



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 8AS0 / pdb_00008as0
Title : PD-1 extracellular domain in complex with Fab fragment from D12 antibody
Authors : Ongaro, T.; Scietti, L.; Pluss, L.; Peissert, F.; Villa, A.; Puca, E.; De Luca, R.; Neri, D.; Forneris, F.
Deposited on : 2022-08-17
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

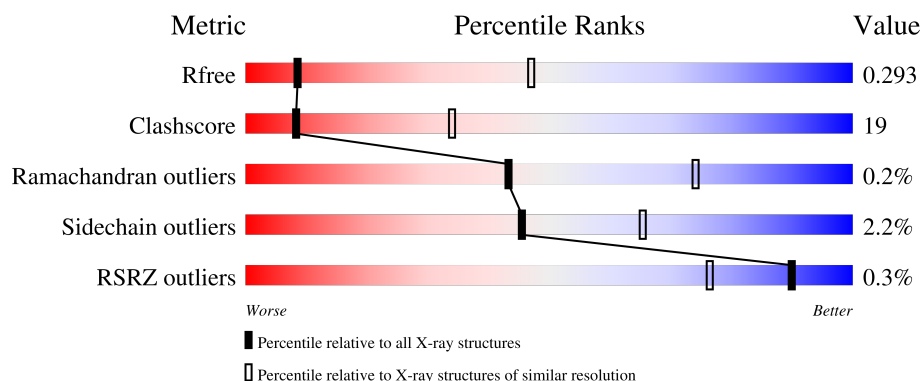
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



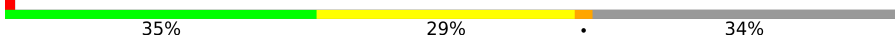
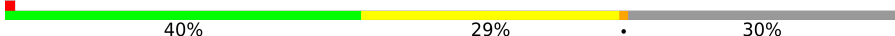
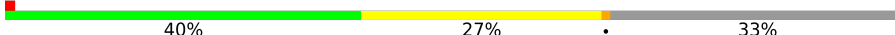
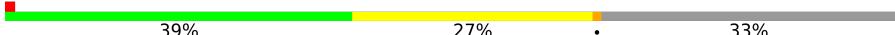
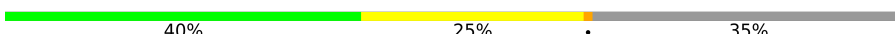
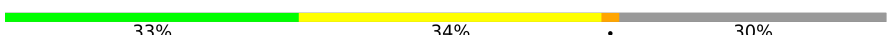
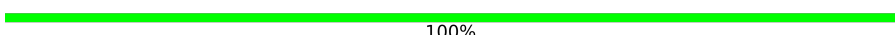
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	C	214	69% 29% .
1	D	214	68% 30% .
1	G	214	71% 27% .
1	J	214	71% 27% .
1	M	214	71% 28% .

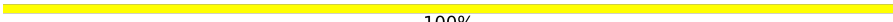
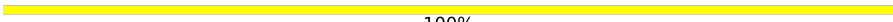
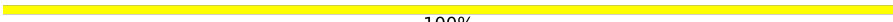
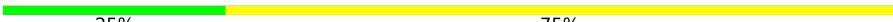
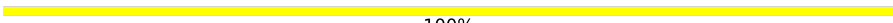
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Mol	Chain	Length	Quality of chain
1	P	214	
1	S	214	
1	V	214	
2	B	225	
2	E	225	
2	H	225	
2	K	225	
2	N	225	
2	Q	225	
2	T	225	
2	W	225	
3	A	168	
3	F	168	
3	I	168	
3	L	168	
3	O	168	
3	R	168	
3	X	168	
3	Y	168	
4	U	4	
5	Z	4	
5	g	4	
5	h	4	
5	k	4	
6	a	3	

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Mol	Chain	Length	Quality of chain
6	e	3	 100%
6	j	3	 100%
7	b	2	 100%
8	c	4	 25%75%
9	d	2	 100%
9	i	2	 50%50%
10	f	6	 50%50%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 33524 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 D12 antibody light chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	D	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	G	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	J	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	M	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	P	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	V	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	S	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			

