	0.41
1:G:15:ILE:HD11	2:H:122:VAL:HG21	2.03	0.41
1:G:172:ASN:HB3	1:G:174:GLU:OE2	2.21	0.41
1:I:164:ILE:O	1:I:246:GLU:HA	2.21	0.41
1:I:216:ARG:HH11	1:I:216:ARG:HD3	1.68	0.41
1:O:37:THR:HG22	1:O:38:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:THR:HB	1:S:209:LEU:N	2.27	0.41
1:S:307:LYS:HB3	2:T:62:GLN:NE2	2.36	0.41
1:U:176:LEU:HD23	1:U:176:LEU:HA	1.85	0.41
2:N:2:LEU:HD13	2:N:109:ASP:OD2	2.20	0.41
2:N:77:ILE:O	2:N:80:LEU:HB3	2.21	0.41
2:Z:97:GLU:OE1	2:b:58:LYS:NZ	2.54	0.41
2:b:77:ILE:HA	2:b:80:LEU:HB3	2.03	0.41
1:A:316:LEU:HD21	2:B:100:VAL:HG22	2.03	0.41
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.83	0.41
1:E:135:VAL:HG22	1:E:146:SER:HA	2.01	0.41
1:I:206:THR:HG22	1:I:207:SER:N	2.36	0.41
1:I:320:LEU:HD13	2:J:6:ILE:HD13	2.02	0.41
1:K:317:ALA:O	2:L:107:THR:HG21	2.21	0.41
1:M:121:ILE:HG21	1:M:121:ILE:HD13	1.75	0.41
1:S:26:VAL:HG12	1:S:315:VAL:HG12	2.03	0.41
1:S:206:THR:CG2	1:S:207:SER:N	2.84	0.41
1:S:265:SER:OG	1:S:266:THR:N	2.53	0.41
1:W:20:ASN:HB2	1:W:21[A]:ASN:H	1.71	0.41
1:W:217:ILE:H	1:W:217:ILE:HD12	1.86	0.41
1:a:20:ASN:HB2	1:a:21[B]:ASN:H	1.75	0.41
1:c:265:SER:OG	1:c:266:THR:N	2.54	0.41
2:H:76:ARG:HH22	2:J:74:GLU:CD	2.28	0.41
2:L:77:ILE:O	2:L:80:LEU:HB3	2.20	0.41
2:T:63:PHE:H	2:T:92:TRP:NE1	2.17	0.41
2:b:59:MET:HE2	2:b:96:ALA:HB2	2.03	0.41
1:A:52:CYS:HB3	1:A:278:ASN:HA	2.02	0.41
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.56	0.41
1:C:107:GLU:O	1:C:111:LEU:HD13	2.21	0.41
1:I:18:HIS:HB2	2:J:21:TRP:HA	2.03	0.41
1:I:37:THR:HG22	1:I:38:HIS:CG	2.56	0.41
1:K:138:ALA:C	1:K:140:PRO:HD3	2.45	0.41
1:K:160:THR:OG1	1:U:165:LYS:NZ	2.46	0.41
1:M:206:THR:HB	1:M:209:LEU:H	1.86	0.41
1:M:283:THR:HG23	1:M:298:HIS:HB3	2.03	0.41
1:O:138:ALA:O	1:O:140:PRO:HD3	2.21	0.41
1:S:76:CYS:O	1:S:78:GLU:N	2.54	0.41
1:S:242:ALA:N	3:t:1:NAG:H82	2.36	0.41
1:W:169:ASN:O	1:W:171:THR:HG23	2.21	0.41
1:Y:124:ILE:HD12	1:Y:254:PRO:HG2	2.03	0.41
1:a:206:THR:HB	1:a:209:LEU:CB	2.51	0.41
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:ASP:OD1	2:L:19:ASP:N	2.54	0.41
2:L:125:GLN:OE1	2:L:155:GLY:HA2	2.21	0.41
2:N:4:GLY:O	2:N:8:GLY:HA3	2.21	0.41
2:P:44:ALA:HA	2:P:110:PHE:HE2	1.85	0.41
2:R:151:SER:O	2:R:157:TYR:N	2.52	0.41
2:V:106:ARG:HG2	2:X:106:ARG:HH22	1.85	0.41
1:A:279:THR:HB	1:A:280:LYS:H	1.66	0.41
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.85	0.41
1:C:206:THR:HG22	1:C:208:THR:H	1.86	0.41
1:E:86:TYR:OH	1:E:282:GLN:HG2	2.21	0.41
1:I:204:VAL:HG12	1:I:209:LEU:HD23	2.03	0.41
1:O:206:THR:CG2	1:O:207:SER:N	2.84	0.41
1:Q:119:GLU:HB2	1:Q:260(A):VAL:HG21	2.03	0.41
1:Q:167:SER:HB2	1:Q:244:ASN:OD1	2.20	0.41
1:Q:212:ARG:HH11	1:Q:212:ARG:HD2	1.72	0.41
1:S:209:LEU:HA	1:S:209:LEU:HD12	1.76	0.41
1:U:61:LEU:H	1:U:61:LEU:HG	1.72	0.41
1:a:20:ASN:HB2	1:a:21[A]:ASN:H	1.75	0.41
1:a:115:ILE:HD13	1:a:260:ILE:HG12	2.02	0.41
2:B:150:GLU:OE2	2:B:153:ARG:HD2	2.20	0.41
2:N:151:SER:O	2:N:156:THR:N	2.53	0.41
2:d:151:SER:O	2:d:156:THR:N	2.54	0.41
1:A:59:LEU:HD23	1:A:87:ILE:HG12	2.03	0.40
1:A:74:PRO:HG3	1:A:147:PHE:O	2.21	0.40
1:C:56:VAL:HB	1:C:85:SER:HB3	2.02	0.40
1:E:317:ALA:O	2:F:107:THR:HG21	2.21	0.40
1:U:200:THR:HA	1:U:248:ASN:OD1	2.21	0.40
1:W:11:ASP:HB2	2:X:140:PHE:HB2	2.04	0.40
1:W:58:PRO:HB3	1:W:86:TYR:CE1	2.56	0.40
1:Y:179:LEU:HD23	1:Y:234:TRP:HB3	2.03	0.40
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.56	0.40
2:D:5:ALA:HA	2:D:9:PHE:CE1	2.56	0.40
2:J:123:ARG:HD2	2:J:132:GLU:OE2	2.21	0.40
2:N:70:PHE:HD1	2:R:76:ARG:HH11	1.67	0.40
2:P:148:CYS:O	2:P:151:SER:OG	2.28	0.40
1:C:29:ILE:HD11	2:D:102:MET:HG2	2.03	0.40
1:C:147:PHE:CE1	1:C:230:MET:HE3	2.56	0.40
1:G:82:VAL:H	1:G:82:VAL:HG23	1.67	0.40
1:G:220:ARG:HD2	1:G:227:SER:O	2.21	0.40
1:I:316:LEU:HD21	2:J:100:VAL:HG22	2.03	0.40
1:M:196:GLN:OE1	1:c:192:THR:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:226:LEU:HD23	1:M:226:LEU:HA	1.84	0.40
1:Q:174:GLU:HG3	1:Q:259:LYS:HB3	2.03	0.40
1:S:230:MET:SD	1:S:252:ILE:CD1	3.07	0.40
1:W:86:TYR:OH	1:W:282:GLN:HG2	2.21	0.40
1:W:320:LEU:HB3	2:X:111:HIS:CG	2.55	0.40
1:c:18:HIS:HD2	2:d:20:GLY:O	2.04	0.40
1:c:136:SER:O	1:c:145:SER:HB2	2.21	0.40
2:D:24:TYR:CE2	2:D:153:ARG:HG2	2.56	0.40
2:F:123:ARG:HH21	2:F:124:LEU:HD21	1.85	0.40
2:H:174:SER:O	2:J:171:GLU:OE2	2.38	0.40
2:d:22:TYR:OH	2:d:111:HIS:HB3	2.21	0.40
1:C:29:ILE:HG22	2:F:51:LYS:HG3	2.02	0.40
1:I:122:GLN:NE2	1:I:125:PRO:HA	2.36	0.40
1:M:203:SER:OG	1:M:246:GLU:HB3	2.21	0.40
1:S:83(A):GLU:HA	1:S:117:HIS:CD2	2.57	0.40
1:U:20:ASN:HB2	1:U:21[B]:ASN:H	1.71	0.40
1:W:181:GLY:C	1:W:252:ILE:HB	2.47	0.40
2:N:76:ARG:HH12	2:P:74:GLU:CD	2.27	0.40
1:G:202:ILE:HD11	1:G:251:PHE:HA	2.03	0.40
1:I:15:ILE:HD11	2:J:122:VAL:HG21	2.03	0.40
1:K:168:TYR:HE2	1:K:176:LEU:CD1	2.33	0.40
1:M:125(A):LYS:HB2	1:M:255:GLU:OE1	2.21	0.40
1:M:181:GLY:C	1:M:252:ILE:HB	2.47	0.40
1:M:314:LEU:HA	1:M:314:LEU:HD23	1.74	0.40
1:O:220:ARG:HD2	1:O:227:SER:O	2.22	0.40
1:W:112:LEU:HD23	1:W:112:LEU:HA	1.77	0.40
1:c:293:PRO:HG2	1:c:294:PHE:HD2	1.86	0.40
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.56	0.40
2:P:58:LYS:HA	2:P:58:LYS:HD3	1.60	0.40
2:X:24:TYR:CD2	2:X:153:ARG:HG2	2.57	0.40
2:X:77:ILE:HA	2:X:80:LEU:HB3	2.03	0.40
1:A:11:ASP:OD2	2:B:144:CYS:N	2.39	0.40
1:A:206:THR:HB	1:A:209:LEU:CB	2.52	0.40
1:I:102:PHE:O	1:I:105:TYR:HB2	2.21	0.40
1:K:98:TYR:CD2	1:K:230:MET:HE2	2.56	0.40
1:K:283:THR:HG23	1:K:284:PRO:HD2	2.03	0.40
1:M:47:HIS:HD2	1:M:297:ILE:HD12	1.87	0.40
1:Q:122:GLN:NE2	1:Q:125:PRO:HA	2.36	0.40
1:Q:133(A):LEU:HD23	1:Q:133(A):LEU:HA	1.85	0.40
1:Q:314:LEU:HD23	1:Q:314:LEU:HA	1.88	0.40
2:R:58:LYS:HD3	2:R:58:LYS:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:94:TYR:CD1	2:R:94:TYR:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	C	323/334 (97%)	305 (94%)	18 (6%)	0	100	100
1	E	323/334 (97%)	302 (94%)	21 (6%)	0	100	100
1	G	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	I	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	K	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	M	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	O	323/334 (97%)	303 (94%)	19 (6%)	1 (0%)	36	59
1	Q	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	36	59
1	S	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	U	323/334 (97%)	305 (94%)	16 (5%)	2 (1%)	21	45
1	W	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	Y	323/334 (97%)	303 (94%)	20 (6%)	0	100	100
1	a	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	c	323/334 (97%)	301 (93%)	21 (6%)	1 (0%)	36	59
2	B	175/181 (97%)	166 (95%)	8 (5%)	1 (1%)	21	45
2	D	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	F	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	H	175/181 (97%)	166 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	L	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	21	45
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	166 (95%)	9 (5%)	0	100	100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	21	45
2	b	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	7003 (94%)	459 (6%)	8 (0%)	48	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	O	248	ASN
1	Q	248	ASN
1	c	248	ASN
2	B	60	ASN
2	Z	176	GLY
1	U	248	ASN
2	L	176	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/300 (97%)	276 (94%)	16 (6%)	19	43
1	C	292/300 (97%)	284 (97%)	8 (3%)	39	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	292/300 (97%)	279 (96%)	13 (4%)	24	50
1	G	292/300 (97%)	279 (96%)	13 (4%)	24	50
1	I	292/300 (97%)	272 (93%)	20 (7%)	14	35
1	K	292/300 (97%)	277 (95%)	15 (5%)	21	47
1	M	292/300 (97%)	279 (96%)	13 (4%)	24	50
1	O	292/300 (97%)	276 (94%)	16 (6%)	19	43
1	Q	292/300 (97%)	277 (95%)	15 (5%)	21	47
1	S	292/300 (97%)	280 (96%)	12 (4%)	27	53
1	U	292/300 (97%)	283 (97%)	9 (3%)	35	59
1	W	292/300 (97%)	281 (96%)	11 (4%)	29	55
1	Y	292/300 (97%)	284 (97%)	8 (3%)	39	64
1	a	292/300 (97%)	279 (96%)	13 (4%)	24	50
1	c	292/300 (97%)	284 (97%)	8 (3%)	39	64
2	B	151/155 (97%)	148 (98%)	3 (2%)	48	71
2	D	151/155 (97%)	148 (98%)	3 (2%)	48	71
2	F	151/155 (97%)	147 (97%)	4 (3%)	40	65
2	H	151/155 (97%)	146 (97%)	5 (3%)	33	58
2	J	151/155 (97%)	148 (98%)	3 (2%)	48	71
2	L	151/155 (97%)	149 (99%)	2 (1%)	61	78
2	N	151/155 (97%)	149 (99%)	2 (1%)	61	78
2	P	151/155 (97%)	146 (97%)	5 (3%)	33	58
2	R	151/155 (97%)	146 (97%)	5 (3%)	33	58
2	T	151/155 (97%)	148 (98%)	3 (2%)	48	71
2	V	151/155 (97%)	146 (97%)	5 (3%)	33	58
2	X	151/155 (97%)	148 (98%)	3 (2%)	48	71
2	Z	151/155 (97%)	145 (96%)	6 (4%)	28	53
2	b	151/155 (97%)	147 (97%)	4 (3%)	40	65
2	d	151/155 (97%)	146 (97%)	5 (3%)	33	58
All	All	6645/6825 (97%)	6397 (96%)	248 (4%)	30	55

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	75	MET
1	A	111	LEU
1	A	112	LEU
1	A	135	VAL
1	A	174	GLU
1	A	206	THR
1	A	219	THR
1	A	252	ILE
1	A	261	LYS
1	A	264	ASP
1	A	268	MET
1	A	283	THR
1	A	300	LEU
1	A	310	LYS
1	A	313	ARG
1	C	28	THR
1	C	46	LYS
1	C	120	LYS
1	C	135	VAL
1	C	174	GLU
1	C	261	LYS
1	C	302	ILE
1	C	310	LYS
1	E	46	LYS
1	E	75	MET
1	E	114	ARG
1	E	135	VAL
1	E	166	ARG
1	E	174	GLU
1	E	199	THR
1	E	219	THR
1	E	230	MET
1	E	261	LYS
1	E	268	MET
1	E	273	GLU
1	E	283	THR
1	G	15	ILE
1	G	28	THR
1	G	75	MET
1	G	80	ILE
1	G	82	VAL
1	G	112	LEU

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Mol	Chain	Res	Type
1	G	167	SER
1	G	174	GLU
1	G	208	THR
1	G	252	ILE
1	G	261	LYS
1	G	283	THR
1	G	313	ARG
1	I	28	THR
1	I	65	SER
1	I	75	MET
1	I	80	ILE
1	I	111	LEU
1	I	135	VAL
1	I	137	SER
1	I	142	GLN
1	I	155	ILE
1	I	166	ARG
1	I	167	SER
1	I	174	GLU
1	I	194	LEU
1	I	206	THR
1	I	208	THR
1	I	261	LYS
1	I	264	ASP
1	I	279	THR
1	I	301	THR
1	I	313	ARG
1	K	28	THR
1	K	46	LYS
1	K	56	VAL
1	K	94	VAL
1	K	135	VAL
1	K	155	ILE
1	K	160	THR
1	K	174	GLU
1	K	187	ASP
1	K	248	ASN
1	K	261	LYS
1	K	273	GLU
1	K	283	THR
1	K	302	ILE
1	K	313	ARG

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Mol	Chain	Res	Type
1	M	28	THR
1	M	56	VAL
1	M	75	MET
1	M	133	SER
1	M	133(A)	LEU
1	M	135	VAL
1	M	174	GLU
1	M	219	THR
1	M	261	LYS
1	M	283	THR
1	M	310	LYS
1	M	311	SER
1	M	313	ARG
1	O	56	VAL
1	O	61	LEU
1	O	75	MET
1	O	80	ILE
1	O	111	LEU
1	O	120	LYS
1	O	135	VAL
1	O	155	ILE
1	O	176	LEU
1	O	208	THR
1	O	209	LEU
1	O	248	ASN
1	O	252	ILE
1	O	261	LYS
1	O	310	LYS
1	O	320	LEU
1	Q	28	THR
1	Q	75	MET
1	Q	94	VAL
1	Q	135	VAL
1	Q	166	ARG
1	Q	167	SER
1	Q	174	GLU
1	Q	176	LEU
1	Q	248	ASN
1	Q	260	ILE
1	Q	260(A)	VAL
1	Q	261	LYS
1	Q	283	THR

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Mol	Chain	Res	Type
1	Q	313	ARG
1	Q	320	LEU
1	S	28	THR
1	S	75	MET
1	S	120	LYS
1	S	135	VAL
1	S	149	ARG
1	S	174	GLU
1	S	208	THR
1	S	261	LYS
1	S	279	THR
1	S	300	LEU
1	S	311	SER
1	S	313	ARG
1	U	28	THR
1	U	75	MET
1	U	111	LEU
1	U	174	GLU
1	U	261	LYS
1	U	268	MET
1	U	272	LEU
1	U	283	THR
1	U	313	ARG
1	W	28	THR
1	W	75	MET
1	W	111	LEU
1	W	149	ARG
1	W	155	ILE
1	W	174	GLU
1	W	264	ASP
1	W	272	LEU
1	W	283	THR
1	W	311	SER
1	W	313	ARG
1	Y	28	THR
1	Y	75	MET
1	Y	114	ARG
1	Y	174	GLU
1	Y	261	LYS
1	Y	272	LEU
1	Y	283	THR
1	Y	309	VAL

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Mol	Chain	Res	Type
1	a	28	THR
1	a	65	SER
1	a	75	MET
1	a	81	ASN
1	a	87	ILE
1	a	114	ARG
1	a	174	GLU
1	a	199	THR
1	a	248	ASN
1	a	261	LYS
1	a	268	MET
1	a	283	THR
1	a	291	SER
1	c	28	THR
1	c	75	MET
1	c	114	ARG
1	c	208	THR
1	c	248	ASN
1	c	261	LYS
1	c	283	THR
1	c	312	ASN
2	B	11	GLU
2	B	41	THR
2	B	93	THR
2	D	41	THR
2	D	113	SER
2	D	150	GLU
2	F	30	GLN
2	F	41	THR
2	F	43	LYS
2	F	150	GLU
2	H	30	GLN
2	H	41	THR
2	H	57	ASP
2	H	94	TYR
2	H	150	GLU
2	J	11	GLU
2	J	41	THR
2	J	85	GLU
2	L	41	THR
2	L	150	GLU
2	N	41	THR

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Mol	Chain	Res	Type
2	N	93	THR
2	P	11	GLU
2	P	41	THR
2	P	85	GLU
2	P	93	THR
2	P	116	LYS
2	R	41	THR
2	R	43	LYS
2	R	50	ASN
2	R	93	THR
2	R	94	TYR
2	T	41	THR
2	T	58	LYS
2	T	150	GLU
2	V	29	GLU
2	V	41	THR
2	V	43	LYS
2	V	93	THR
2	V	94	TYR
2	X	41	THR
2	X	93	THR
2	X	94	TYR
2	Z	30	GLN
2	Z	41	THR
2	Z	57	ASP
2	Z	66	VAL
2	Z	77	ILE
2	Z	80	LEU
2	b	41	THR
2	b	77	ILE
2	b	80	LEU
2	b	93	THR
2	d	19	ASP
2	d	30	GLN
2	d	41	THR
2	d	86	ASP
2	d	93	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS

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Mol	Chain	Res	Type
1	A	117	HIS
1	A	197	ASN
1	A	211	GLN
1	C	20	ASN
1	C	38	HIS
1	C	116	ASN
1	C	122	GLN
1	C	210	ASN
1	C	211	GLN
1	C	278	ASN
1	C	282	GLN
1	C	298	HIS
1	E	25	GLN
1	E	103	ASN
1	E	110	HIS
1	E	197	ASN
1	E	244	ASN
1	E	278	ASN
1	G	117	HIS
1	G	210	ASN
1	I	12	GLN
1	I	122	GLN
1	I	197	ASN
1	I	248	ASN
1	K	20	ASN
1	K	38	HIS
1	K	196	GLN
1	K	197	ASN
1	K	211	GLN
1	K	248	ASN
1	M	12	GLN
1	M	116	ASN
1	M	197	ASN
1	M	211	GLN
1	M	322	ASN
1	O	150	ASN
1	O	197	ASN
1	O	210	ASN
1	O	211	GLN
1	Q	25	GLN
1	Q	117	HIS
1	Q	197	ASN

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Mol	Chain	Res	Type
1	Q	248	ASN
1	S	110	HIS
1	S	116	ASN
1	S	117	HIS
1	S	122	GLN
1	S	211	GLN
1	U	122	GLN
1	U	211	GLN
1	W	12	GLN
1	W	81	ASN
1	W	150	ASN
1	Y	38	HIS
1	Y	197	ASN
1	Y	211	GLN
1	a	38	HIS
1	a	197	ASN
1	a	278	ASN
1	c	18	HIS
1	c	278	ASN
2	B	30	GLN
2	B	50	ASN
2	B	60	ASN
2	D	42	GLN
2	D	72	ASN
2	D	161	GLN
2	F	42	GLN
2	J	15	GLN
2	J	30	GLN
2	L	42	GLN
2	N	25	HIS
2	N	26	HIS
2	N	30	GLN
2	N	62	GLN
2	P	28	ASN
2	P	62	GLN
2	P	125	GLN
2	P	142	HIS
2	R	25	HIS
2	R	30	GLN
2	R	62	GLN
2	R	161	GLN
2	T	15	GLN

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Mol	Chain	Res	Type
2	V	30	GLN
2	V	50	ASN
2	V	117	ASN
2	b	42	GLN
2	b	62	GLN
2	b	142	HIS
2	d	30	GLN
2	d	142	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