- Molecule 2 is a protein called D12 antibody heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1593	1007	265	314	7			
2	E	214	Total	C	N	O	S	0	0	0
			1593	1007	265	314	7			
2	H	210	Total	C	N	O	S	0	0	0
			1562	988	260	307	7			
2	K	212	Total	C	N	O	S	0	0	0
			1578	998	262	311	7			
2	N	209	Total	C	N	O	S	0	0	0
			1555	983	259	306	7			
2	Q	210	Total	C	N	O	S	0	0	0
			1562	988	260	307	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	206	Total	C	N	O	S	0	0	0
			1540	975	256	302	7			
2	T	212	Total	C	N	O	S	0	0	0
			1578	998	262	311	7			

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	111	Total	C	N	O	S	0	0	0
			879	549	159	166	5			
3	F	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	I	113	Total	C	N	O	S	0	0	0
			891	555	161	170	5			
3	L	112	Total	C	N	O	S	0	0	0
			887	553	160	169	5			
3	O	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	R	110	Total	C	N	O	S	0	0	0
			870	544	157	164	5			
3	X	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	Y	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q15116
A	172	LEU	-	expression tag	UNP Q15116
A	173	ASN	-	expression tag	UNP Q15116
A	174	ASP	-	expression tag	UNP Q15116
A	175	ILE	-	expression tag	UNP Q15116
A	176	PHE	-	expression tag	UNP Q15116
A	177	GLU	-	expression tag	UNP Q15116
A	178	ALA	-	expression tag	UNP Q15116
A	179	GLN	-	expression tag	UNP Q15116
A	180	LYS	-	expression tag	UNP Q15116
A	181	ILE	-	expression tag	UNP Q15116
A	182	GLU	-	expression tag	UNP Q15116
A	183	TRP	-	expression tag	UNP Q15116
A	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLU	-	expression tag	UNP Q15116
A	186	HIS	-	expression tag	UNP Q15116
A	187	HIS	-	expression tag	UNP Q15116
A	188	HIS	-	expression tag	UNP Q15116
A	189	HIS	-	expression tag	UNP Q15116
A	190	HIS	-	expression tag	UNP Q15116
A	191	HIS	-	expression tag	UNP Q15116
F	171	GLY	-	expression tag	UNP Q15116
F	172	LEU	-	expression tag	UNP Q15116
F	173	ASN	-	expression tag	UNP Q15116
F	174	ASP	-	expression tag	UNP Q15116
F	175	ILE	-	expression tag	UNP Q15116
F	176	PHE	-	expression tag	UNP Q15116
F	177	GLU	-	expression tag	UNP Q15116
F	178	ALA	-	expression tag	UNP Q15116
F	179	GLN	-	expression tag	UNP Q15116
F	180	LYS	-	expression tag	UNP Q15116
F	181	ILE	-	expression tag	UNP Q15116
F	182	GLU	-	expression tag	UNP Q15116
F	183	TRP	-	expression tag	UNP Q15116
F	184	HIS	-	expression tag	UNP Q15116
F	185	GLU	-	expression tag	UNP Q15116
F	186	HIS	-	expression tag	UNP Q15116
F	187	HIS	-	expression tag	UNP Q15116