58 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	0	1	1,4	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
4	NAG	0	2	4	14,14,15	0.43	0	17,19,21	0.44	0
3	NAG	e	1	3,1	14,14,15	1.10	1 (7%)	17,19,21	1.12	2 (11%)
3	NAG	e	2	3	14,14,15	0.31	0	17,19,21	0.52	0
3	BMA	e	3	3	11,11,12	1.64	3 (27%)	15,15,17	1.20	2 (13%)
4	NAG	f	1	1,4	14,14,15	0.99	1 (7%)	17,19,21	1.21	2 (11%)
4	NAG	f	2	4	14,14,15	1.48	2 (14%)	17,19,21	1.20	1 (5%)
3	NAG	g	1	3,1	14,14,15	0.36	0	17,19,21	0.58	0
3	NAG	g	2	3	14,14,15	0.57	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	g	3	3	11,11,12	2.12	5 (45%)	15,15,17	1.49	4 (26%)
3	NAG	h	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	h	2	3	14,14,15	1.23	1 (7%)	17,19,21	1.27	2 (11%)
3	BMA	h	3	3	11,11,12	1.57	1 (9%)	15,15,17	1.62	3 (20%)
4	NAG	i	1	1,4	14,14,15	1.19	1 (7%)	17,19,21	1.39	3 (17%)
4	NAG	i	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.48	0
3	NAG	j	1	3,1	14,14,15	1.63	2 (14%)	17,19,21	1.36	2 (11%)
3	NAG	j	2	3	14,14,15	0.85	1 (7%)	17,19,21	0.80	0
3	BMA	j	3	3	11,11,12	1.97	5 (45%)	15,15,17	1.10	1 (6%)
4	NAG	k	1	1,4	14,14,15	1.24	1 (7%)	17,19,21	1.36	2 (11%)
4	NAG	k	2	4	14,14,15	0.65	0	17,19,21	0.41	0
3	NAG	l	1	3,1	14,14,15	1.40	1 (7%)	17,19,21	1.27	2 (11%)
3	NAG	l	2	3	14,14,15	0.99	1 (7%)	17,19,21	0.82	1 (5%)
3	BMA	l	3	3	11,11,12	2.38	4 (36%)	15,15,17	1.58	3 (20%)
4	NAG	m	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	m	2	4	14,14,15	1.62	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	n	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
3	NAG	n	2	3	14,14,15	0.43	0	17,19,21	0.80	0
3	BMA	n	3	3	11,11,12	2.23	5 (45%)	15,15,17	1.57	2 (13%)
3	NAG	o	1	3,1	14,14,15	0.62	0	17,19,21	0.70	0
3	NAG	o	2	3	14,14,15	0.94	1 (7%)	17,19,21	0.83	1 (5%)
3	BMA	o	3	3	11,11,12	1.97	3 (27%)	15,15,17	1.55	2 (13%)
3	NAG	p	1	3,1	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
3	NAG	p	2	3	14,14,15	0.64	0	17,19,21	0.38	0
3	BMA	p	3	3	11,11,12	1.62	3 (27%)	15,15,17	1.32	2 (13%)
4	NAG	q	1	1,4	14,14,15	1.17	1 (7%)	17,19,21	1.13	2 (11%)
4	NAG	q	2	4	14,14,15	0.46	0	17,19,21	0.71	1 (5%)
3	NAG	r	1	3,1	14,14,15	0.60	1 (7%)	17,19,21	0.76	1 (5%)
3	NAG	r	2	3	14,14,15	0.23	0	17,19,21	0.54	0
3	BMA	r	3	3	11,11,12	0.70	0	15,15,17	1.78	4 (26%)
4	NAG	s	1	1,4	14,14,15	1.13	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	s	2	4	14,14,15	0.51	0	17,19,21	0.53	0
3	NAG	t	1	3,1	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
3	NAG	t	2	3	14,14,15	0.48	0	17,19,21	0.84	0
3	BMA	t	3	3	11,11,12	1.90	2 (18%)	15,15,17	1.74	5 (33%)
4	NAG	u	1	1,4	14,14,15	0.55	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	u	2	4	14,14,15	1.54	3 (21%)	17,19,21	1.19	1 (5%)
3	NAG	v	1	3,1	14,14,15	0.42	0	17,19,21	0.57	0
3	NAG	v	2	3	14,14,15	1.49	2 (14%)	17,19,21	1.09	1 (5%)
3	BMA	v	3	3	11,11,12	1.16	0	15,15,17	1.68	2 (13%)
4	NAG	w	1	1,4	14,14,15	0.46	0	17,19,21	0.53	0
4	NAG	w	2	4	14,14,15	0.42	0	17,19,21	0.41	0
3	NAG	x	1	3,1	14,14,15	0.63	0	17,19,21	0.98	2 (11%)
3	NAG	x	2	3	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
3	BMA	x	3	3	11,11,12	0.58	0	15,15,17	0.69	0
4	NAG	y	1	1,4	14,14,15	1.31	1 (7%)	17,19,21	1.40	2 (11%)
4	NAG	y	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.72	0
4	NAG	z	1	1,4	14,14,15	0.38	0	17,19,21	0.41	0
4	NAG	z	2	4	14,14,15	0.35	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
4	NAG	0	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	0	2	4	-	2/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	BMA	e	3	3	-	0/2/19/22	0/1/1/1
4	NAG	f	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	1/6/23/26	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
4	NAG	k	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	k	2	4	-	0/6/23/26	0/1/1/1
3	NAG	l	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1
3	BMA	l	3	3	-	0/2/19/22	0/1/1/1
4	NAG	m	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	0/6/23/26	0/1/1/1
3	NAG	n	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	BMA	n	3	3	-	0/2/19/22	0/1/1/1
3	NAG	o	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1
3	BMA	o	3	3	-	2/2/19/22	0/1/1/1
3	NAG	p	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	p	2	3	-	1/6/23/26	0/1/1/1
3	BMA	p	3	3	-	2/2/19/22	0/1/1/1
4	NAG	q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	q	2	4	-	0/6/23/26	0/1/1/1
3	NAG	r	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1
3	BMA	r	3	3	-	2/2/19/22	0/1/1/1
4	NAG	s	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	s	2	4	-	2/6/23/26	0/1/1/1
3	NAG	t	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	t	2	3	-	2/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
4	NAG	u	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	u	2	4	-	0/6/23/26	0/1/1/1
3	NAG	v	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	v	2	3	-	2/6/23/26	0/1/1/1
3	BMA	v	3	3	-	2/2/19/22	0/1/1/1
4	NAG	w	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	w	2	4	-	1/6/23/26	0/1/1/1
3	NAG	x	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	x	2	3	-	0/6/23/26	0/1/1/1
3	BMA	x	3	3	-	2/2/19/22	0/1/1/1
4	NAG	y	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	y	2	4	-	0/6/23/26	0/1/1/1
4	NAG	z	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	z	2	4	-	1/6/23/26	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	1	NAG	O5-C1	-5.52	1.34	1.43
3	v	2	NAG	O5-C1	-4.77	1.35	1.43
4	u	2	NAG	O5-C1	-4.71	1.35	1.43
3	l	1	NAG	O5-C1	-4.68	1.35	1.43
3	l	3	BMA	C4-C3	4.61	1.64	1.52
4	y	1	NAG	O5-C1	-4.55	1.36	1.43
4	m	2	NAG	O5-C1	4.44	1.51	1.43
3	g	3	BMA	C4-C5	4.40	1.62	1.53
4	k	1	NAG	O5-C1	-4.38	1.36	1.43
3	l	3	BMA	C4-C5	4.34	1.62	1.53
4	f	2	NAG	C1-C2	4.27	1.58	1.52
4	i	1	NAG	O5-C1	-4.26	1.36	1.43
3	t	3	BMA	C2-C3	4.20	1.58	1.52
3	o	3	BMA	C4-C5	4.19	1.62	1.53
3	n	3	BMA	C4-C3	4.18	1.63	1.52
3	h	2	NAG	O5-C1	-4.08	1.36	1.43
4	m	2	NAG	C1-C2	3.94	1.57	1.52
4	s	1	NAG	O5-C1	-3.92	1.37	1.43
3	n	3	BMA	C4-C5	3.89	1.61	1.53
3	t	3	BMA	C1-C2	3.85	1.61	1.52
3	j	3	BMA	C4-C3	3.85	1.62	1.52
4	q	1	NAG	O5-C1	-3.82	1.37	1.43
3	e	3	BMA	C1-C2	3.63	1.60	1.52
3	h	3	BMA	C1-C2	3.58	1.60	1.52
3	e	1	NAG	C1-C2	3.58	1.57	1.52
3	l	2	NAG	O5-C1	-3.44	1.37	1.43
3	p	3	BMA	C4-C5	3.43	1.60	1.53
4	f	1	NAG	O5-C1	-3.40	1.38	1.43
3	o	3	BMA	C4-C3	3.29	1.60	1.52
4	f	2	NAG	O5-C1	3.16	1.49	1.43
3	g	3	BMA	C4-C3	3.15	1.60	1.52
3	j	2	NAG	O5-C1	-3.09	1.38	1.43
3	g	3	BMA	C1-C2	3.00	1.59	1.52
3	j	3	BMA	C4-C5	2.94	1.59	1.53
3	n	3	BMA	C6-C5	2.64	1.60	1.51
3	p	3	BMA	O5-C1	-2.58	1.39	1.43
3	e	3	BMA	C4-C3	2.54	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	n	3	BMA	O3-C3	2.51	1.49	1.43
3	o	2	NAG	O5-C1	-2.50	1.39	1.43
4	i	2	NAG	C1-C2	2.49	1.55	1.52
4	m	1	NAG	O5-C1	-2.46	1.39	1.43
3	l	3	BMA	C1-C2	2.44	1.58	1.52
3	v	2	NAG	C1-C2	2.39	1.55	1.52
3	j	3	BMA	C2-C3	2.39	1.56	1.52
3	h	1	NAG	O5-C1	2.36	1.47	1.43
4	u	2	NAG	C1-C2	2.36	1.55	1.52
3	o	3	BMA	O5-C1	-2.31	1.39	1.43
3	n	1	NAG	C1-C2	2.29	1.55	1.52
3	g	3	BMA	O3-C3	2.24	1.48	1.43
3	p	3	BMA	C4-C3	2.23	1.58	1.52
3	e	3	BMA	C2-C3	2.21	1.55	1.52
3	l	3	BMA	O2-C2	2.20	1.47	1.43
3	r	1	NAG	O5-C1	-2.19	1.40	1.43
3	g	3	BMA	C6-C5	2.13	1.59	1.51
4	u	2	NAG	C3-C2	2.12	1.57	1.52
3	j	1	NAG	C3-C2	2.09	1.56	1.52
4	y	2	NAG	C1-C2	2.07	1.55	1.52
3	n	3	BMA	O5-C5	2.04	1.47	1.43
3	j	3	BMA	C1-C2	2.03	1.57	1.52
3	j	3	BMA	O5-C5	2.01	1.47	1.43

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	v	3	BMA	C1-O5-C5	4.91	118.76	112.19
4	f	2	NAG	C1-O5-C5	4.45	118.15	112.19
3	j	1	NAG	C4-C3-C2	4.25	117.25	111.02
3	r	3	BMA	C3-C4-C5	4.16	117.78	110.23
4	k	1	NAG	C3-C4-C5	3.99	117.46	110.23
3	n	3	BMA	C1-O5-C5	3.89	117.40	112.19
3	o	3	BMA	C3-C4-C5	3.88	117.28	110.23
3	h	2	NAG	C3-C4-C5	3.88	117.27	110.23
4	u	2	NAG	C4-C3-C2	3.88	116.71	111.02
3	l	3	BMA	C3-C4-C5	3.77	117.07	110.23
3	t	3	BMA	C1-C2-C3	3.72	115.07	109.64
4	y	1	NAG	C3-C4-C5	3.71	116.97	110.23
4	f	1	NAG	C3-C4-C5	3.64	116.83	110.23
4	y	1	NAG	C4-C3-C2	3.60	116.30	111.02
4	i	1	NAG	C4-C3-C2	3.55	116.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	1	NAG	C4-C3-C2	3.45	116.08	111.02
3	h	1	NAG	C1-O5-C5	3.45	116.81	112.19
4	m	1	NAG	C3-C4-C5	3.42	116.44	110.23
3	h	3	BMA	O2-C2-C1	3.34	116.88	109.22
4	m	2	NAG	C1-O5-C5	3.24	116.53	112.19
3	r	3	BMA	O3-C3-C4	-3.22	102.78	110.38
4	k	1	NAG	C4-C3-C2	3.12	115.59	111.02
3	p	1	NAG	C1-O5-C5	3.10	116.34	112.19
3	r	3	BMA	O3-C3-C2	3.01	116.19	110.05
4	i	1	NAG	C3-C4-C5	2.96	115.60	110.23
3	h	3	BMA	C1-O5-C5	2.93	116.12	112.19
4	q	1	NAG	C4-C3-C2	2.81	115.14	111.02
3	l	3	BMA	C2-C3-C4	2.72	115.65	110.86
3	t	3	BMA	C1-O5-C5	2.66	115.75	112.19
3	e	1	NAG	C1-O5-C5	2.64	115.73	112.19
3	r	1	NAG	C1-O5-C5	2.61	115.69	112.19
3	t	3	BMA	C2-C3-C4	2.61	115.44	110.86
3	h	3	BMA	O2-C2-C3	-2.58	104.80	110.15
3	j	1	NAG	C3-C4-C5	2.58	114.90	110.23
3	v	2	NAG	C4-C3-C2	2.54	114.74	111.02
3	o	2	NAG	C1-O5-C5	-2.54	108.78	112.19
3	l	3	BMA	O2-C2-C1	2.54	115.03	109.22
3	h	2	NAG	C4-C3-C2	2.52	114.72	111.02
4	f	1	NAG	C4-C3-C2	2.52	114.70	111.02
3	v	3	BMA	O2-C2-C3	-2.46	105.06	110.15
4	0	1	NAG	C4-C3-C2	2.43	114.58	111.02
4	i	1	NAG	C1-O5-C5	-2.42	108.94	112.19
3	p	3	BMA	C1-O5-C5	2.42	115.42	112.19
4	m	1	NAG	C4-C3-C2	2.37	114.50	111.02
4	q	1	NAG	C1-O5-C5	-2.34	109.04	112.19
3	g	3	BMA	O2-C2-C3	-2.33	105.32	110.15
4	q	2	NAG	C1-O5-C5	2.31	115.29	112.19
3	g	3	BMA	C3-C4-C5	2.31	114.41	110.23
3	n	3	BMA	O2-C2-C3	-2.29	105.40	110.15
3	r	3	BMA	O5-C1-C2	-2.26	105.39	110.79
3	x	1	NAG	C1-O5-C5	2.24	115.19	112.19
3	l	1	NAG	C1-O5-C5	-2.23	109.19	112.19
3	g	3	BMA	O2-C2-C1	2.22	114.32	109.22
3	p	3	BMA	C3-C4-C5	2.18	114.19	110.23
3	e	1	NAG	O5-C1-C2	-2.18	107.92	111.29
3	t	3	BMA	O5-C1-C2	2.13	115.87	110.79
3	j	3	BMA	C3-C4-C5	2.12	114.08	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	3	BMA	O2-C2-C3	-2.11	105.79	110.15
3	t	1	NAG	C1-O5-C5	2.10	115.01	112.19
4	s	1	NAG	C4-C3-C2	2.09	114.09	111.02
3	l	2	NAG	C1-O5-C5	-2.06	109.42	112.19
3	t	3	BMA	O2-C2-C1	2.05	113.91	109.22
3	x	2	NAG	O7-C7-C8	-2.04	118.42	122.05
3	e	3	BMA	O2-C2-C1	2.01	113.82	109.22
3	e	3	BMA	C1-C2-C3	2.01	112.57	109.64
3	g	3	BMA	C1-O5-C5	2.00	114.87	112.19
3	x	1	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	x	3	BMA	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	s	1	NAG	C4-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
3	v	2	NAG	O5-C5-C6-O6
3	v	3	BMA	O5-C5-C6-O6
3	p	3	BMA	O5-C5-C6-O6
3	v	2	NAG	C4-C5-C6-O6
4	s	1	NAG	O5-C5-C6-O6
3	x	3	BMA	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
4	0	1	NAG	O5-C5-C6-O6
4	s	2	NAG	O5-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
4	0	1	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	s	2	NAG	C4-C5-C6-O6
4	z	1	NAG	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	p	1	NAG	C4-C5-C6-O6
4	z	1	NAG	C4-C5-C6-O6
3	p	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	v	3	BMA	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
4	0	2	NAG	C4-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
3	p	1	NAG	O5-C5-C6-O6
4	w	1	NAG	C4-C5-C6-O6
3	r	3	BMA	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
3	r	2	NAG	C4-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
3	l	1	NAG	C4-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	w	1	NAG	O5-C5-C6-O6
4	w	2	NAG	O5-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
3	t	1	NAG	C4-C5-C6-O6
4	k	1	NAG	C4-C5-C6-O6
3	r	3	BMA	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	p	2	NAG	C4-C5-C6-O6
4	z	2	NAG	C4-C5-C6-O6
4	u	1	NAG	C4-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6
3	o	3	BMA	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 11 short contacts:

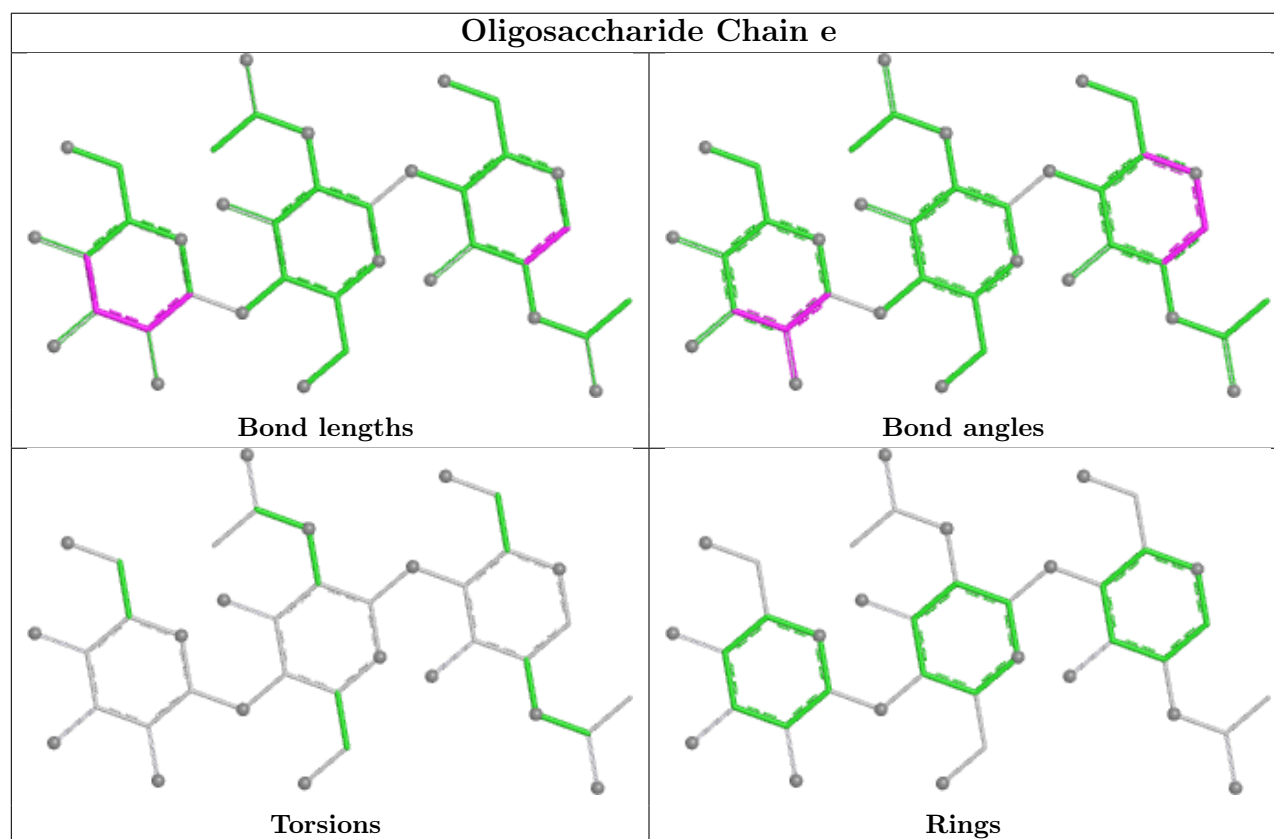
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	s	2	NAG	1	0
4	y	1	NAG	1	0

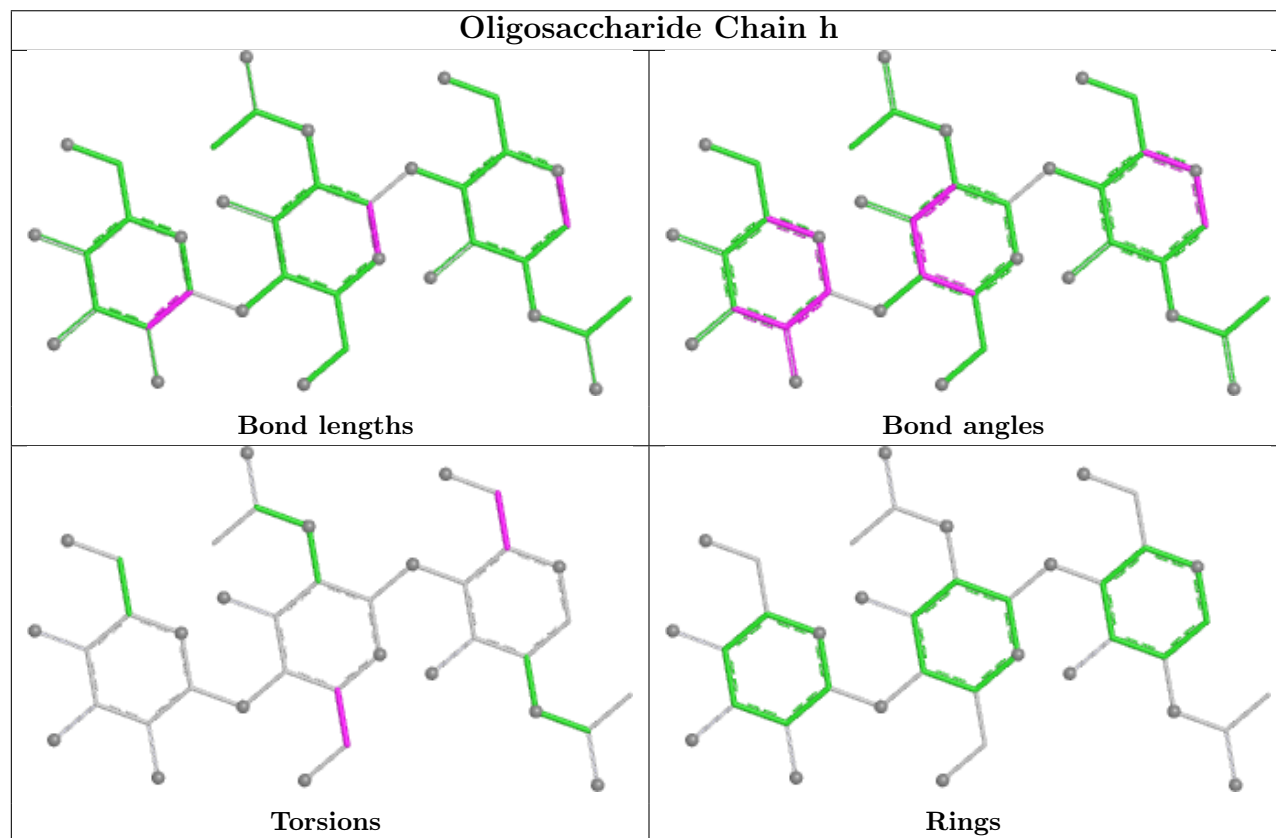
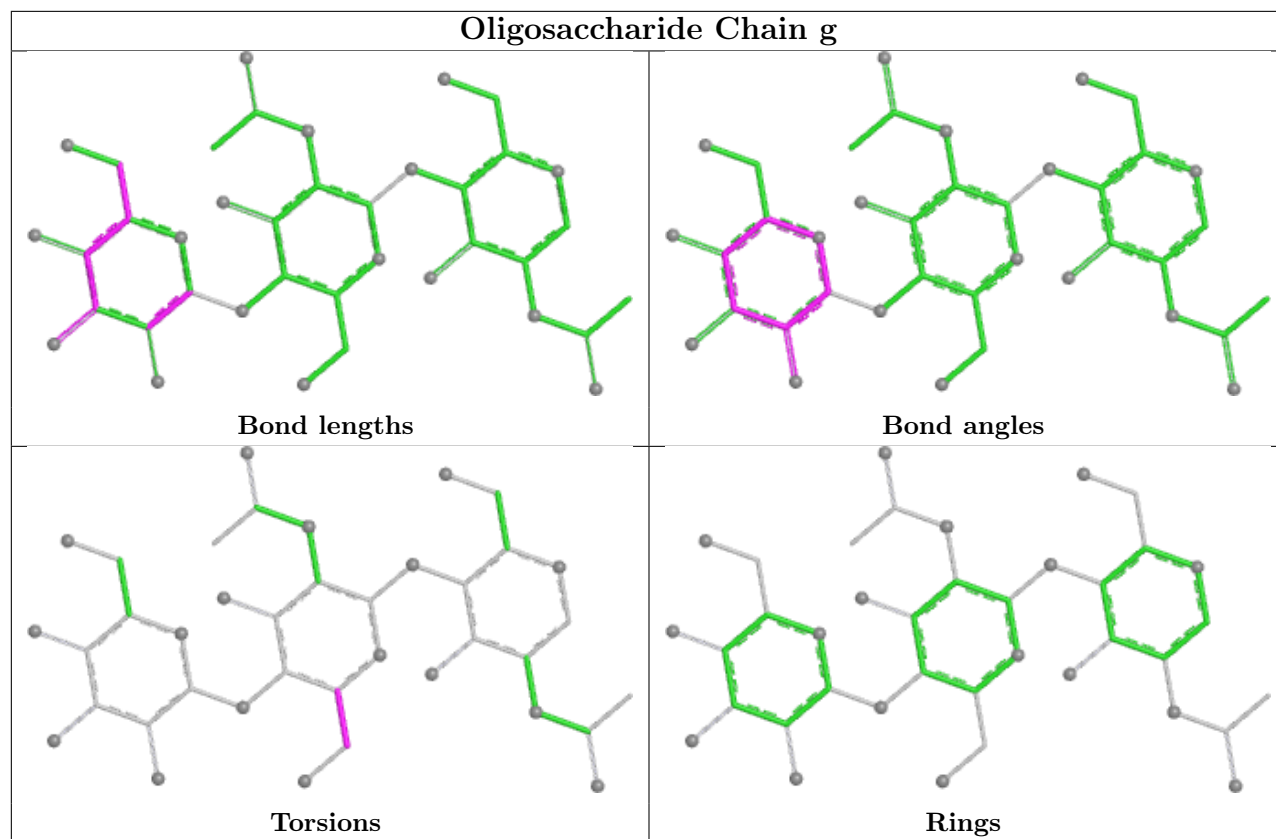
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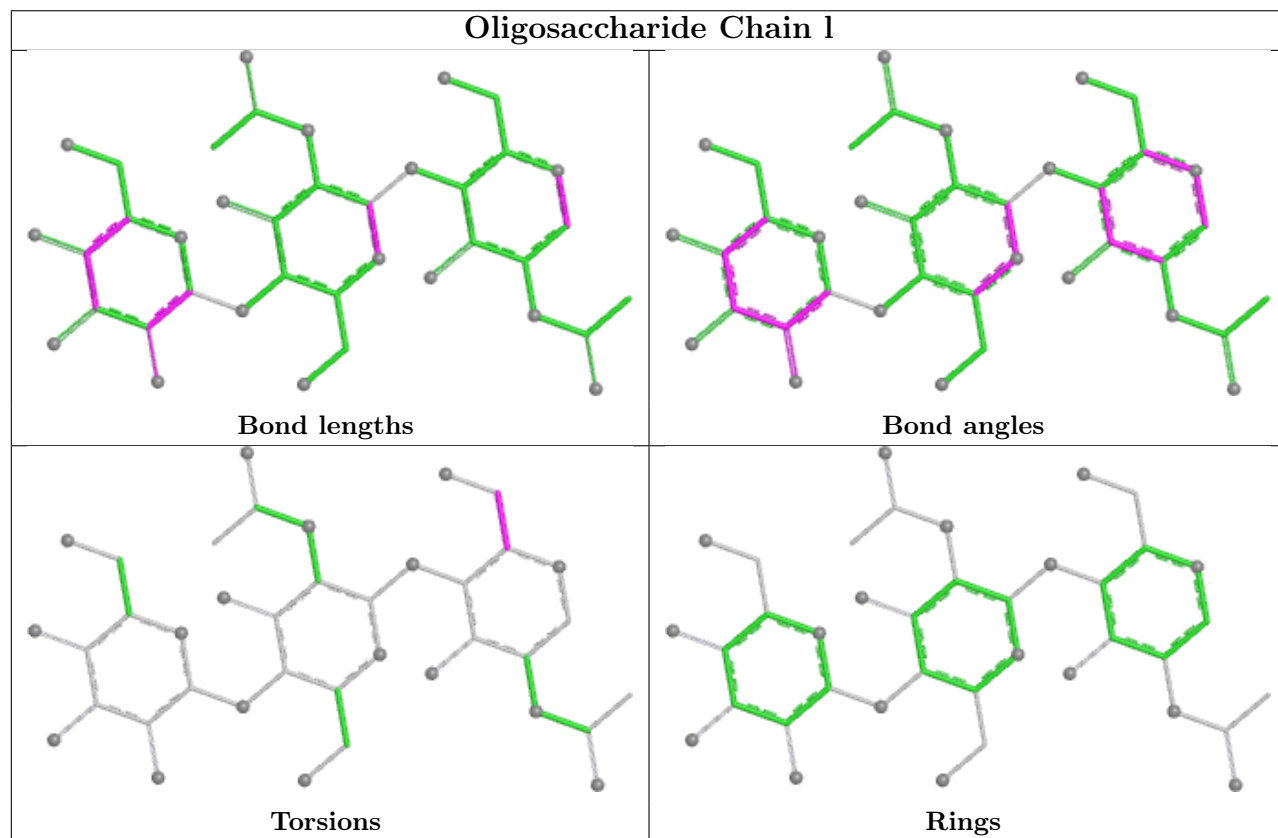
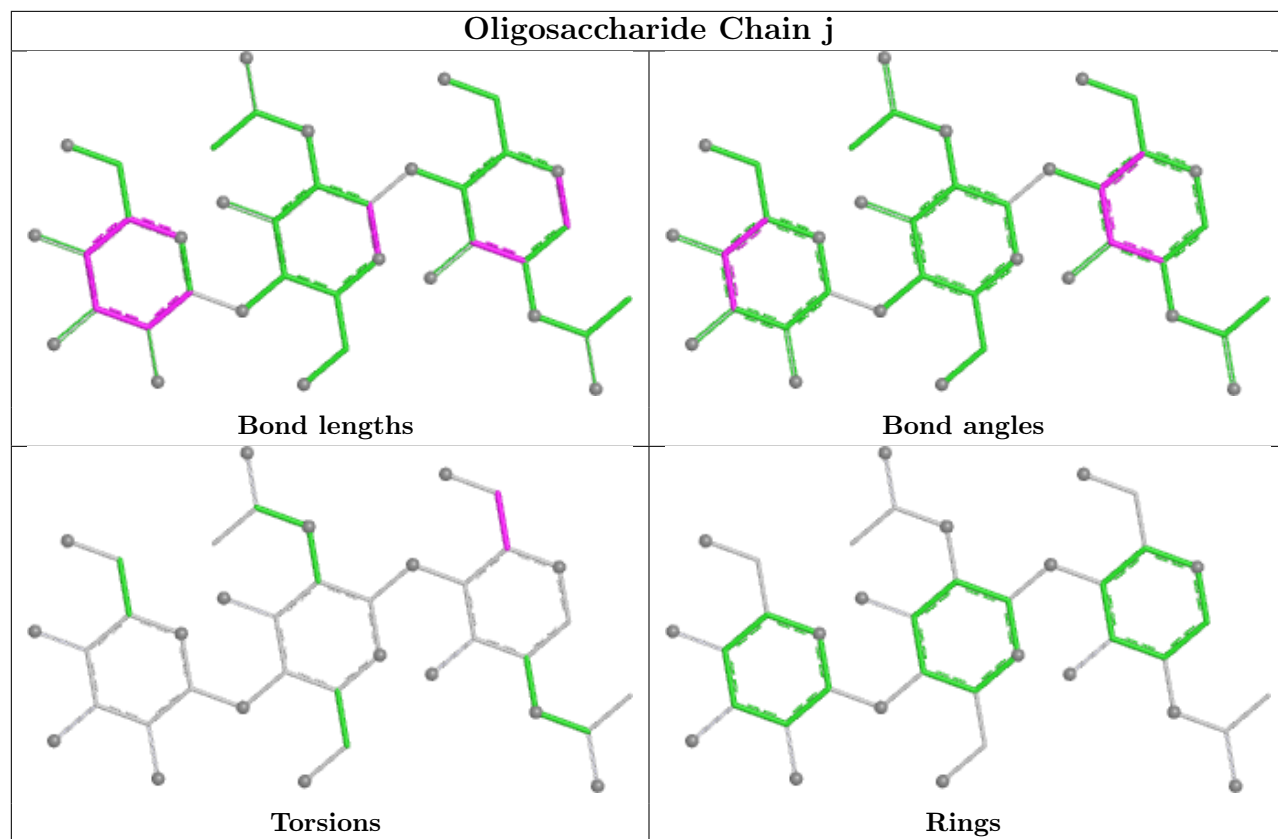
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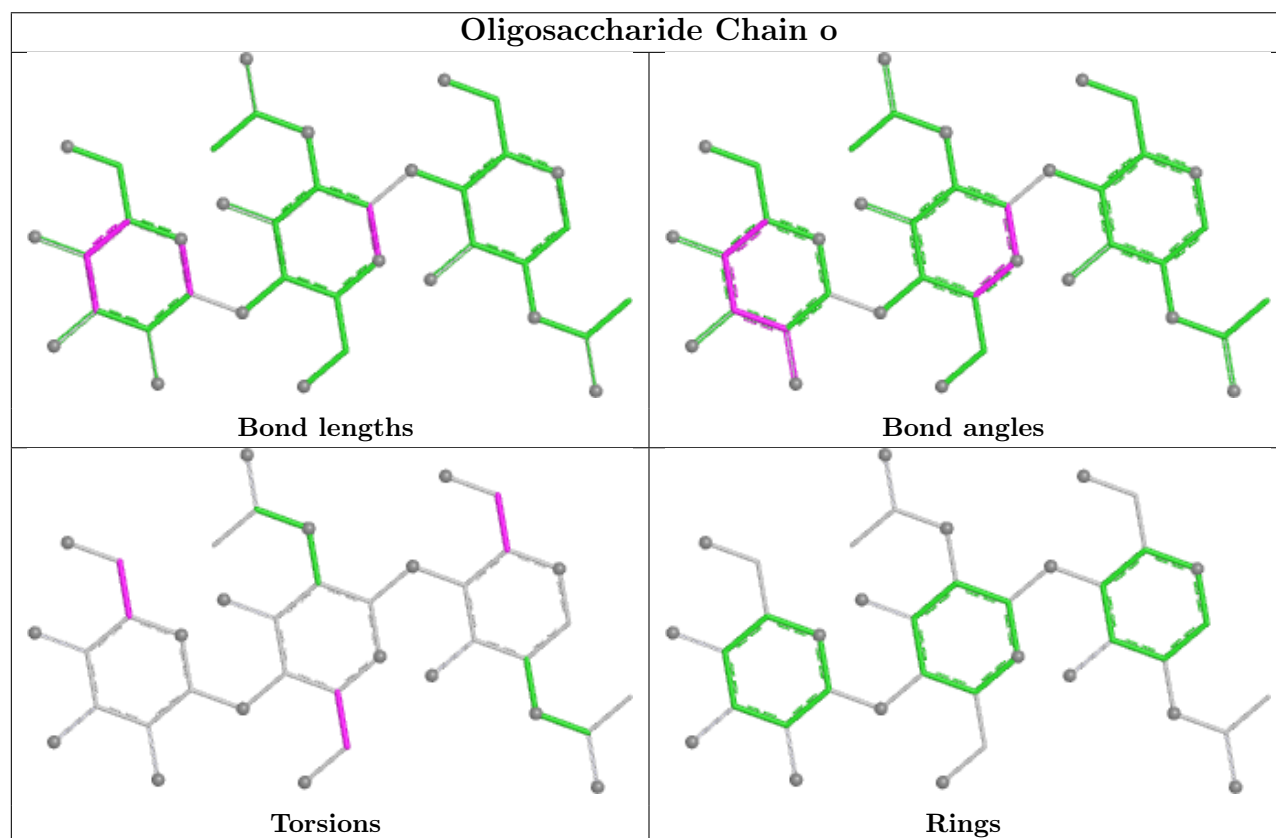
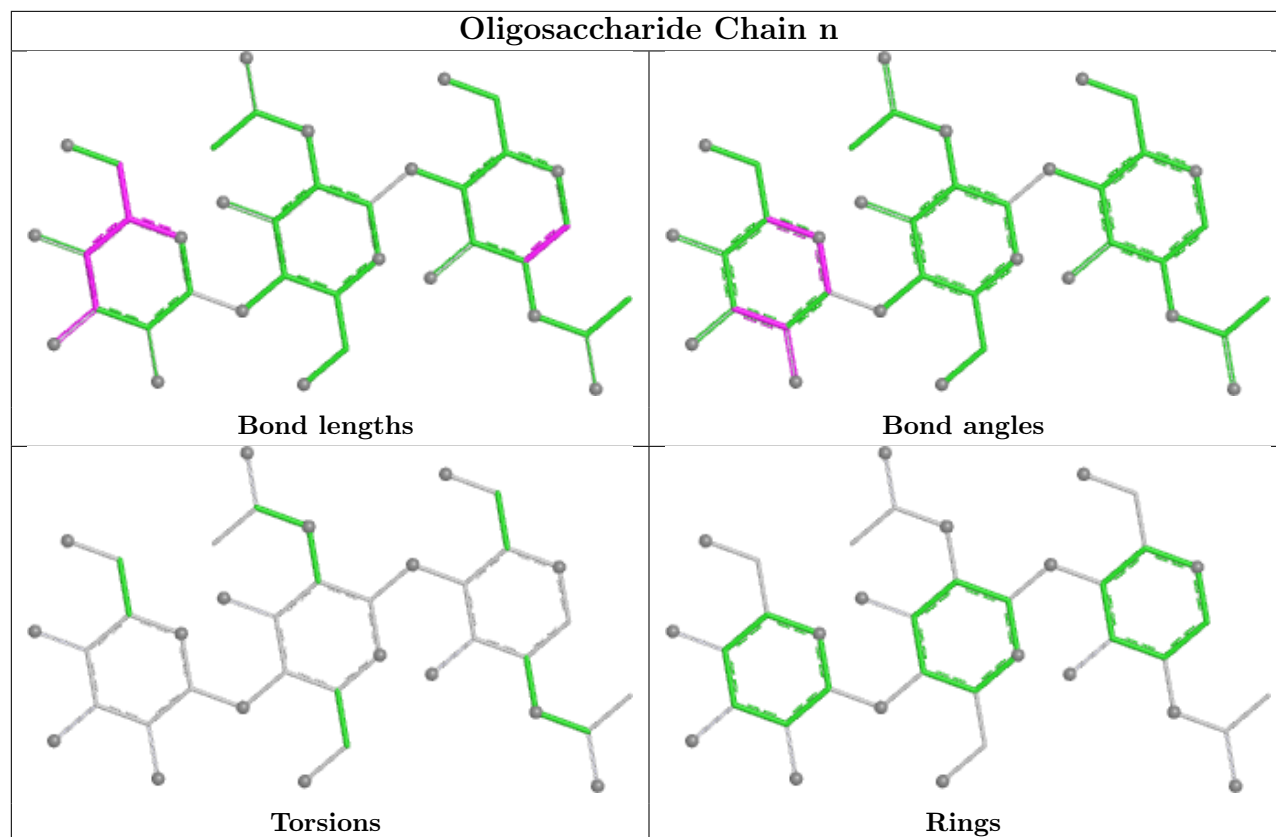
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	h	1	NAG	1	0
4	m	1	NAG	1	0
4	s	1	NAG	1	0
4	z	2	NAG	1	0
4	k	1	NAG	1	0
3	t	1	NAG	1	0
4	k	2	NAG	1	0
3	j	1	NAG	1	0
4	u	1	NAG	1	0
4	u	2	NAG	1	0
4	z	1	NAG	1	0
4	y	2	NAG	1	0
4	0	1	NAG	1	0
4	m	2	NAG	1	0
3	e	1	NAG	1	0
3	h	2	NAG	1	0

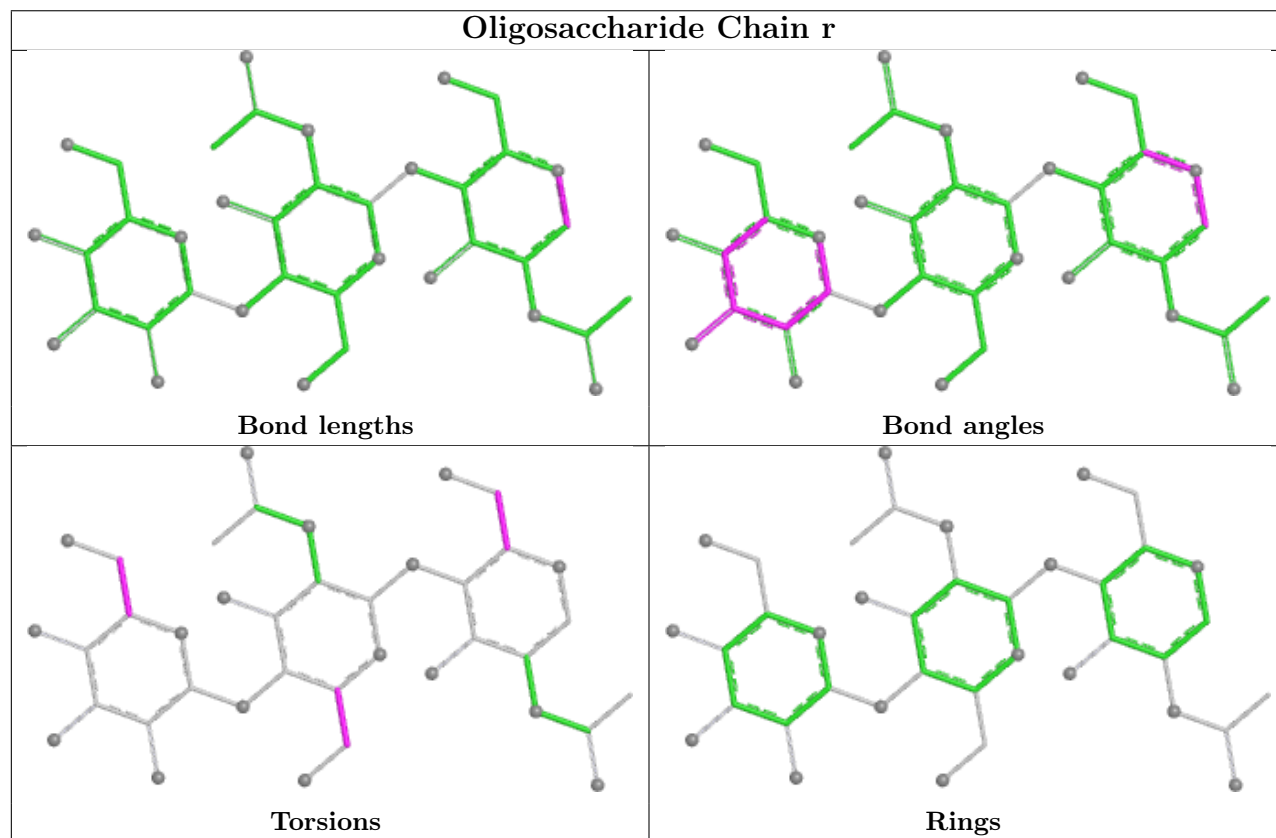
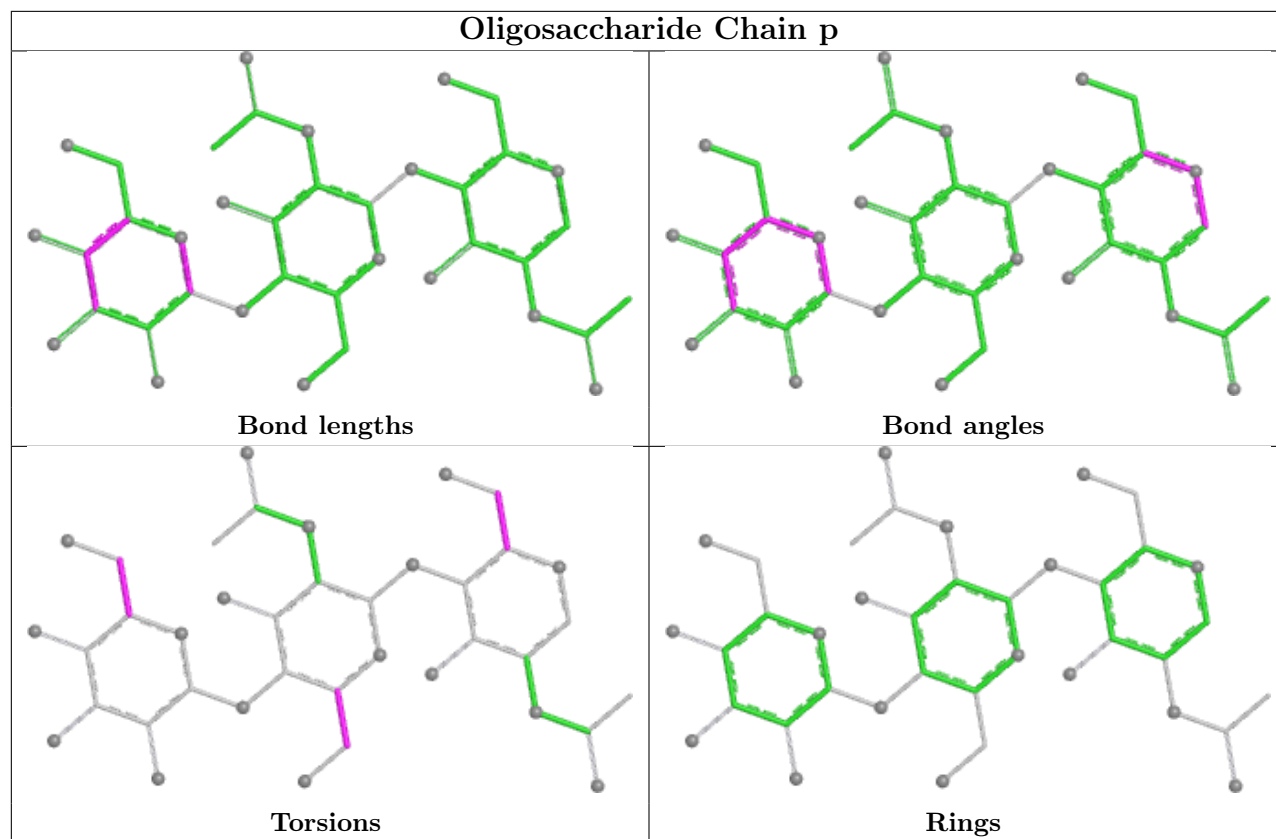
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