F	188	HIS	-	expression tag	UNP Q15116
F	189	HIS	-	expression tag	UNP Q15116
F	190	HIS	-	expression tag	UNP Q15116
F	191	HIS	-	expression tag	UNP Q15116
I	171	GLY	-	expression tag	UNP Q15116
I	172	LEU	-	expression tag	UNP Q15116
I	173	ASN	-	expression tag	UNP Q15116
I	174	ASP	-	expression tag	UNP Q15116
I	175	ILE	-	expression tag	UNP Q15116
I	176	PHE	-	expression tag	UNP Q15116
I	177	GLU	-	expression tag	UNP Q15116
I	178	ALA	-	expression tag	UNP Q15116
I	179	GLN	-	expression tag	UNP Q15116
I	180	LYS	-	expression tag	UNP Q15116
I	181	ILE	-	expression tag	UNP Q15116
I	182	GLU	-	expression tag	UNP Q15116
I	183	TRP	-	expression tag	UNP Q15116
I	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
I	185	GLU	-	expression tag	UNP Q15116
I	186	HIS	-	expression tag	UNP Q15116
I	187	HIS	-	expression tag	UNP Q15116
I	188	HIS	-	expression tag	UNP Q15116
I	189	HIS	-	expression tag	UNP Q15116
I	190	HIS	-	expression tag	UNP Q15116
I	191	HIS	-	expression tag	UNP Q15116
L	171	GLY	-	expression tag	UNP Q15116
L	172	LEU	-	expression tag	UNP Q15116
L	173	ASN	-	expression tag	UNP Q15116
L	174	ASP	-	expression tag	UNP Q15116
L	175	ILE	-	expression tag	UNP Q15116
L	176	PHE	-	expression tag	UNP Q15116
L	177	GLU	-	expression tag	UNP Q15116
L	178	ALA	-	expression tag	UNP Q15116
L	179	GLN	-	expression tag	UNP Q15116
L	180	LYS	-	expression tag	UNP Q15116
L	181	ILE	-	expression tag	UNP Q15116
L	182	GLU	-	expression tag	UNP Q15116
L	183	TRP	-	expression tag	UNP Q15116
L	184	HIS	-	expression tag	UNP Q15116
L	185	GLU	-	expression tag	UNP Q15116
L	186	HIS	-	expression tag	UNP Q15116
L	187	HIS	-	expression tag	UNP Q15116
L	188	HIS	-	expression tag	UNP Q15116
L	189	HIS	-	expression tag	UNP Q15116
L	190	HIS	-	expression tag	UNP Q15116
L	191	HIS	-	expression tag	UNP Q15116
O	171	GLY	-	expression tag	UNP Q15116
O	172	LEU	-	expression tag	UNP Q15116
O	173	ASN	-	expression tag	UNP Q15116
O	174	ASP	-	expression tag	UNP Q15116
O	175	ILE	-	expression tag	UNP Q15116
O	176	PHE	-	expression tag	UNP Q15116
O	177	GLU	-	expression tag	UNP Q15116
O	178	ALA	-	expression tag	UNP Q15116
O	179	GLN	-	expression tag	UNP Q15116
O	180	LYS	-	expression tag	UNP Q15116
O	181	ILE	-	expression tag	UNP Q15116
O	182	GLU	-	expression tag	UNP Q15116
O	183	TRP	-	expression tag	UNP Q15116
O	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
O	185	GLU	-	expression tag	UNP Q15116
O	186	HIS	-	expression tag	UNP Q15116
O	187	HIS	-	expression tag	UNP Q15116
O	188	HIS	-	expression tag	UNP Q15116