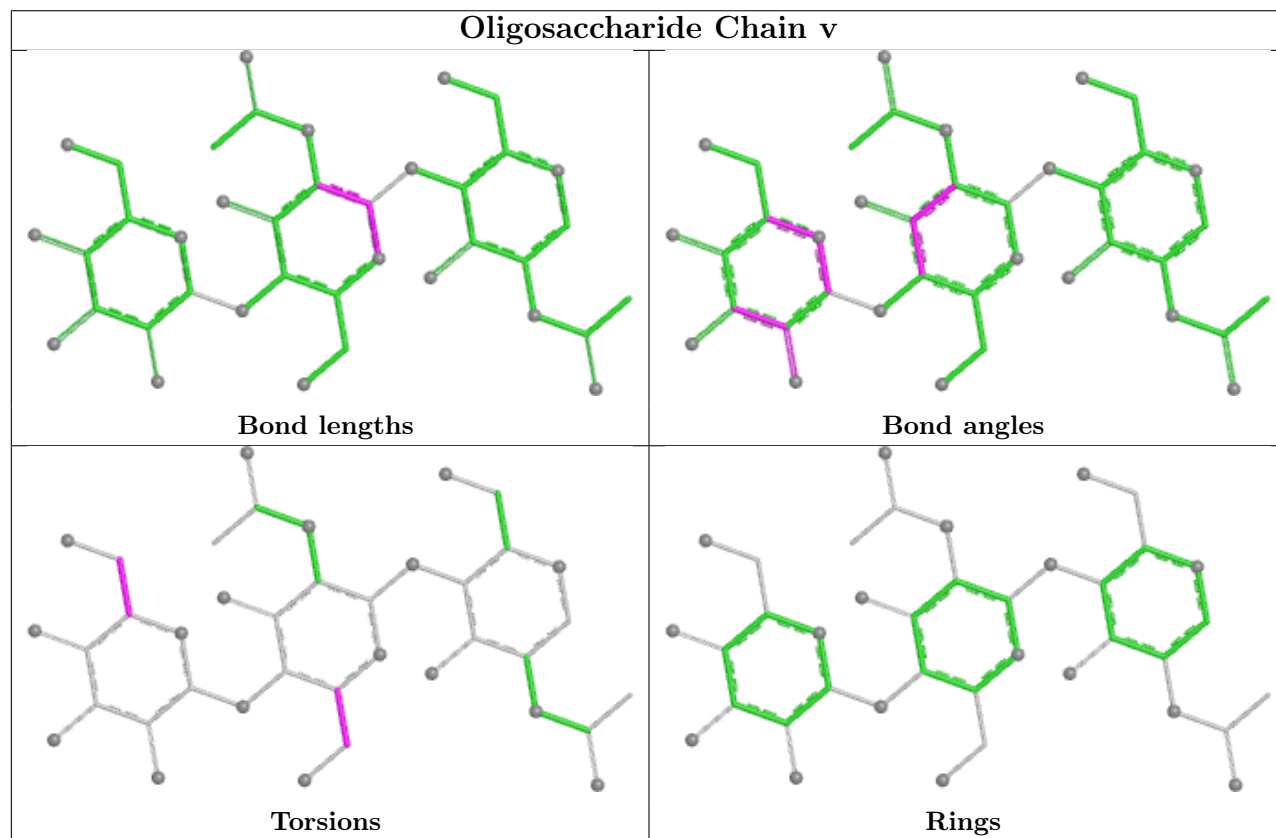
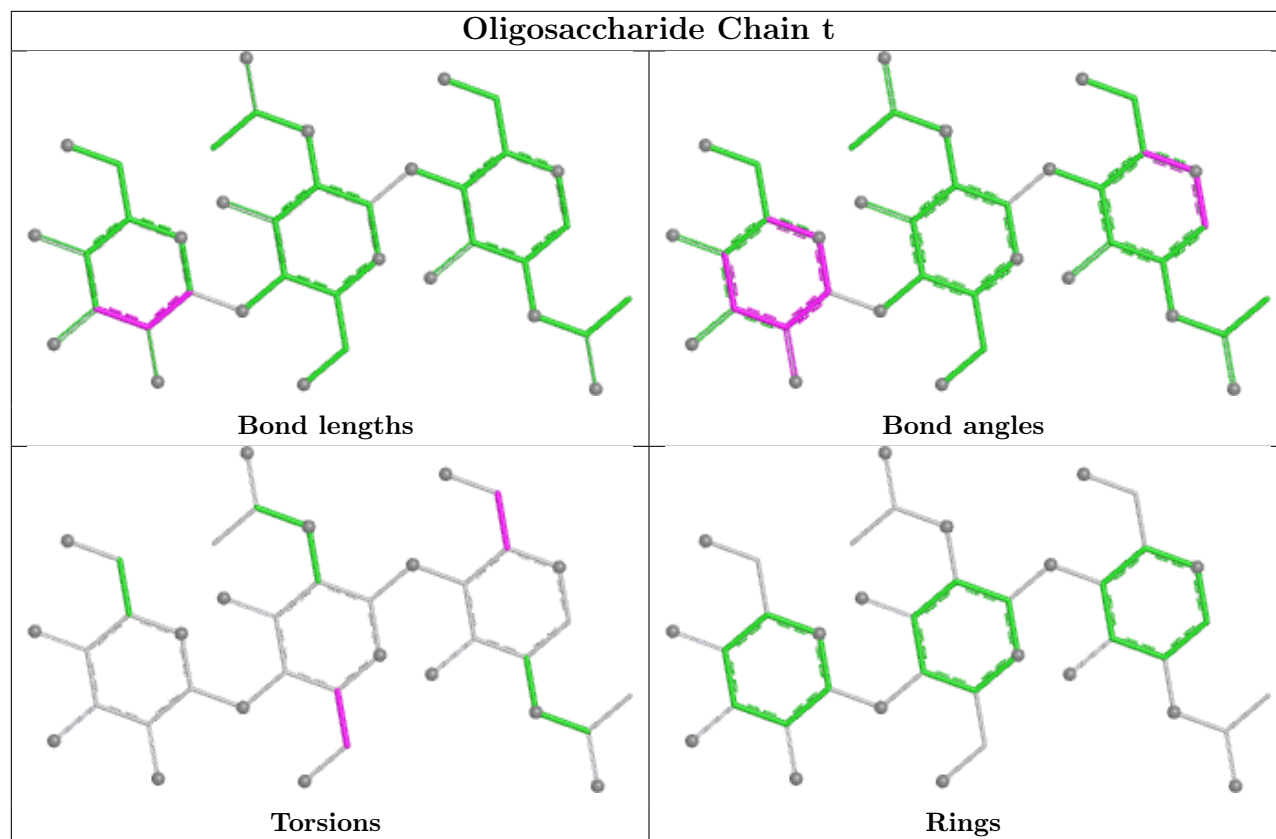


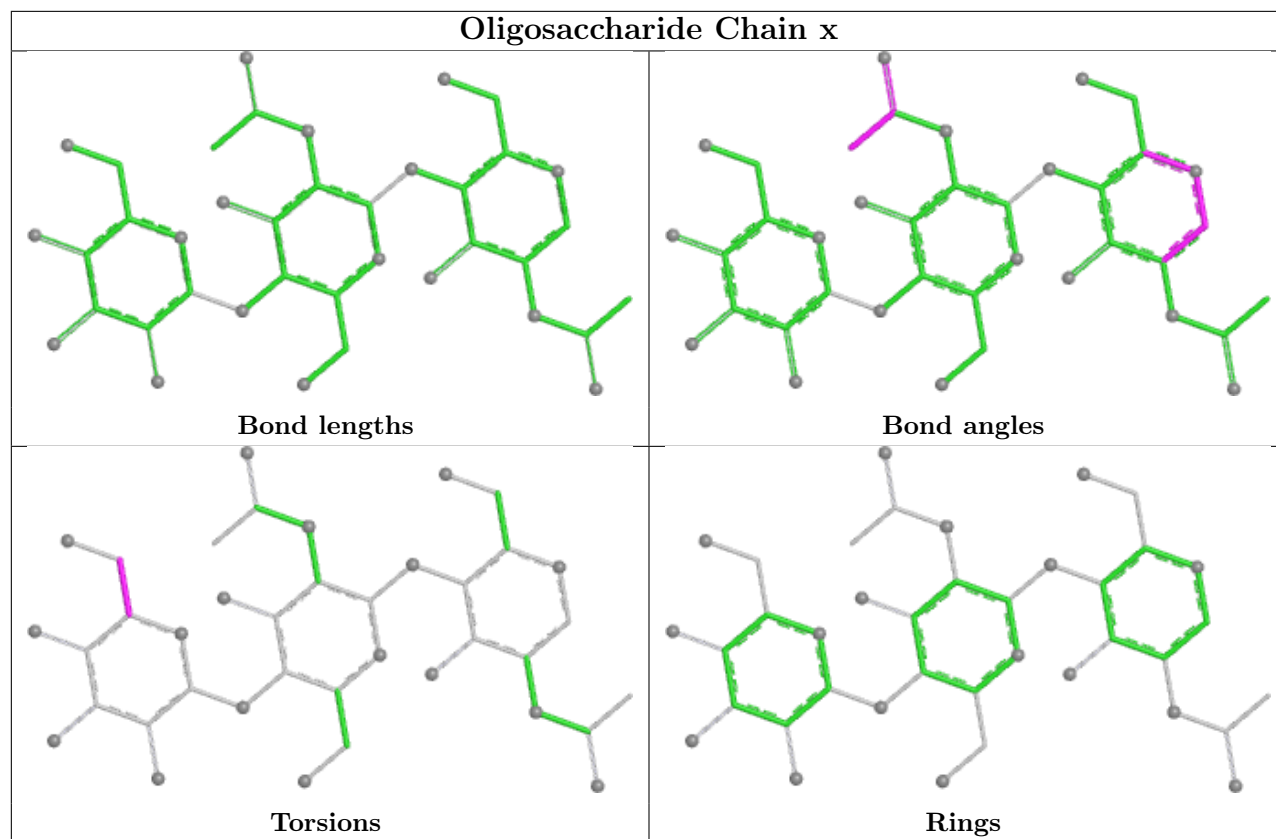


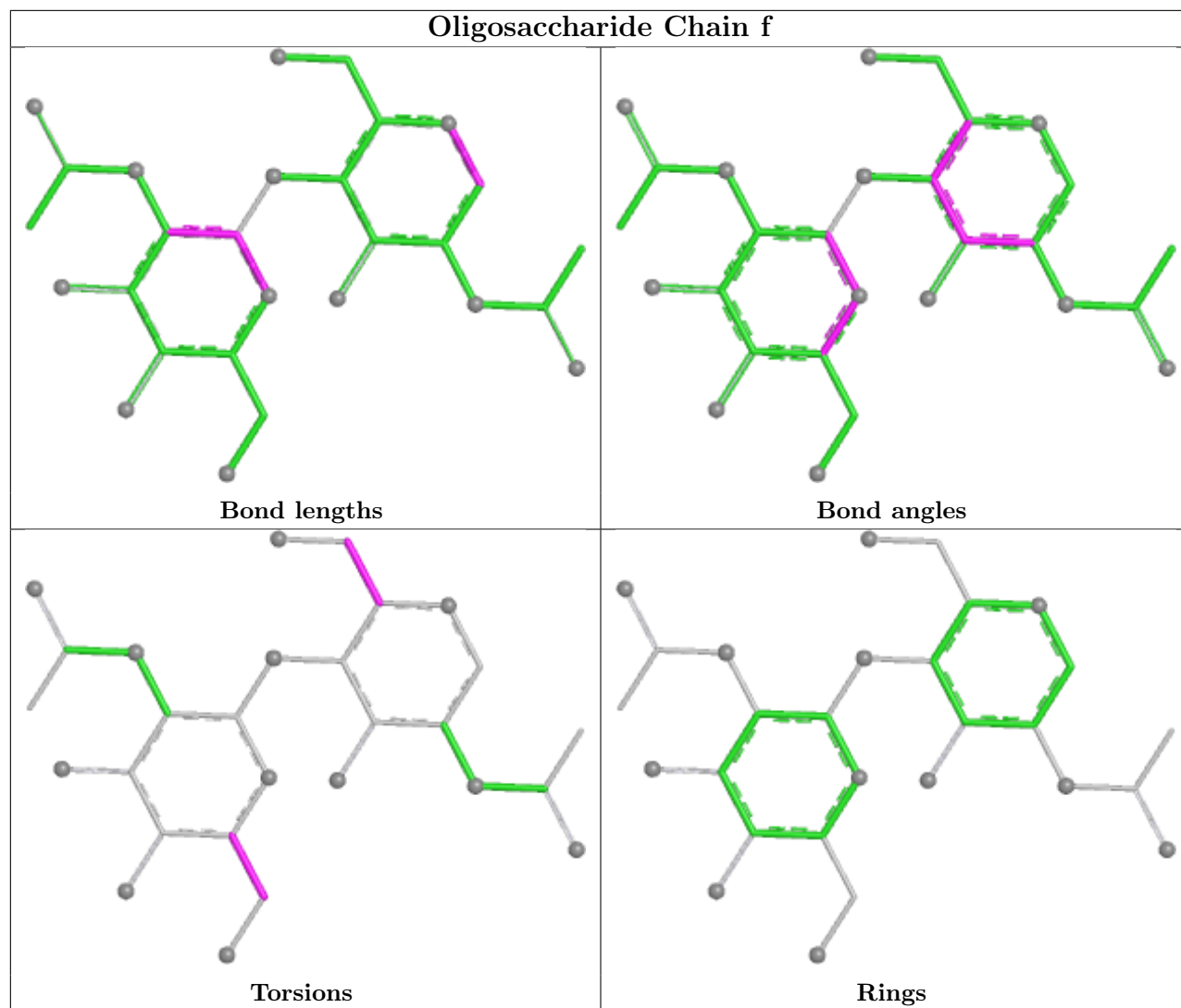


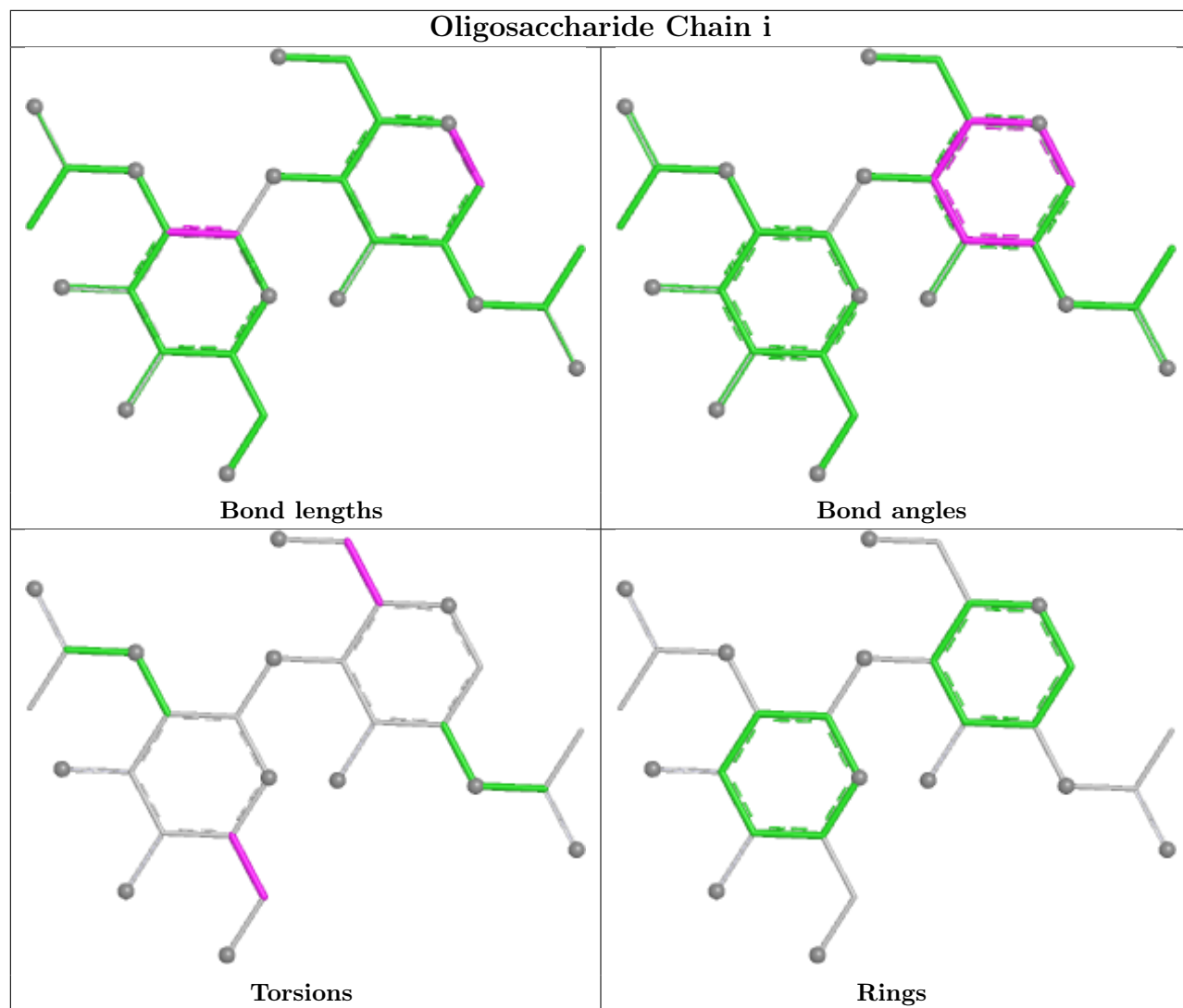


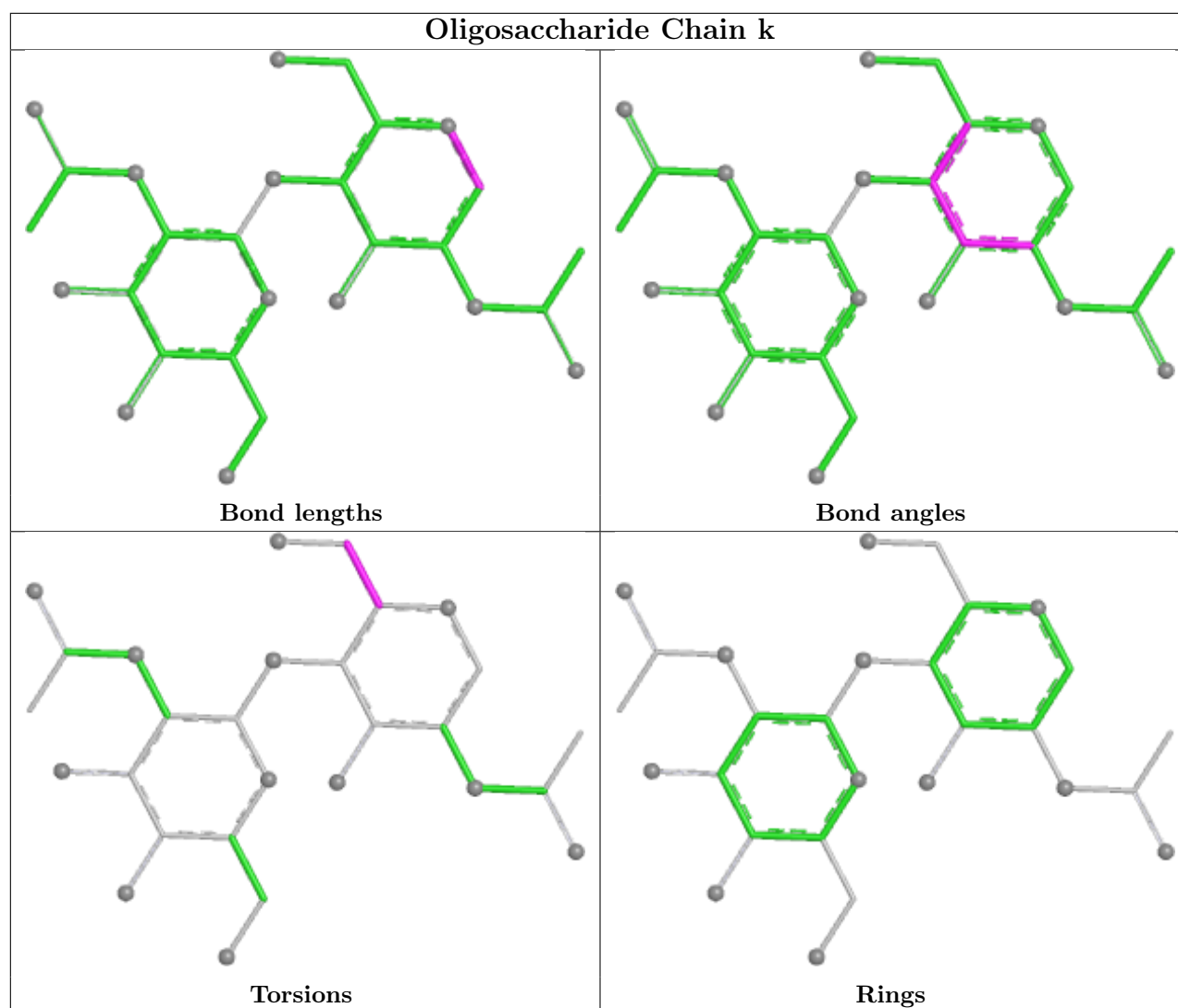


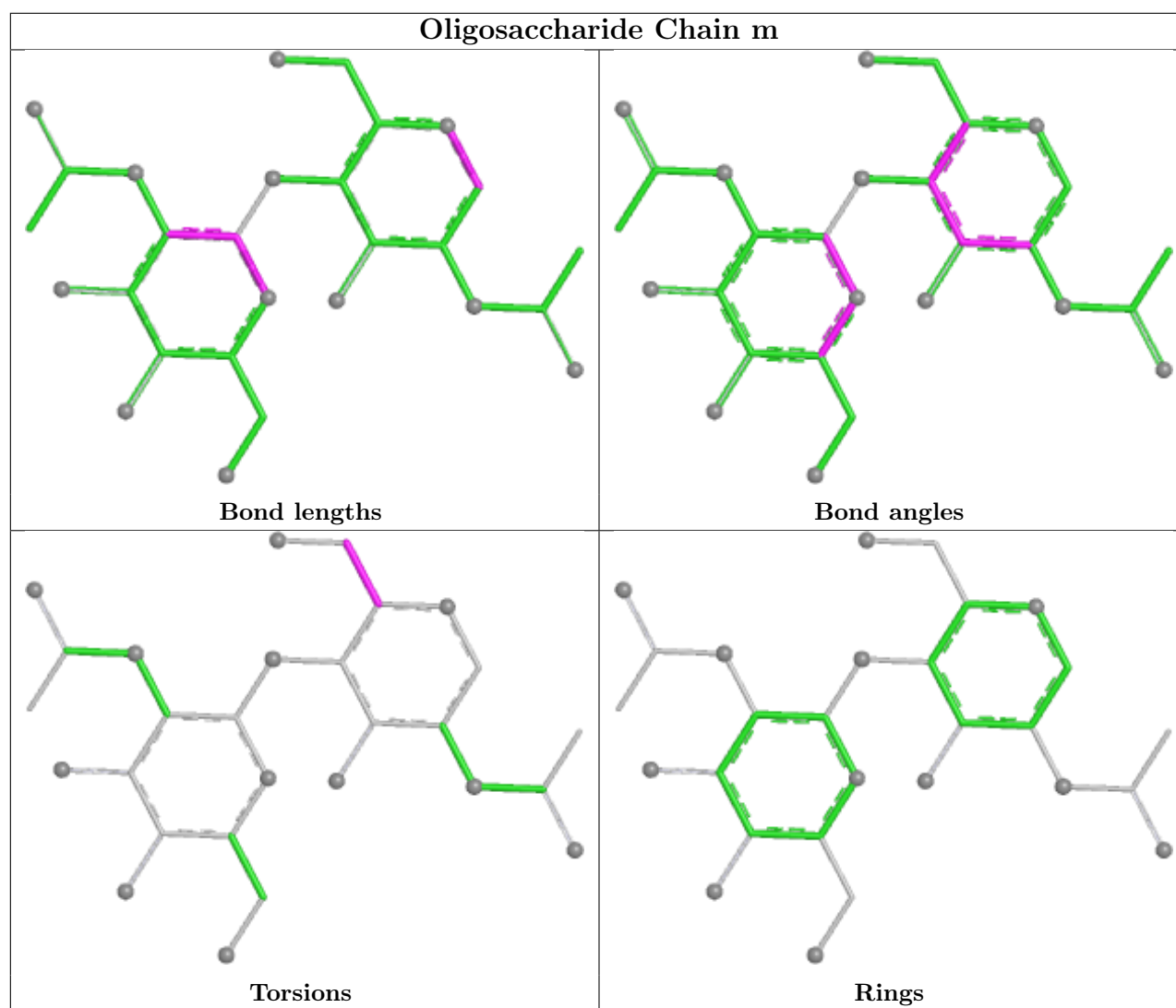


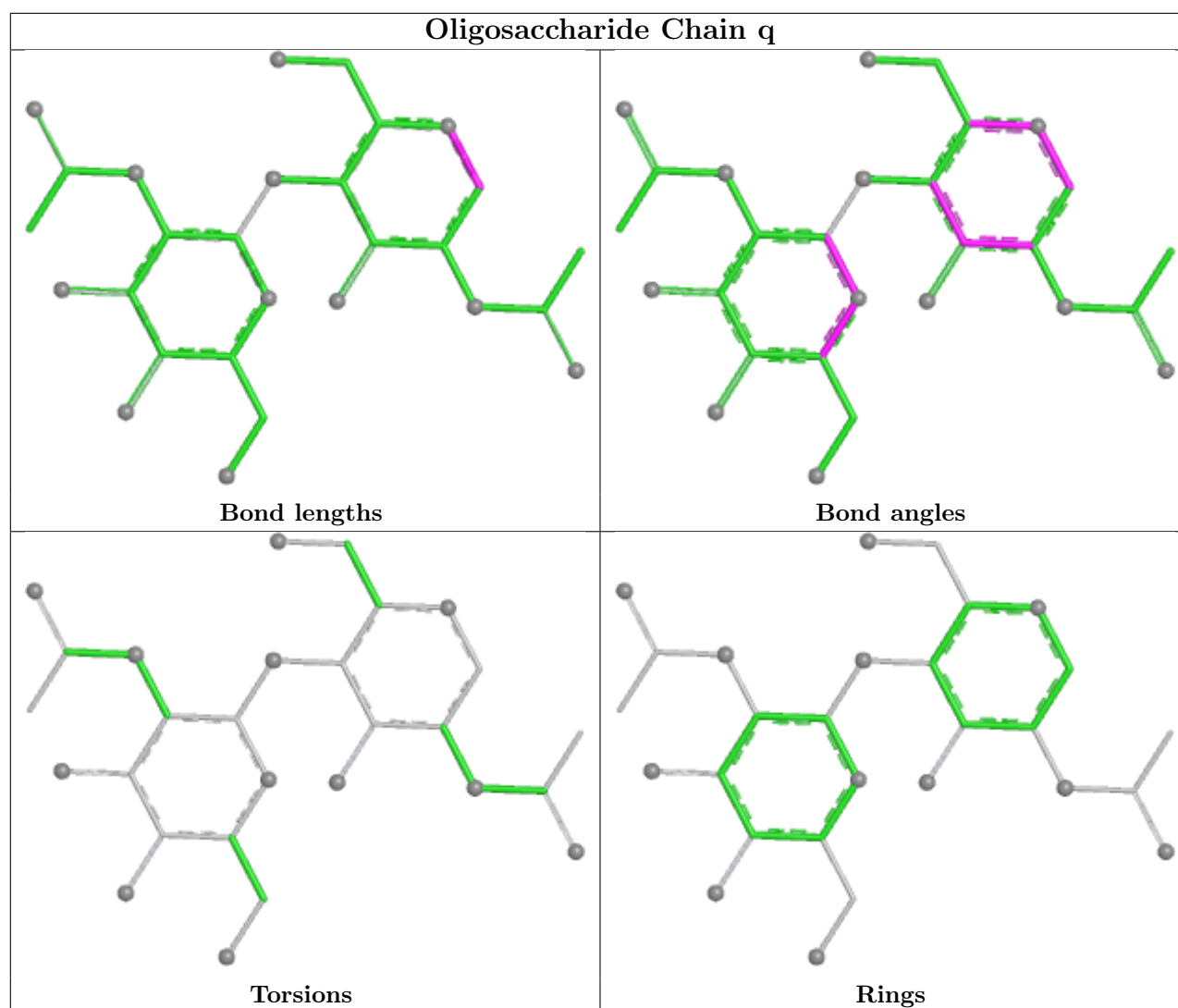


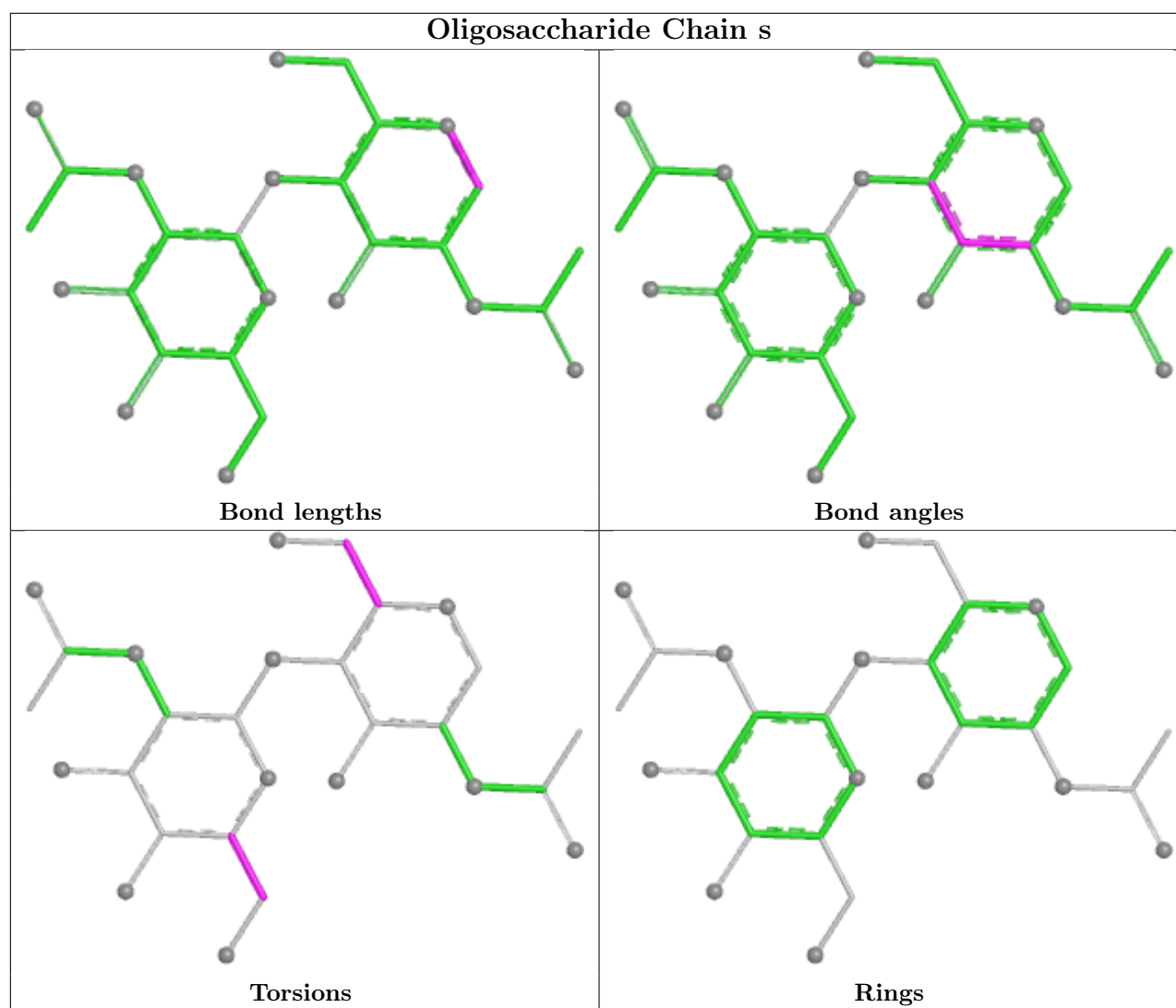


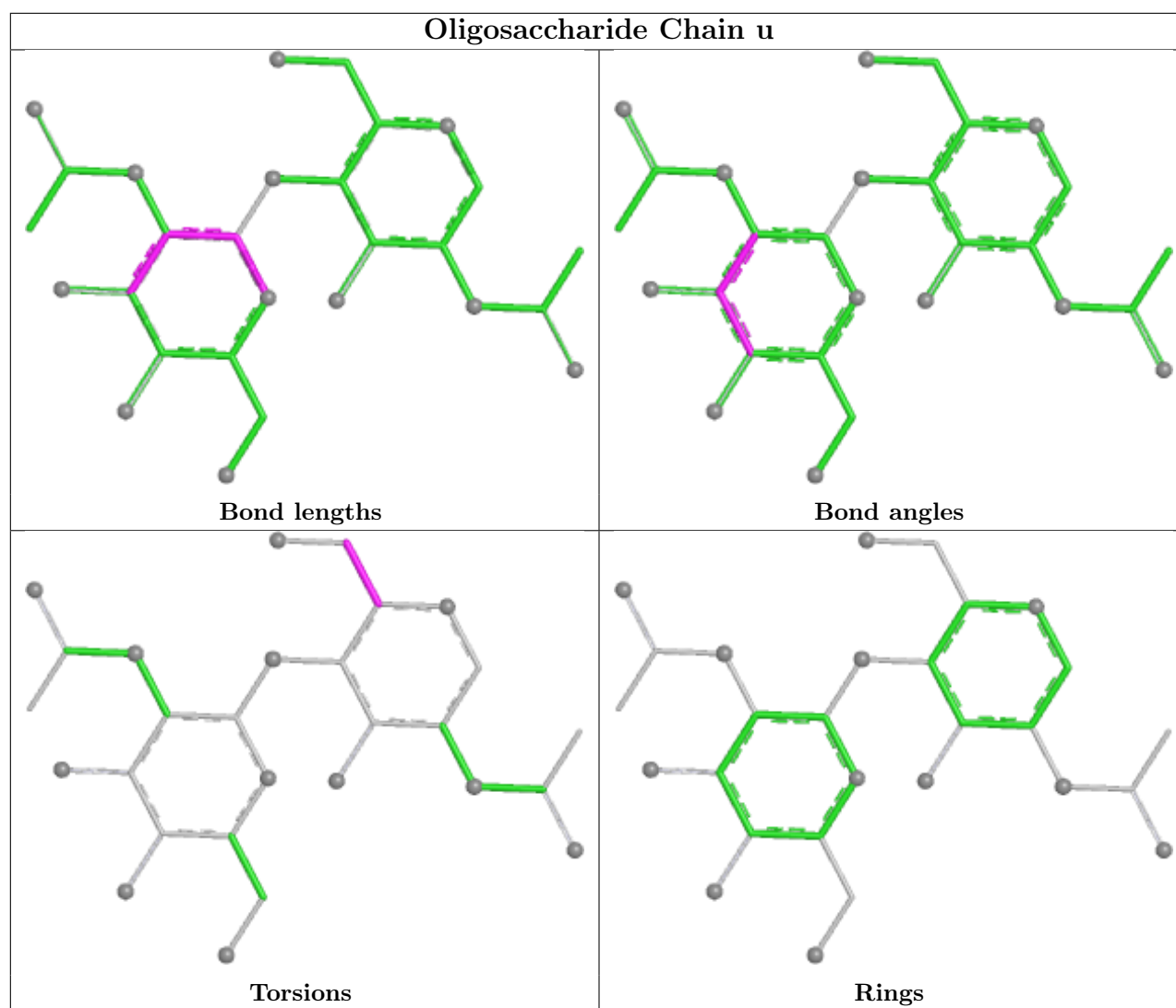


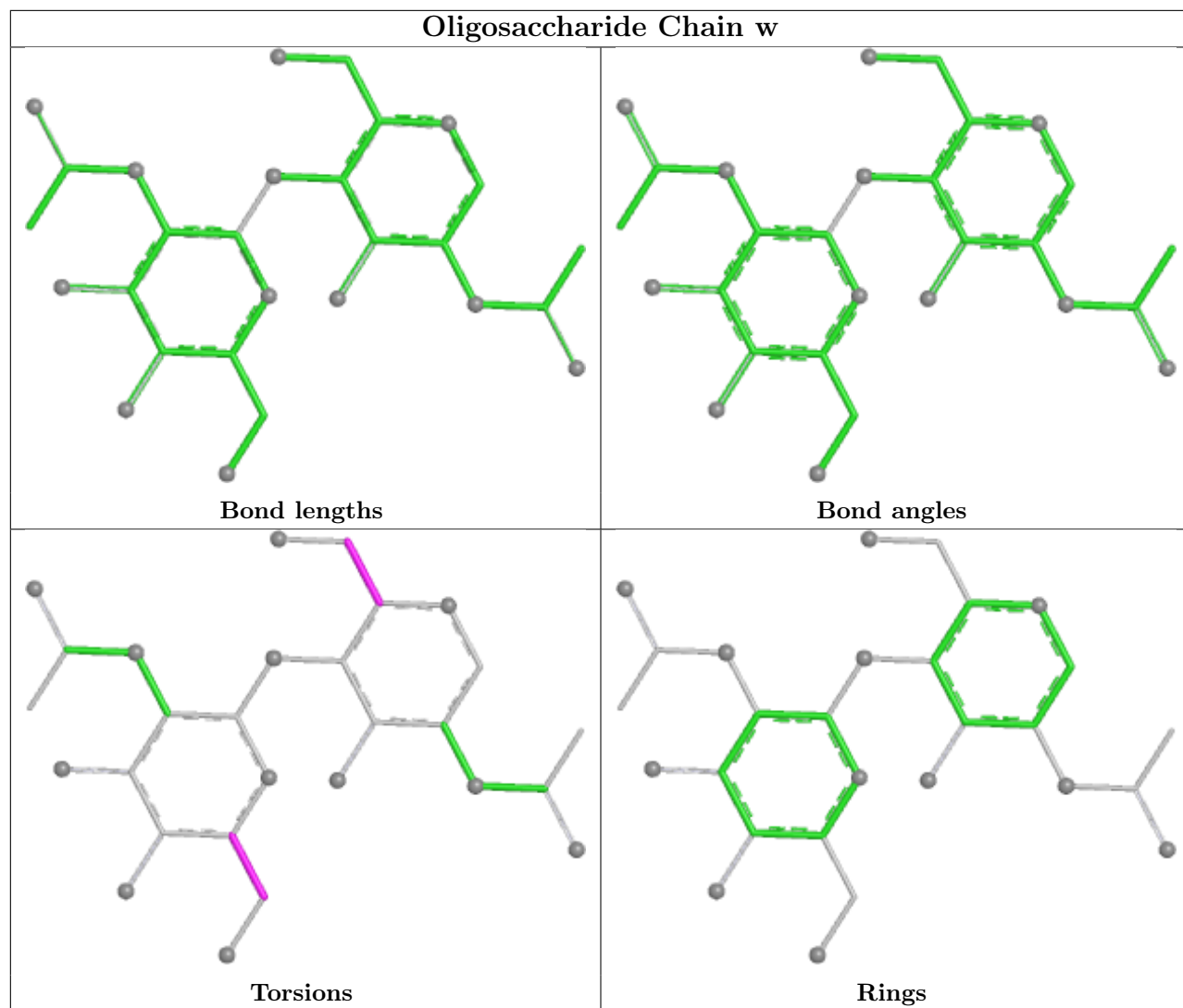


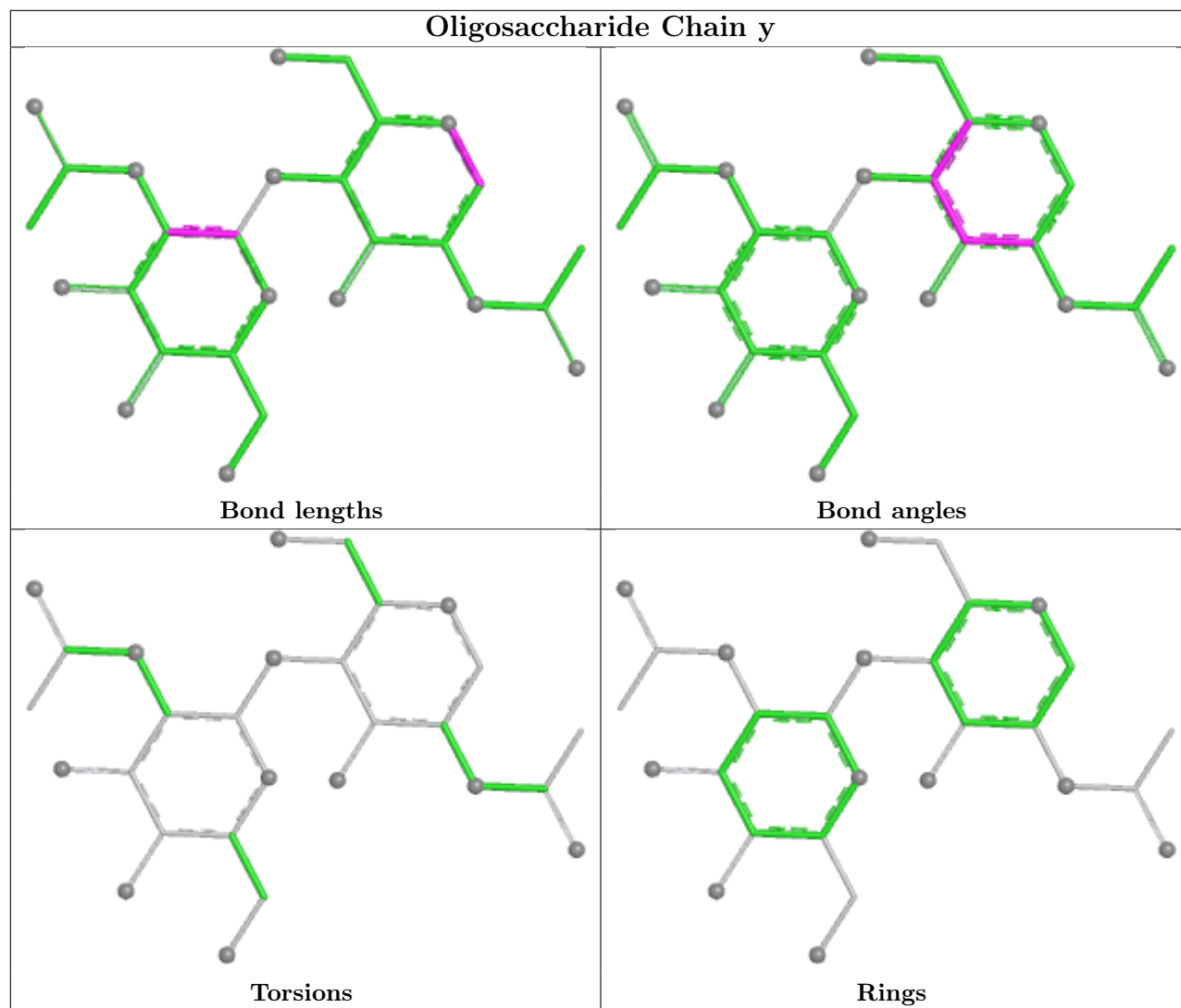


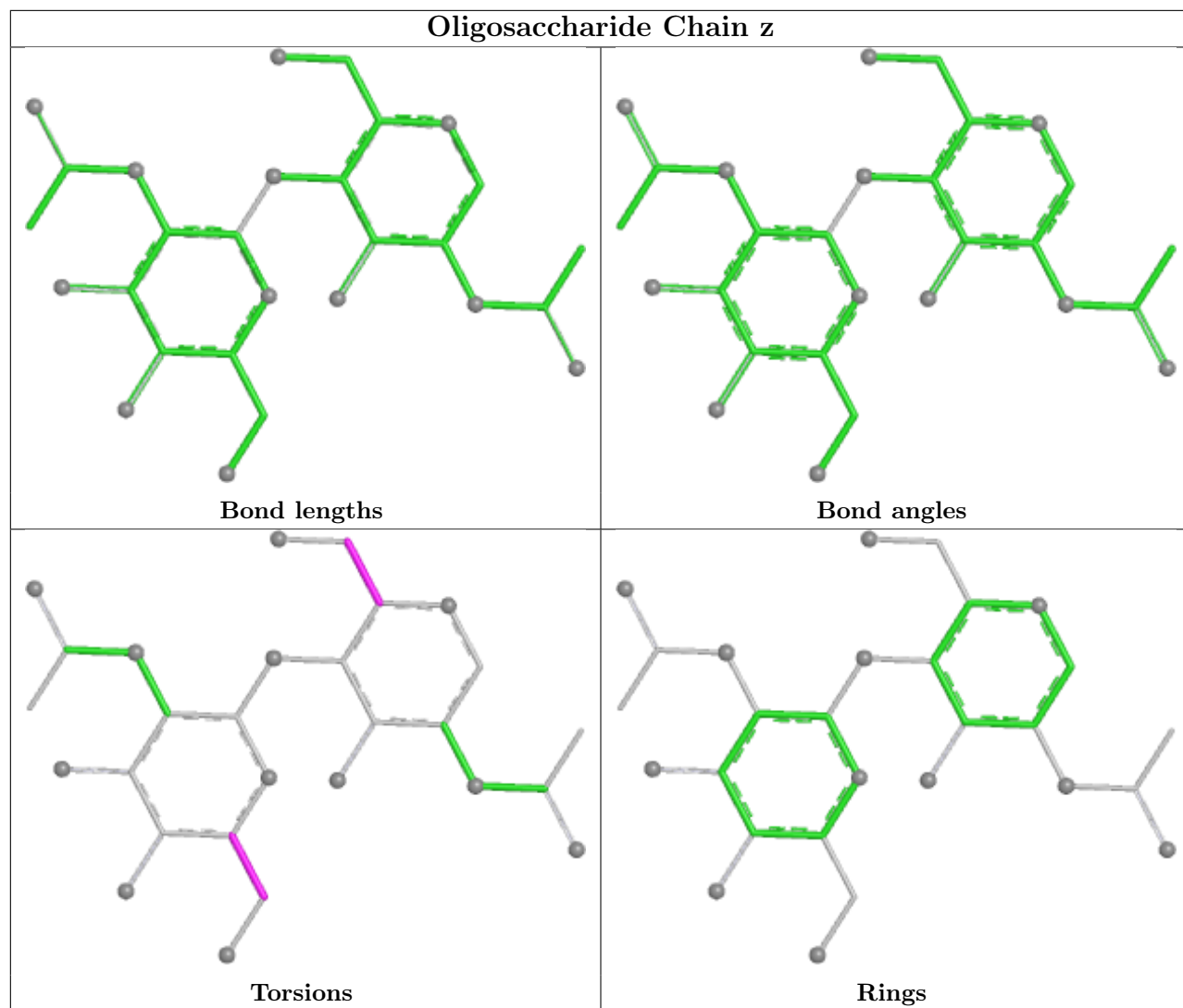


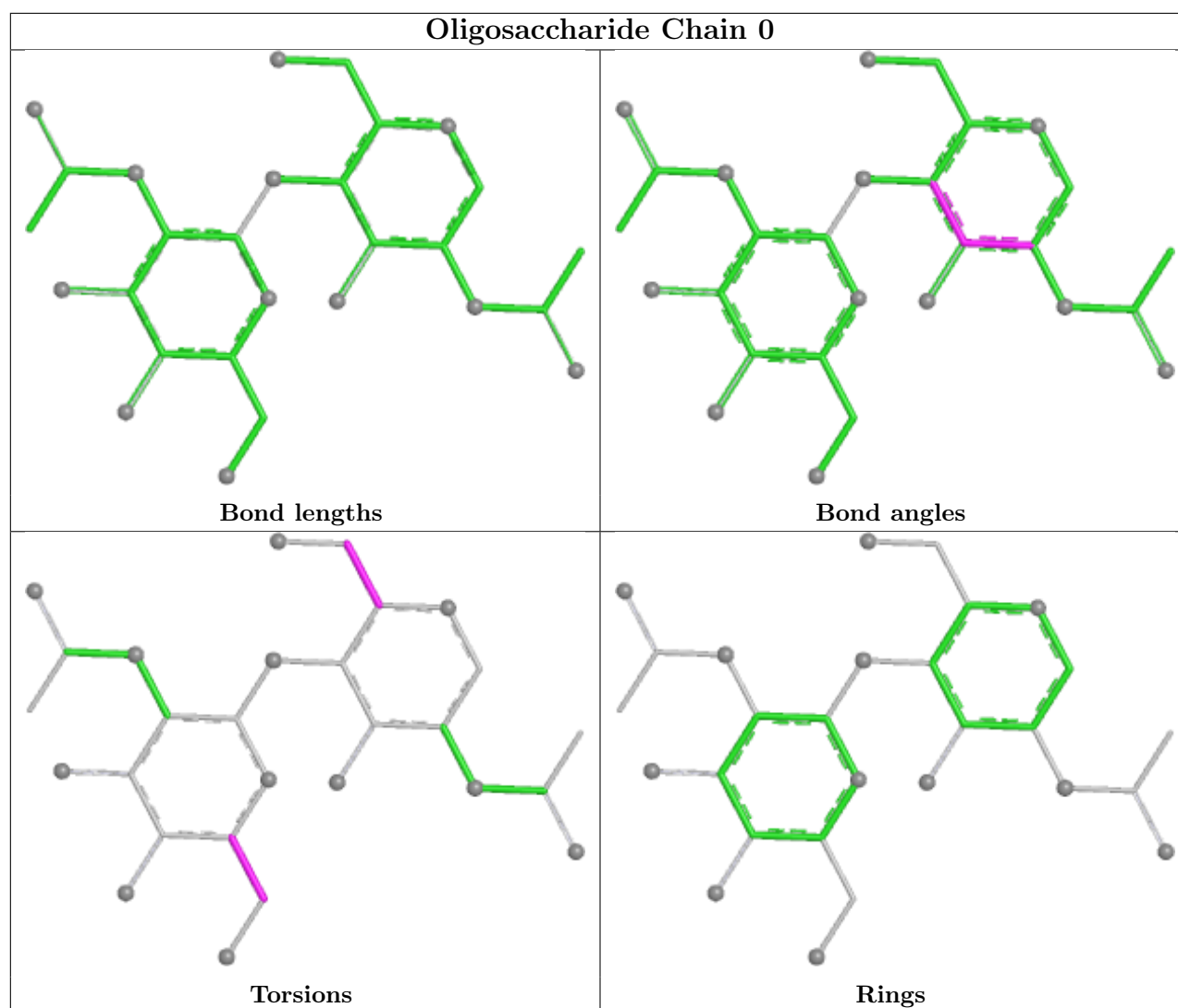












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	a	2001	1	14,14,15	0.60	0	17,19,21	0.68	1 (5%)
5	NAG	O	2006	1	14,14,15	1.00	1 (7%)	17,19,21	0.99	2 (11%)
5	NAG	M	2004	1	14,14,15	0.32	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	2004	1	14,14,15	0.88	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	Y	2001	1	14,14,15	0.37	0	17,19,21	0.98	1 (5%)
5	NAG	K	2004	1	14,14,15	0.65	0	17,19,21	0.58	0
5	NAG	c	2001	1	14,14,15	0.62	1 (7%)	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	a	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	O	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	M	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2006	NAG	O5-C1	-2.90	1.38	1.43
5	C	2004	NAG	O5-C1	-2.43	1.39	1.43
5	c	2001	NAG	O5-C1	-2.09	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	2001	NAG	C1-O5-C5	3.49	116.86	112.19
5	O	2006	NAG	C4-C3-C2	2.76	115.06	111.02
5	O	2006	NAG	C3-C4-C5	2.26	114.34	110.23
5	a	2001	NAG	C1-O5-C5	2.21	115.15	112.19
5	C	2004	NAG	C4-C3-C2	2.18	114.21	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2006	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	a	2001	NAG	O5-C5-C6-O6
5	O	2006	NAG	O5-C5-C6-O6
5	a	2001	NAG	C4-C5-C6-O6
5	M	2004	NAG	C4-C5-C6-O6
5	M	2004	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/334 (97%)	-1.49	0 100 100	32, 52, 86, 162	1 (0%)
1	C	324/334 (97%)	-1.46	0 100 100	38, 63, 122, 185	1 (0%)
1	E	324/334 (97%)	-1.49	0 100 100	36, 58, 115, 196	1 (0%)
1	G	324/334 (97%)	-1.53	0 100 100	28, 51, 91, 170	1 (0%)
1	I	324/334 (97%)	-1.55	0 100 100	27, 49, 93, 166	1 (0%)
1	K	324/334 (97%)	-1.40	0 100 100	37, 59, 112, 178	1 (0%)
1	M	324/334 (97%)	-1.47	0 100 100	28, 54, 113, 206	1 (0%)
1	O	324/334 (97%)	-1.45	0 100 100	32, 54, 116, 190	1 (0%)
1	Q	324/334 (97%)	-1.50	0 100 100	34, 53, 116, 181	1 (0%)
1	S	324/334 (97%)	-1.46	0 100 100	37, 62, 125, 177	1 (0%)
1	U	324/334 (97%)	-1.43	0 100 100	36, 66, 123, 186	1 (0%)
1	W	324/334 (97%)	-1.41	0 100 100	41, 64, 124, 183	1 (0%)
1	Y	324/334 (97%)	-1.27	2 (0%) 85 82	57, 83, 178, 247	1 (0%)
1	a	324/334 (97%)	-1.30	1 (0%) 90 88	59, 86, 197, 263	1 (0%)
1	c	324/334 (97%)	-1.29	0 100 100	55, 87, 180, 267	1 (0%)
2	B	177/181 (97%)	-1.29	0 100 100	36, 94, 134, 165	0
2	D	177/181 (97%)	-1.19	0 100 100	42, 124, 175, 199	0
2	F	177/181 (97%)	-1.17	0 100 100	45, 123, 173, 182	0
2	H	177/181 (97%)	-1.26	0 100 100	35, 97, 139, 151	0
2	J	177/181 (97%)	-1.35	0 100 100	36, 95, 136, 152	0
2	L	177/181 (97%)	-1.25	0 100 100	42, 122, 163, 171	0
2	N	177/181 (97%)	-1.17	0 100 100	37, 123, 176, 197	0
2	P	177/181 (97%)	-1.18	0 100 100	31, 120, 174, 185	0
2	R	177/181 (97%)	-1.14	0 100 100	42, 122, 189, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	177/181 (97%)	-1.24	0 100 100	48, 123, 166, 184	0
2	V	177/181 (97%)	-1.11	0 100 100	45, 123, 167, 180	0
2	X	177/181 (97%)	-1.14	0 100 100	46, 123, 171, 182	0