O	189	HIS	-	expression tag	UNP Q15116
O	190	HIS	-	expression tag	UNP Q15116
O	191	HIS	-	expression tag	UNP Q15116
R	171	GLY	-	expression tag	UNP Q15116
R	172	LEU	-	expression tag	UNP Q15116
R	173	ASN	-	expression tag	UNP Q15116
R	174	ASP	-	expression tag	UNP Q15116
R	175	ILE	-	expression tag	UNP Q15116
R	176	PHE	-	expression tag	UNP Q15116
R	177	GLU	-	expression tag	UNP Q15116
R	178	ALA	-	expression tag	UNP Q15116
R	179	GLN	-	expression tag	UNP Q15116
R	180	LYS	-	expression tag	UNP Q15116
R	181	ILE	-	expression tag	UNP Q15116
R	182	GLU	-	expression tag	UNP Q15116
R	183	TRP	-	expression tag	UNP Q15116
R	184	HIS	-	expression tag	UNP Q15116
R	185	GLU	-	expression tag	UNP Q15116
R	186	HIS	-	expression tag	UNP Q15116
R	187	HIS	-	expression tag	UNP Q15116
R	188	HIS	-	expression tag	UNP Q15116
R	189	HIS	-	expression tag	UNP Q15116
R	190	HIS	-	expression tag	UNP Q15116
R	191	HIS	-	expression tag	UNP Q15116
X	171	GLY	-	expression tag	UNP Q15116
X	172	LEU	-	expression tag	UNP Q15116
X	173	ASN	-	expression tag	UNP Q15116
X	174	ASP	-	expression tag	UNP Q15116
X	175	ILE	-	expression tag	UNP Q15116
X	176	PHE	-	expression tag	UNP Q15116
X	177	GLU	-	expression tag	UNP Q15116
X	178	ALA	-	expression tag	UNP Q15116
X	179	GLN	-	expression tag	UNP Q15116
X	180	LYS	-	expression tag	UNP Q15116
X	181	ILE	-	expression tag	UNP Q15116
X	182	GLU	-	expression tag	UNP Q15116
X	183	TRP	-	expression tag	UNP Q15116
X	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
X	185	GLU	-	expression tag	UNP Q15116
X	186	HIS	-	expression tag	UNP Q15116
X	187	HIS	-	expression tag	UNP Q15116
X	188	HIS	-	expression tag	UNP Q15116
X	189	HIS	-	expression tag	UNP Q15116
X	190	HIS	-	expression tag	UNP Q15116
X	191	HIS	-	expression tag	UNP Q15116
Y	171	GLY	-	expression tag	UNP Q15116
Y	172	LEU	-	expression tag	UNP Q15116
Y	173	ASN	-	expression tag	UNP Q15116
Y	174	ASP	-	expression tag	UNP Q15116
Y	175	ILE	-	expression tag	UNP Q15116
Y	176	PHE	-	expression tag	UNP Q15116
Y	177	GLU	-	expression tag	UNP Q15116
Y	178	ALA	-	expression tag	UNP Q15116
Y	179	GLN	-	expression tag	UNP Q15116
Y	180	LYS	-	expression tag	UNP Q15116
Y	181	ILE	-	expression tag	UNP Q15116
Y	182	GLU	-	expression tag	UNP Q15116
Y	183	TRP	-	expression tag	UNP Q15116
Y	184	HIS	-	expression tag	UNP Q15116
Y	185	GLU	-	expression tag	UNP Q15116
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Y	188	HIS	-	expression tag	UNP Q15116
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Y	191	HIS	-	expression tag	UNP Q15116