2	Z	177/181 (97%)	-0.34	9 (5%) 33 28	68, 193, 265, 299	0
2	b	177/181 (97%)	-0.65	3 (1%) 69 62	74, 189, 251, 272	0
2	d	177/181 (97%)	-0.54	6 (3%) 48 41	68, 193, 239, 274	0
All	All	7515/7725 (97%)	-1.30	21 (0%) 90 88	27, 75, 185, 299	15 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	35	ALA	8.7
2	Z	23	GLY	7.6
1	Y	16	GLY	7.2
2	Z	9	PHE	7.0
2	d	36	ALA	6.1
2	b	141	TYR	5.7
2	Z	24	TYR	5.3
2	b	152	VAL	4.9
2	d	24	TYR	4.8
2	d	35	ALA	4.7
2	Z	8	GLY	3.8
2	b	131	LYS	3.2
1	Y	15	ILE	3.2
1	a	15	ILE	2.9
2	Z	36	ALA	2.6
2	Z	10	ILE	2.4
2	d	153	ARG	2.3
2	d	128	ASP	2.2
2	Z	7	ALA	2.2
2	Z	115	VAL	2.1
2	d	23	GLY	2.0

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	e	1	14/15	-	-	49,69,79,82	0
3	NAG	e	2	14/15	-	-	59,82,94,97	0
3	BMA	e	3	11/12	-	-	81,83,101,101	0
3	NAG	g	1	14/15	-	-	70,89,102,112	0
3	NAG	g	2	14/15	-	-	98,106,110,110	0
3	BMA	g	3	11/12	-	-	48,70,90,94	0
3	NAG	h	1	14/15	-	-	74,93,116,124	0
3	NAG	h	2	14/15	-	-	103,121,127,128	0
3	BMA	h	3	11/12	-	-	74,81,103,103	0
3	NAG	j	1	14/15	-	-	57,65,73,85	0
3	NAG	j	2	14/15	-	-	49,63,83,84	0
3	BMA	j	3	11/12	-	-	63,85,93,95	0
3	NAG	l	1	14/15	-	-	50,58,78,80	0
3	NAG	l	2	14/15	-	-	44,57,67,71	0
3	BMA	l	3	11/12	-	-	56,83,91,91	0
3	NAG	n	1	14/15	-	-	56,78,99,101	0
3	NAG	n	2	14/15	-	-	81,97,102,102	0
3	BMA	n	3	11/12	-	-	67,77,85,86	0
3	NAG	o	1	14/15	-	-	50,58,79,79	0
3	NAG	o	2	14/15	-	-	76,91,113,128	0
3	BMA	o	3	11/12	-	-	105,121,134,135	0
3	NAG	p	1	14/15	-	-	58,72,90,97	0
3	NAG	p	2	14/15	-	-	83,102,117,123	0
3	BMA	p	3	11/12	-	-	119,127,132,132	0
3	NAG	r	1	14/15	-	-	52,67,75,77	0
3	NAG	r	2	14/15	-	-	67,88,103,115	0
3	BMA	r	3	11/12	-	-	116,120,126,127	0
3	NAG	t	1	14/15	-	-	57,81,97,97	0
3	NAG	t	2	14/15	-	-	87,110,127,135	0
3	BMA	t	3	11/12	-	-	110,125,137,139	0
3	NAG	v	1	14/15	-	-	59,71,87,99	0
3	NAG	v	2	14/15	-	-	89,104,121,126	0
3	BMA	v	3	11/12	-	-	114,127,131,133	0
3	NAG	x	1	14/15	-	-	64,71,80,92	0
3	NAG	x	2	14/15	-	-	77,96,107,119	0
3	BMA	x	3	11/12	-	-	113,124,130,135	0
4	NAG	f	1	14/15	-	-	93,112,119,119	0

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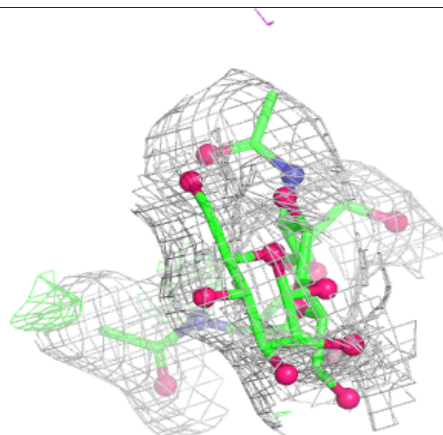
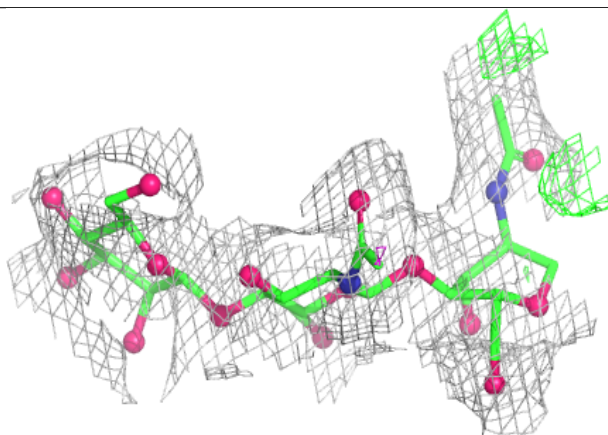
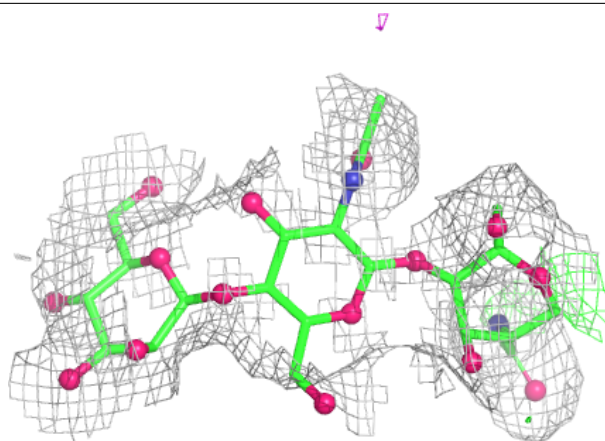
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	f	2	14/15	-	-	112,122,129,132	0
4	NAG	i	1	14/15	-	-	112,124,125,126	0
4	NAG	i	2	14/15	-	-	106,128,134,134	0
4	NAG	k	1	14/15	-	-	102,107,113,114	0
4	NAG	k	2	14/15	-	-	106,120,127,128	0
4	NAG	m	1	14/15	-	-	89,94,103,109	0
4	NAG	m	2	14/15	-	-	111,117,124,133	0
4	NAG	q	1	14/15	-	-	123,134,139,143	0
4	NAG	q	2	14/15	-	-	117,139,146,146	0
4	NAG	s	1	14/15	-	-	101,118,133,146	0
4	NAG	s	2	14/15	-	-	120,148,158,161	0
4	NAG	u	1	14/15	-	-	128,150,163,163	0
4	NAG	u	2	14/15	-	-	150,164,166,166	0
4	NAG	w	1	14/15	-	-	130,142,151,153	0
4	NAG	w	2	14/15	-	-	136,154,160,165	0
4	NAG	y	1	14/15	-	-	114,128,139,141	0
4	NAG	y	2	14/15	-	-	122,134,141,141	0
4	NAG	z	1	14/15	-	-	155,161,168,175	0
4	NAG	z	2	14/15	-	-	159,180,187,187	0
4	NAG	0	1	14/15	-	-	159,180,187,188	0
4	NAG	0	2	14/15	-	-	168,181,188,188	0

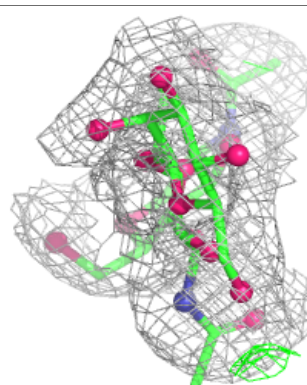
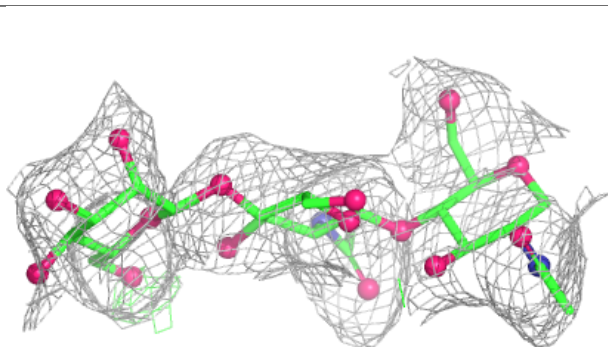
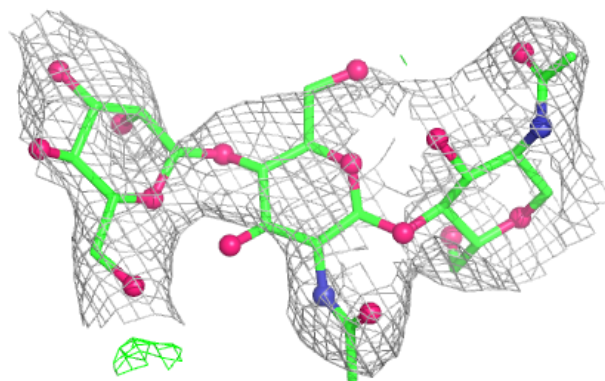
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

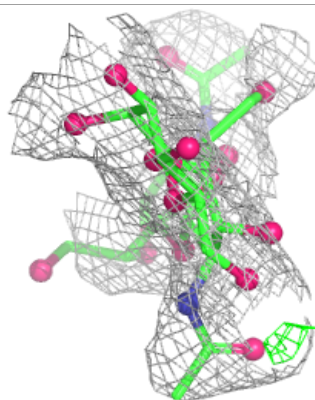
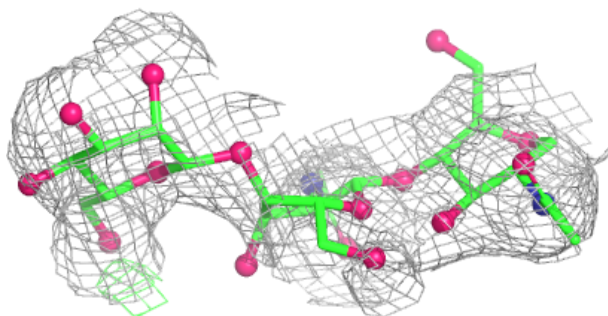
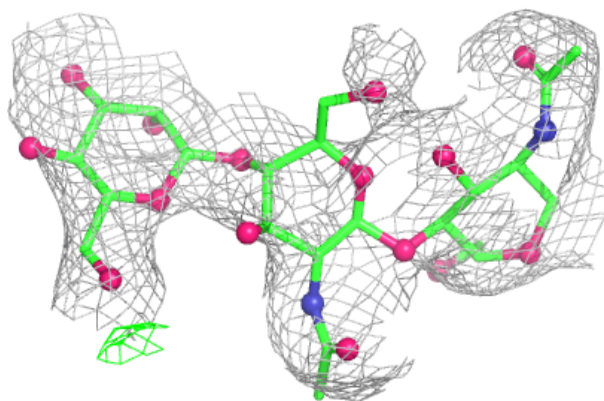
**Electron density around Chain g:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