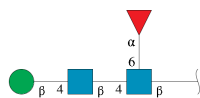
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

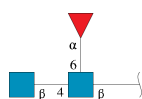
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



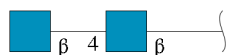
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Z	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	g	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	h	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	k	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	e	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	j	3	Total	C	N	O	0	0	0
			38	22	2	14			

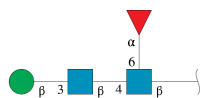
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



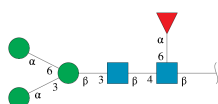
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	c	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	d	2	Total	C	N	O	0	0	0
			24	14	1	9			
9	i	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	f	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

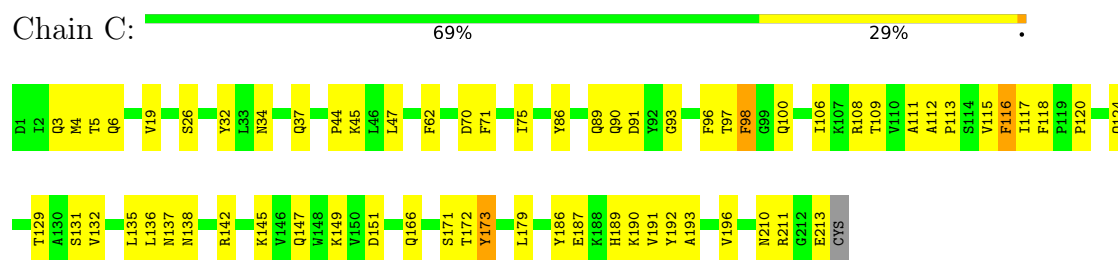


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	F	1	Total	C	N	O	0	0
			14	8	1	5		
11	I	1	Total	C	N	O	0	0
			14	8	1	5		
11	L	1	Total	C	N	O	0	0
			14	8	1	5		
11	L	1	Total	C	N	O	0	0
			14	8	1	5		
11	O	1	Total	C	N	O	0	0
			14	8	1	5		
11	R	1	Total	C	N	O	0	0
			14	8	1	5		
11	Y	1	Total	C	N	O	0	0
			14	8	1	5		
11	Y	1	Total	C	N	O	0	0
			14	8	1	5		

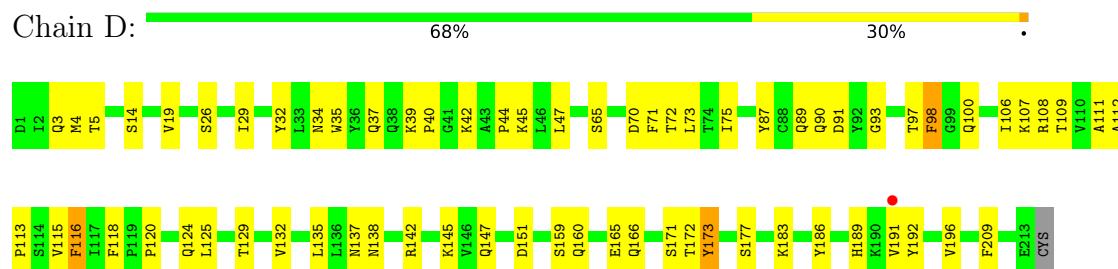
3 Residue-property plots

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.

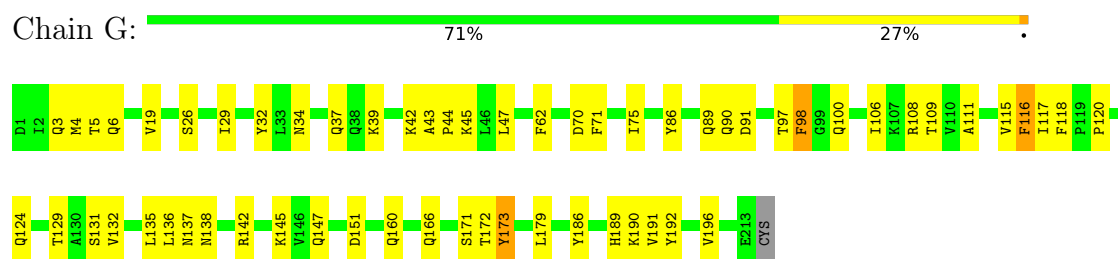
- Molecule 1: D12 antibody light chain, Fab fragment



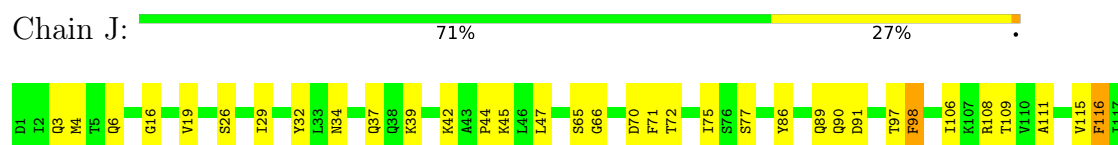
- Molecule 1: D12 antibody light chain, Fab fragment



- Molecule 1: D12 antibody light chain, Fab fragment



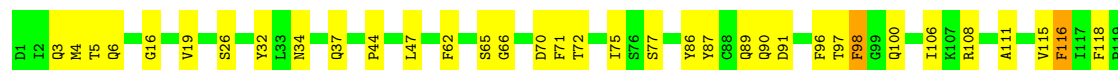
- Molecule 1: D12 antibody light chain, Fab fragment





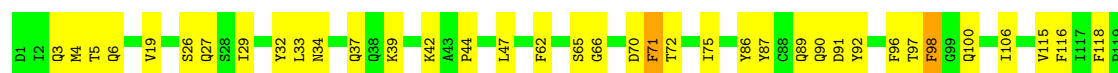
- Molecule 1: D12 antibody light chain, Fab fragment

Chain M: 71% 28%



- Molecule 1: D12 antibody light chain, Fab fragment

Chain P: 70% 28%



- Molecule 1: D12 antibody light chain, Fab fragment

Chain V: 72% 25%



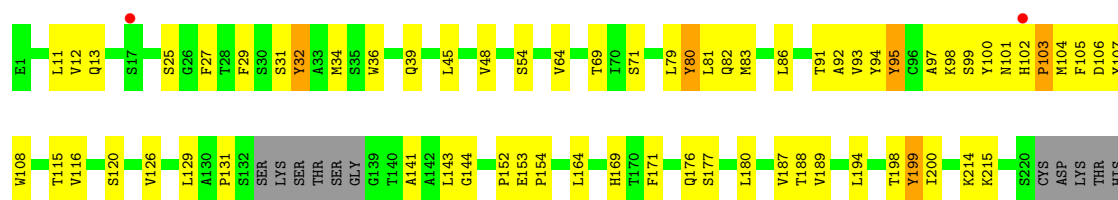
- Molecule 1: D12 antibody light chain, Fab fragment

Chain S: 71% 27%



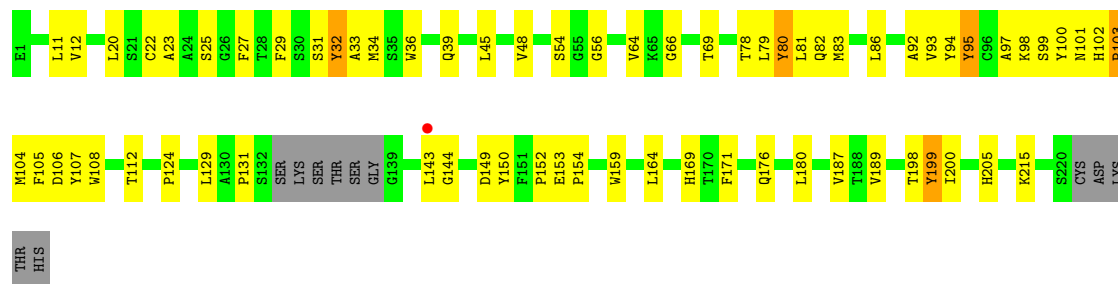
- Molecule 2: D12 antibody heavy chain, Fab fragment

Chain B: 65% 28% 5%



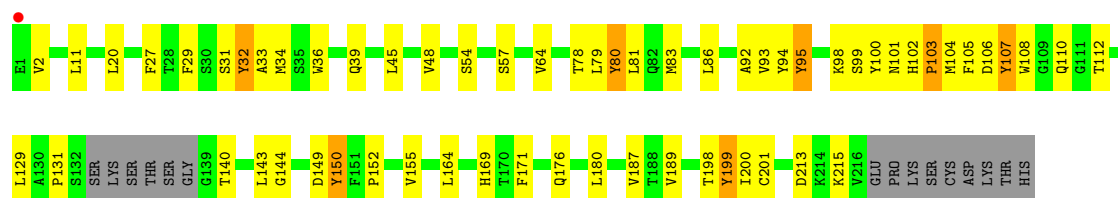
- Molecule 2: D12 antibody heavy chain, Fab fragment