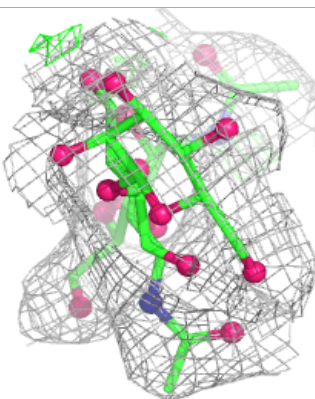
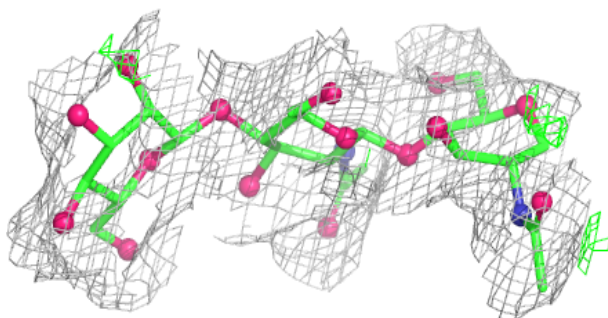
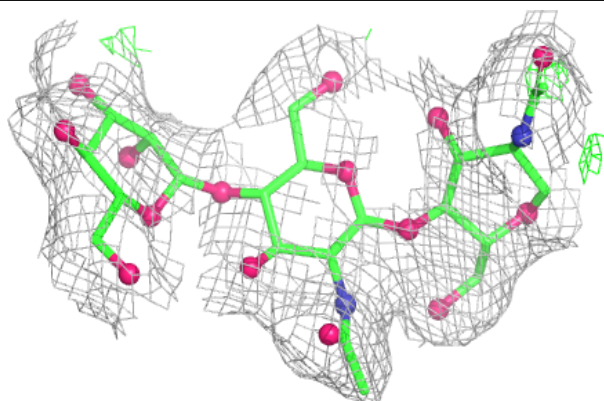


Electron density around Chain h:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

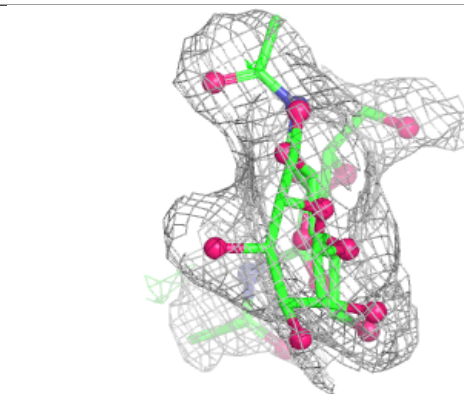
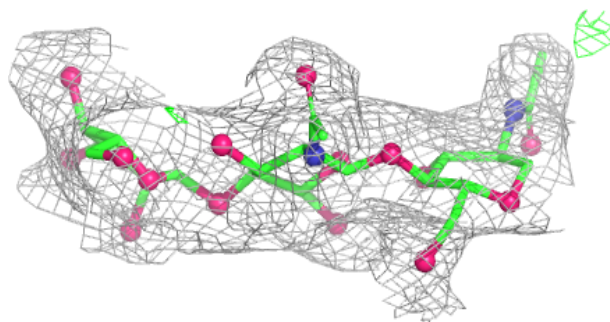
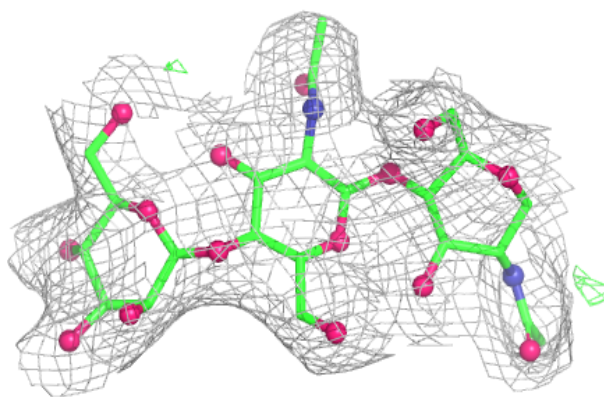
**Electron density around Chain j:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

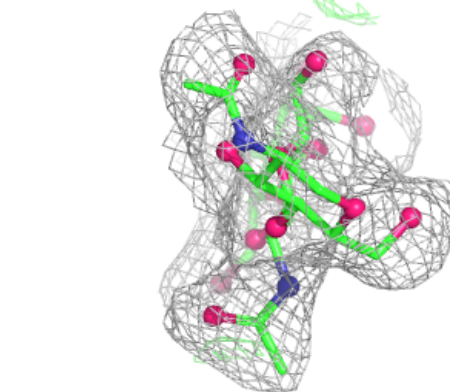
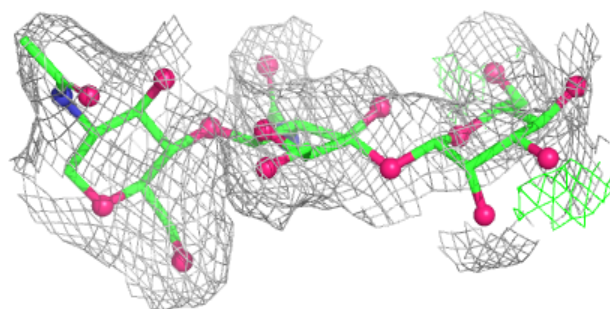
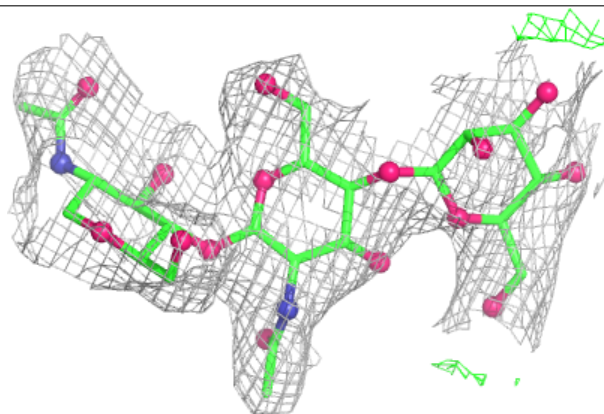


Electron density around Chain 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

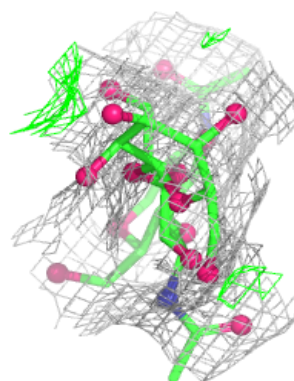
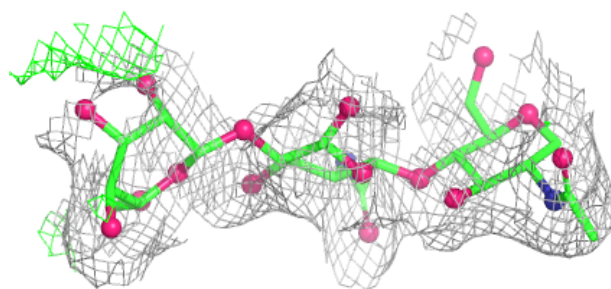
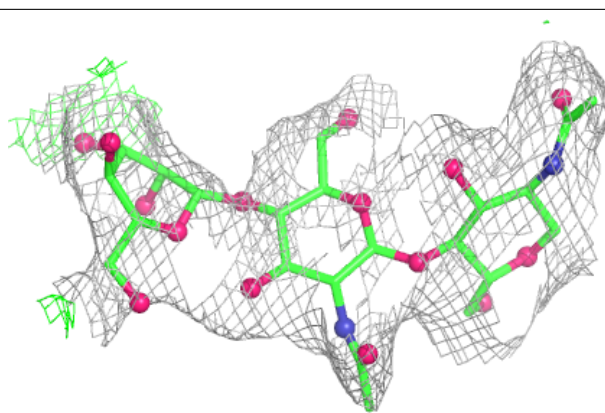
**Electron density around Chain n:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

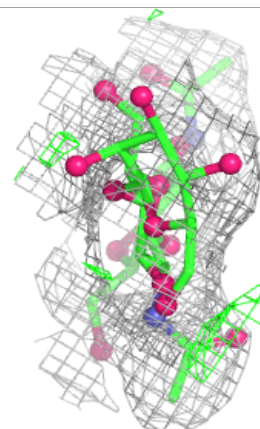
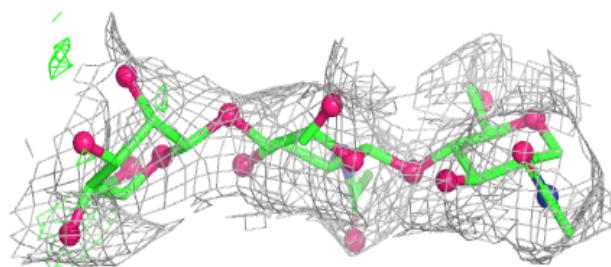
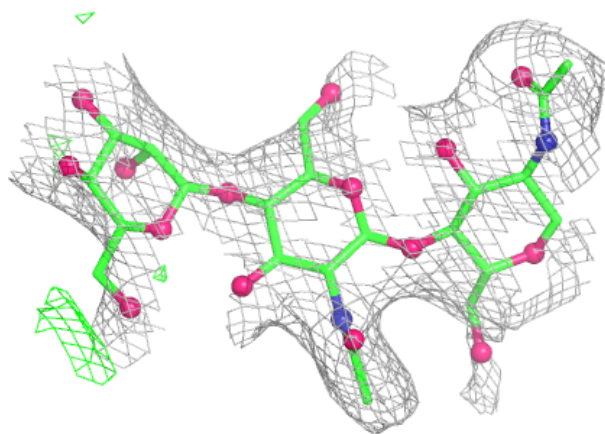


Electron density around Chain o:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

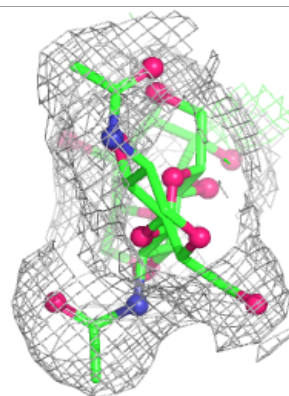
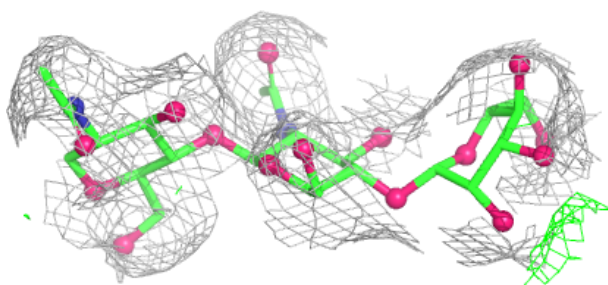
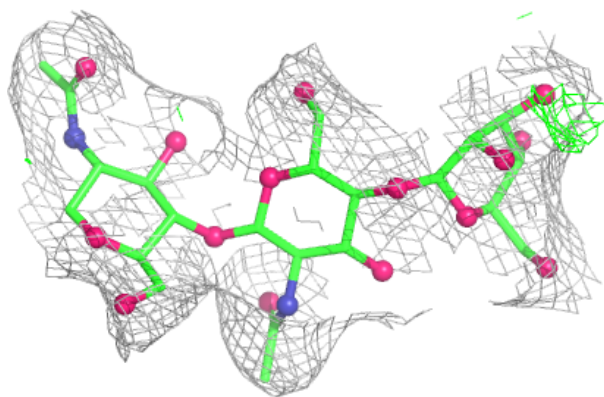
**Electron density around Chain p:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

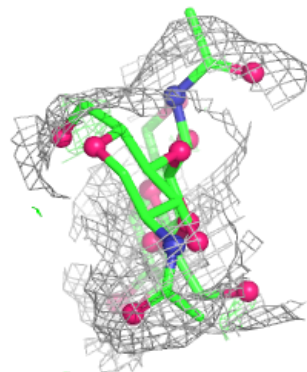
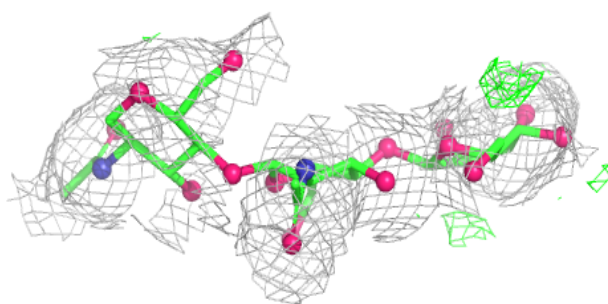
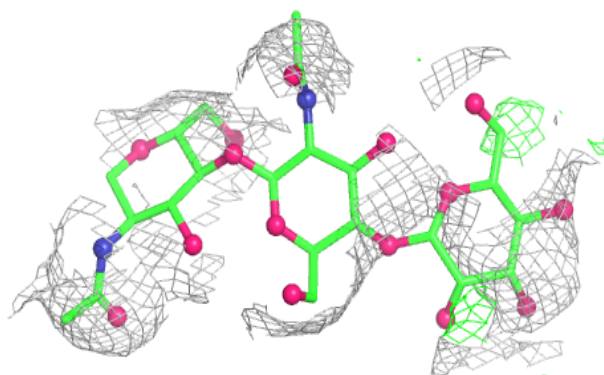


Electron density around Chain r:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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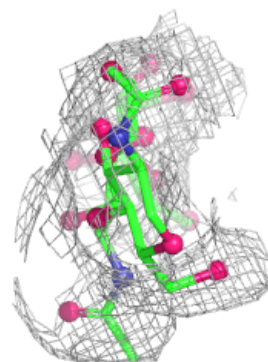
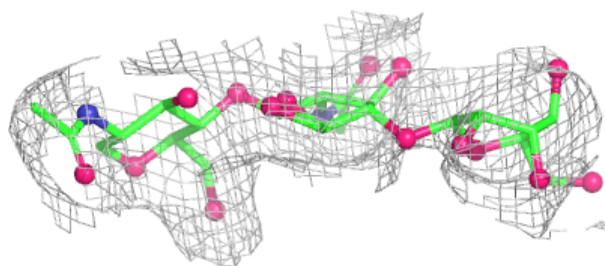
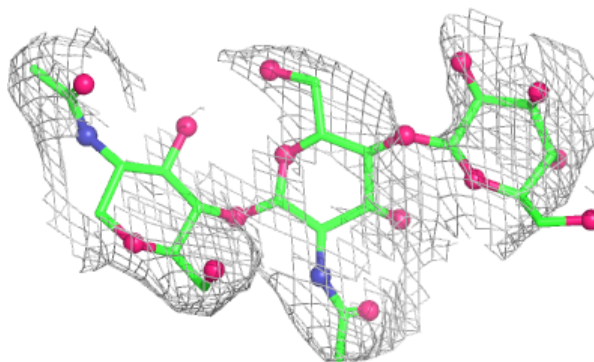
**Electron density around Chain t:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

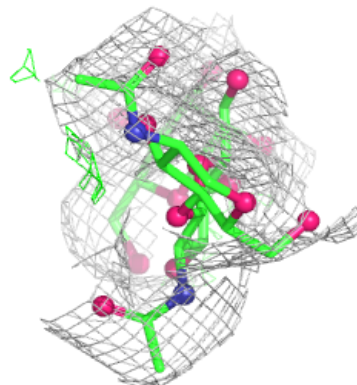
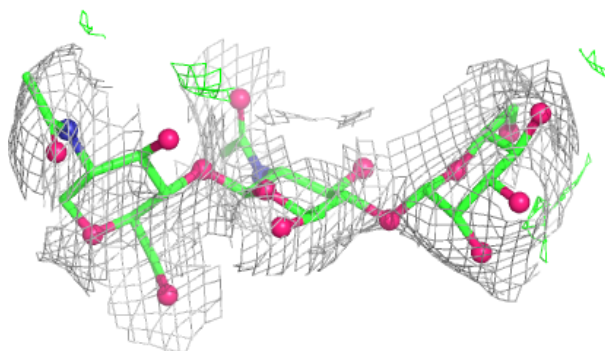
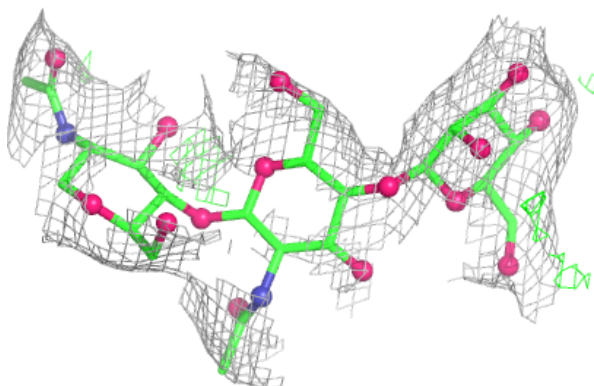


Electron density around Chain v:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

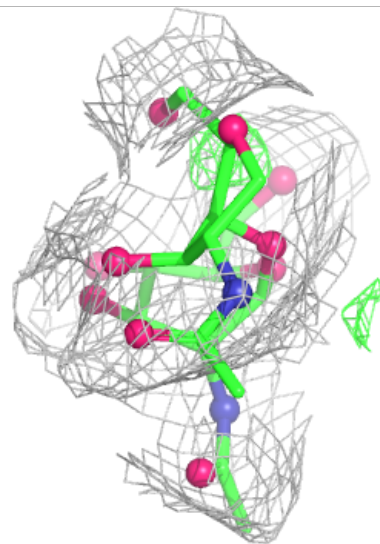
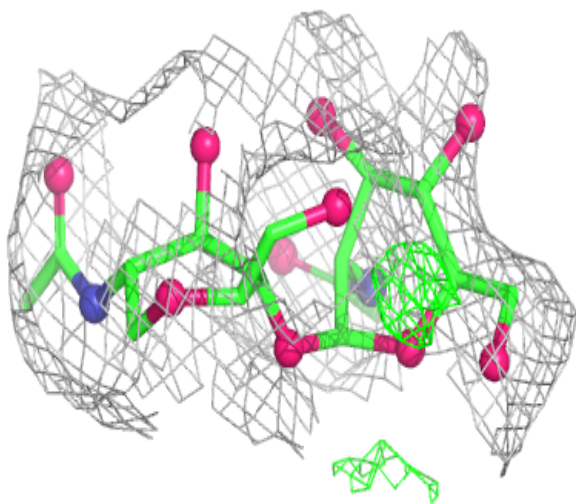
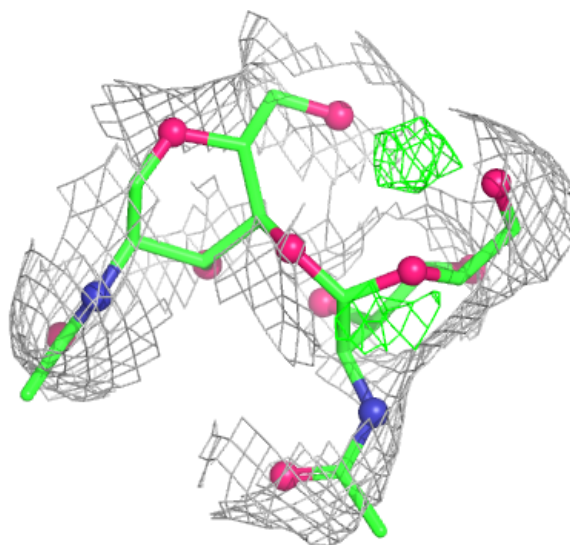
**Electron density around Chain x:**

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and green (positive)



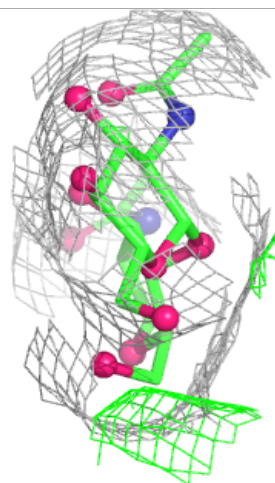
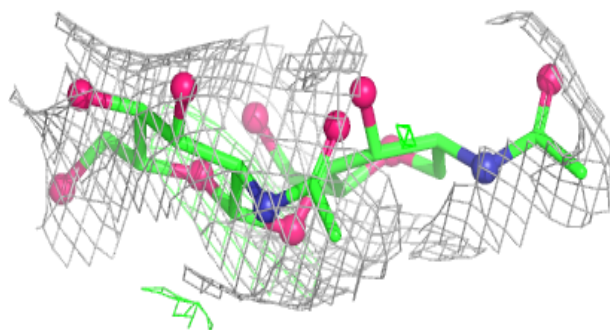
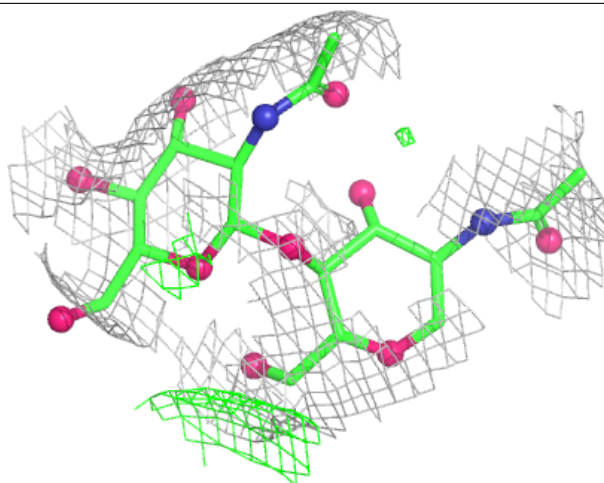
Electron density around Chain f:

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and green (positive)



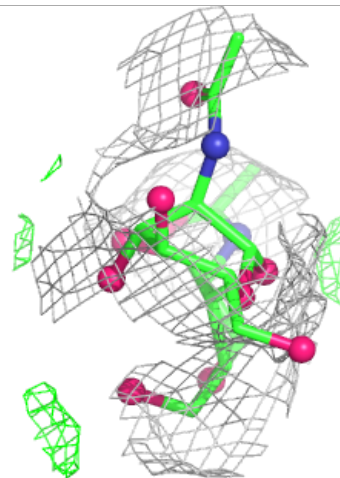
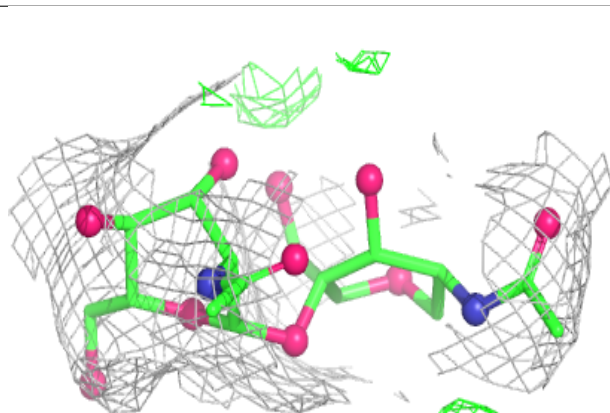
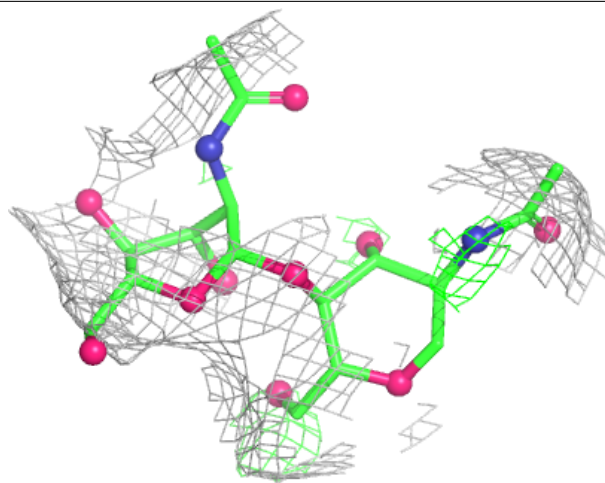
Electron density around Chain i:

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and green (positive)



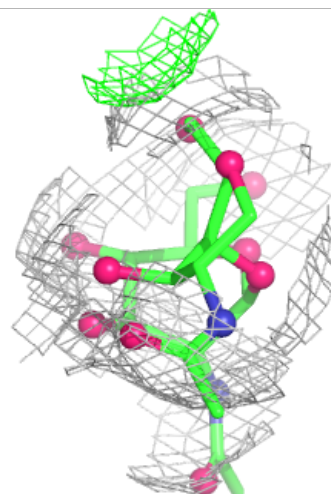
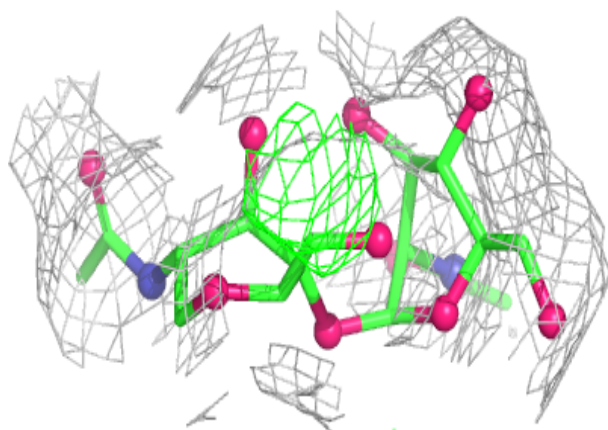
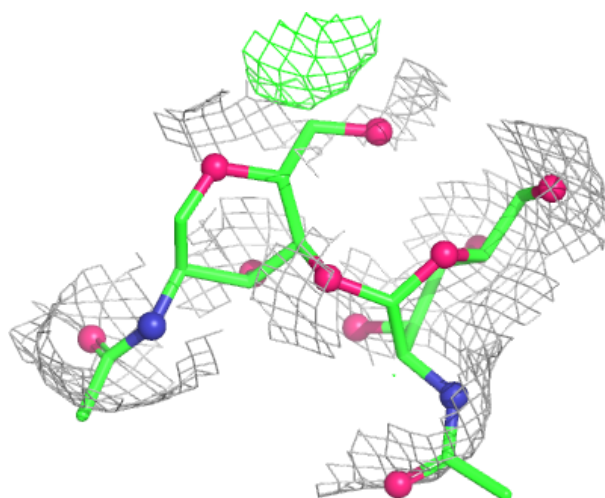
Electron density around Chain k:

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and green (positive)



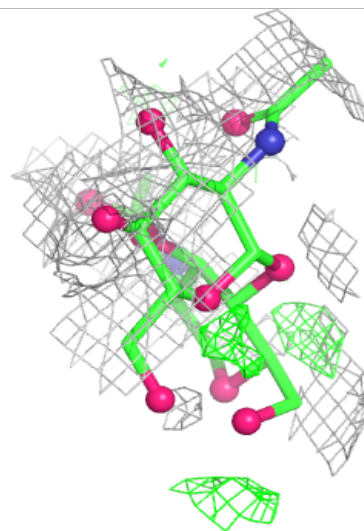
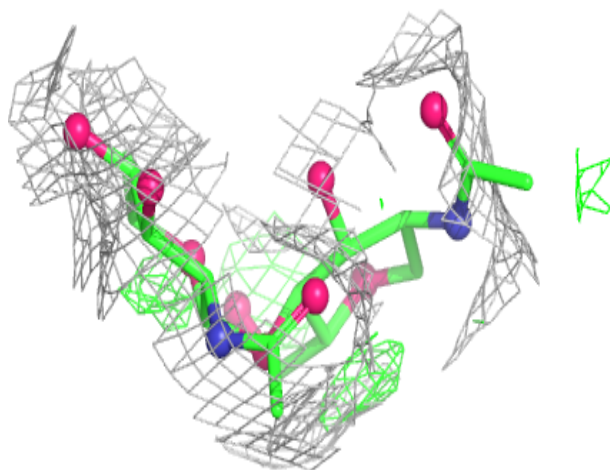
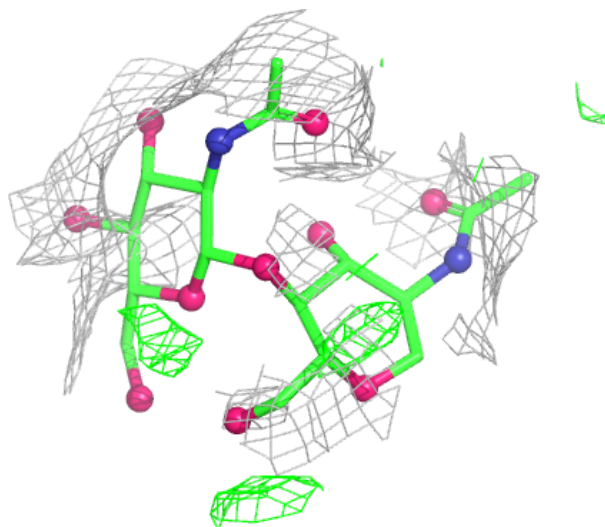
Electron density around Chain m:

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and green (positive)



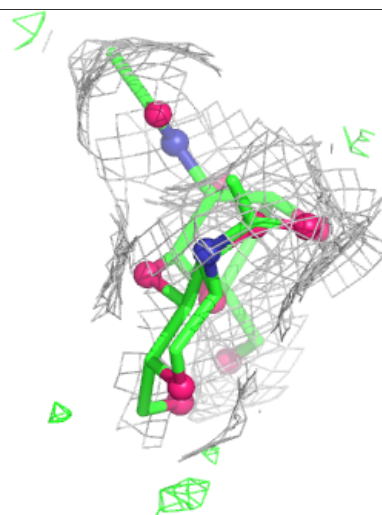
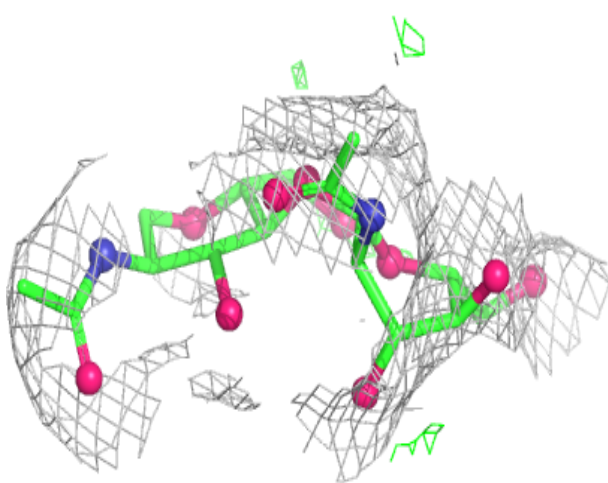
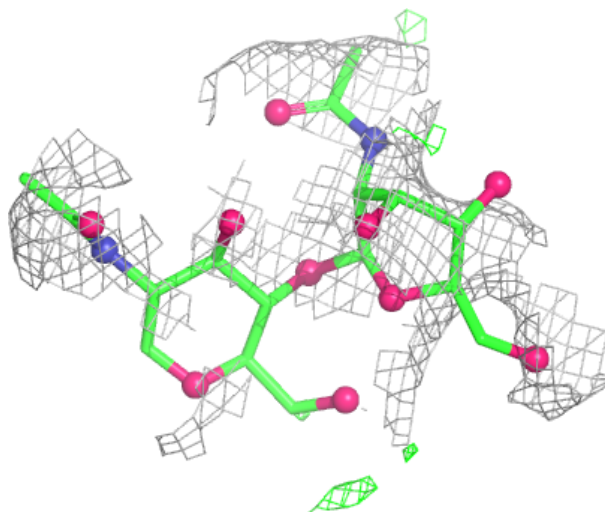
Electron density around Chain q:

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and green (positive)



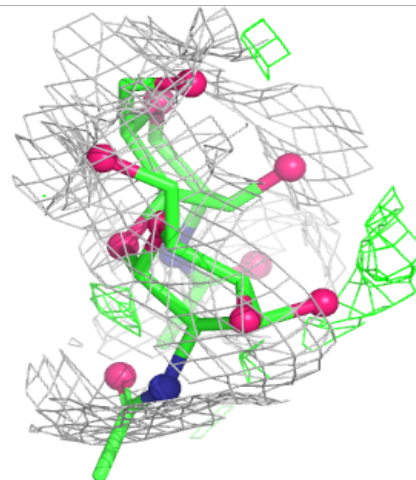
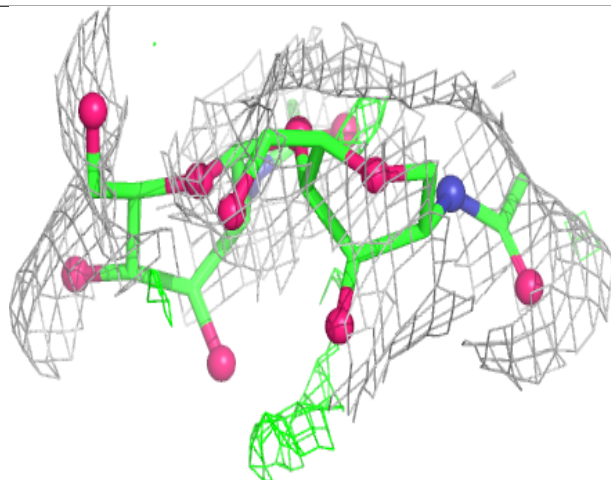
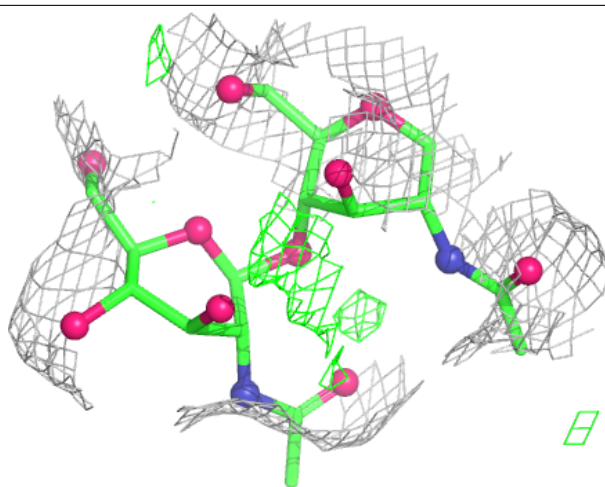
Electron density around Chain s:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



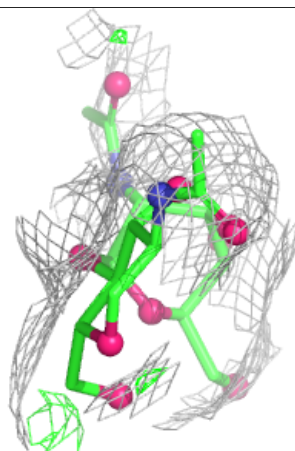
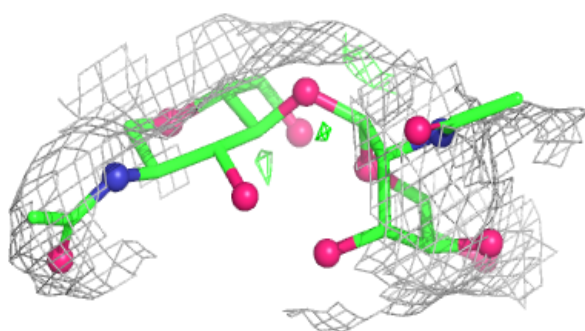
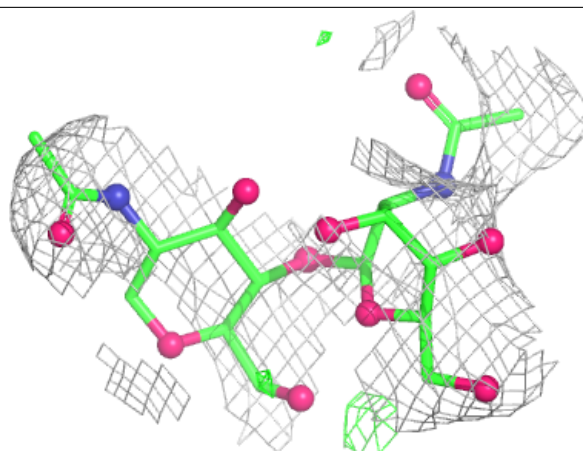
Electron density around Chain u:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



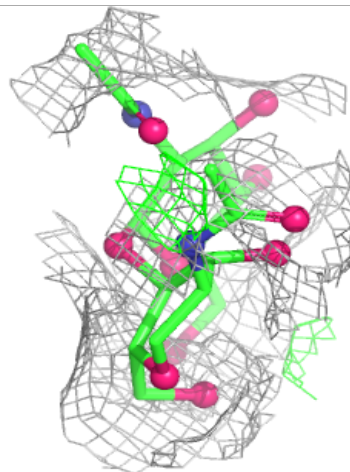
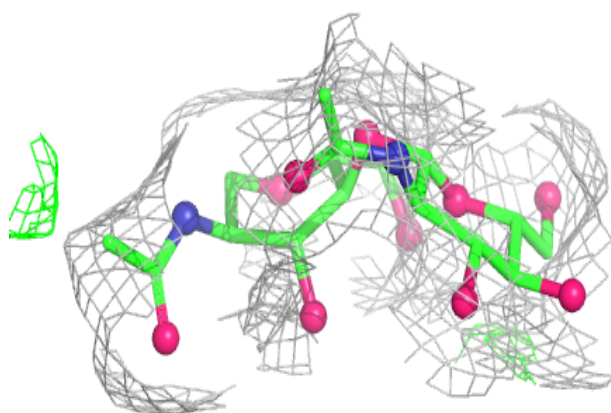
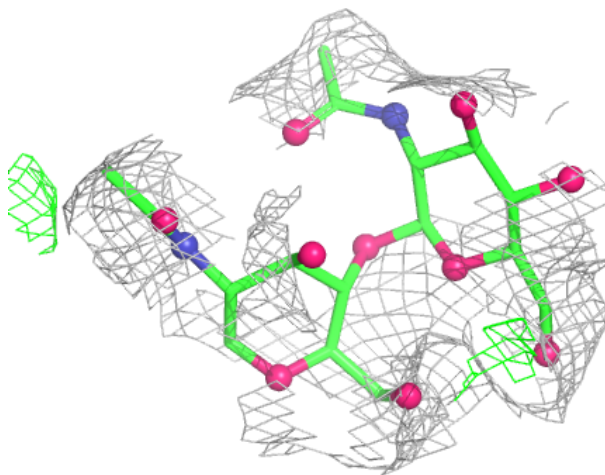
Electron density around Chain w:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



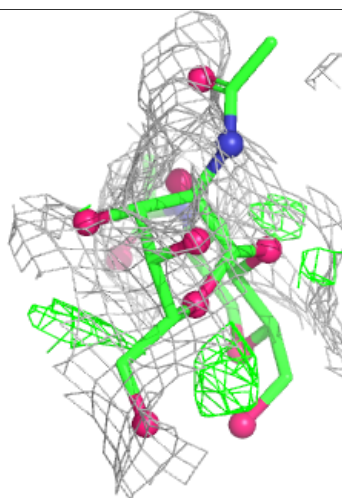
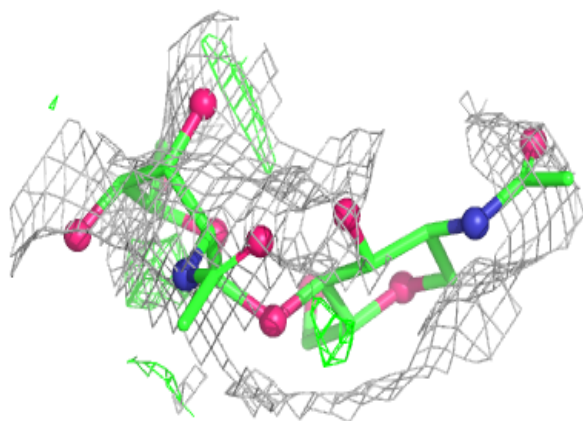
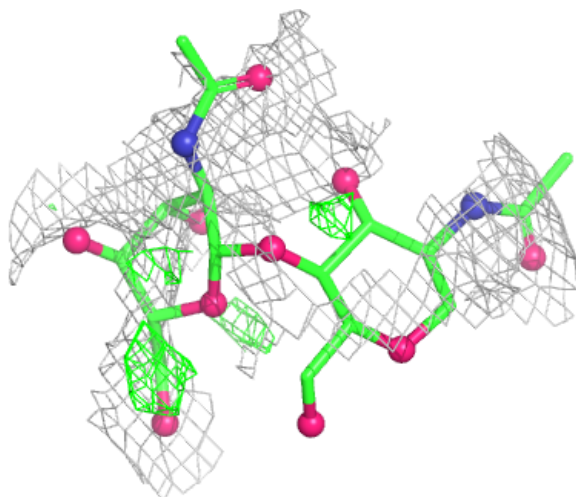
Electron density around Chain y:

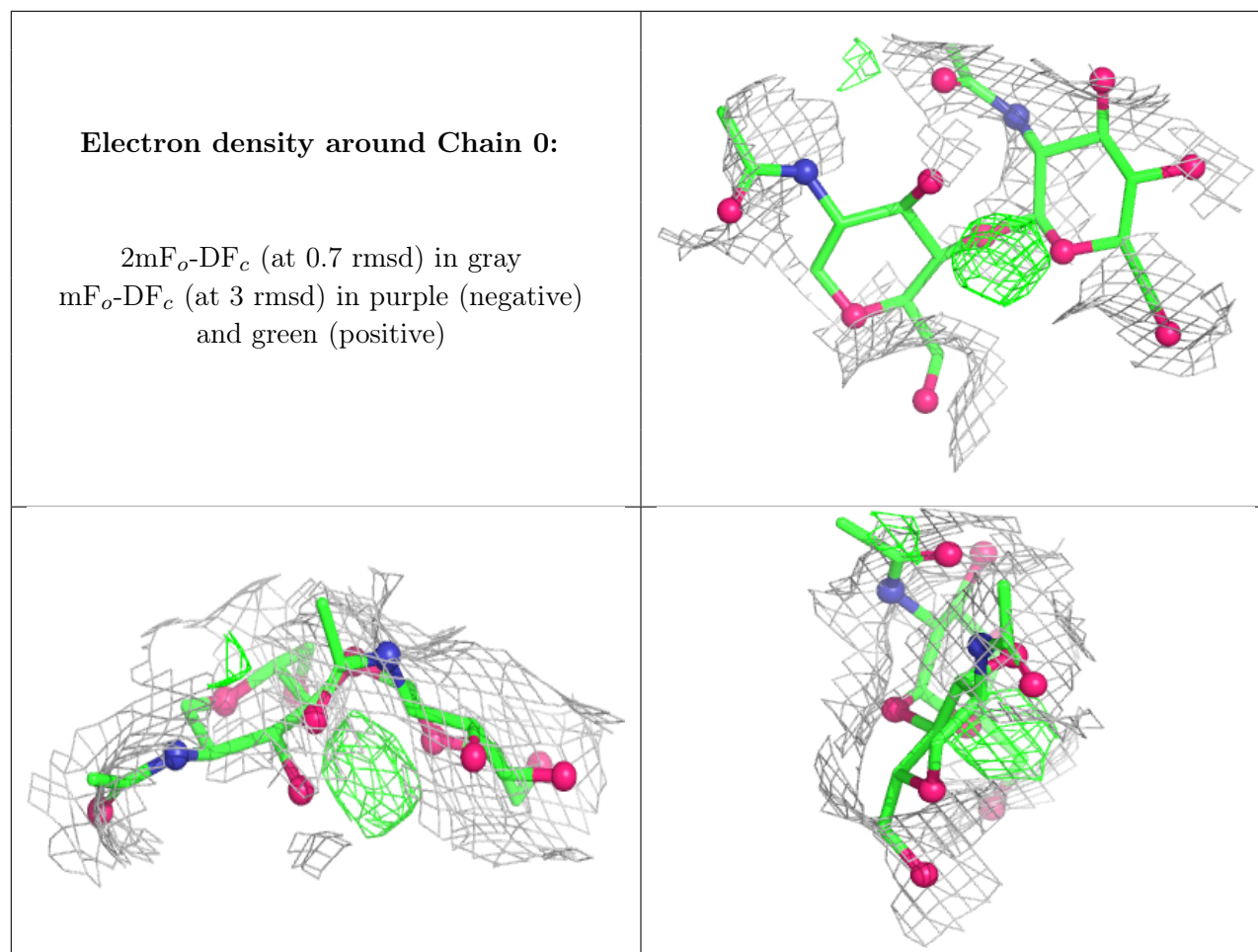
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	M	2004	14/15	0.95	0.04	119,135,154,161	0
5	NAG	K	2004	14/15	0.97	0.05	127,135,145,149	0
5	NAG	O	2006	14/15	0.97	0.06	96,105,117,126	0
5	NAG	C	2004	14/15	0.98	0.04	125,149,153,153	0
5	NAG	a	2001	14/15	0.98	0.04	92,112,119,128	0
5	NAG	Y	2001	14/15	0.99	0.04	75,93,108,120	0
5	NAG	c	2001	14/15	0.99	0.04	91,102,120,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.