Chain E: 65% 28% 5%



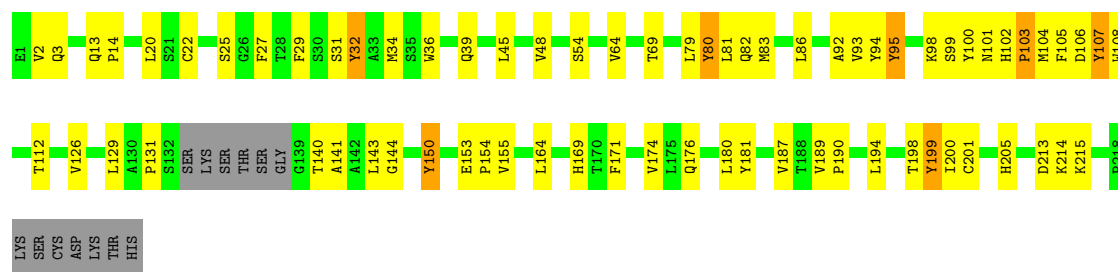
- Molecule 2: D12 antibody heavy chain, Fab fragment

Chain H: 66% 24% 7%



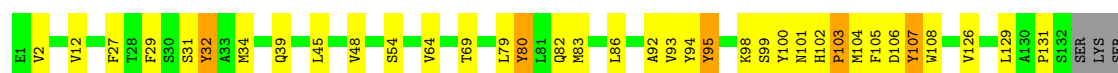
- Molecule 2: D12 antibody heavy chain, Fab fragment

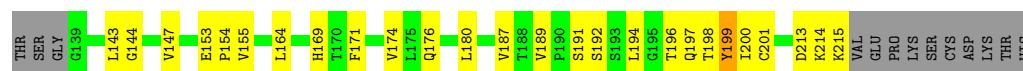
Chain K: 63% 28% 6%



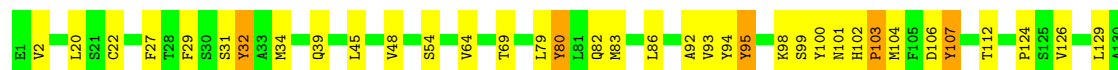
- Molecule 2: D12 antibody heavy chain, Fab fragment

Chain N: 65% 25% 7%

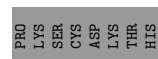




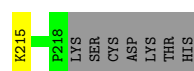
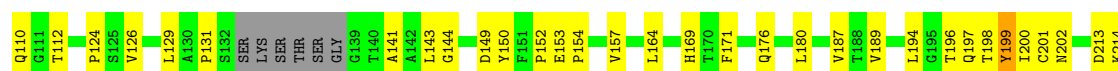
- Molecule 2: D12 antibody heavy chain, Fab fragment



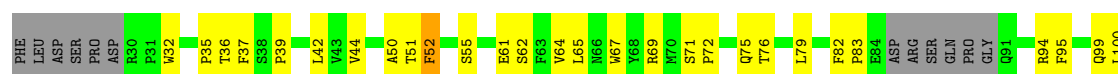
- Molecule 2: D12 antibody heavy chain, Fab fragment



- Molecule 2: D12 antibody heavy chain, Fab fragment



- Molecule 3: Programmed cell death protein 1



LEU
ASN
ASP
ILE
SER
PHE
PRO
GLU
ALA
GLN
LYS
ILE
GLU
TRP
HIS
GLU
HIS
HIS
HIS
HIS

• Molecule 3: Programmed cell death protein 1



PHE
LEU
ASP
SER
PHE
PRO
ASP
R30
P31
W32
N33
P34
P35
T36
F37
S38
P39
L42
N49
A50
T51
F52
S55
E61
S62
F63
V64
L65
W66
W67
Y68
R69
M70
S71
P72
Q75
T76
L79
F82
P83
T84
S87
Q88
R94
F95
R96
Q99
L100
F106
H107

V110
V111
R115
N116
D117
T120
Y121
L122
L128
A129
P130
K131
A132
E136
S137
L138
R139
L142
T145
E146
ARG
ALA
GLU
VAL
PRO
THR
ALA
HIS
PRO
SER
PRO
SER
PRO
ARG
PRO
ALA
GLY
GLN
PHE
GLN
THR
LEU
VAL
LEU
ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
ILE

GLU
TRP
HIS
GLU
HIS
HIS
HIS
HIS

• Molecule 3: Programmed cell death protein 1



PHE
LEU
ASP
SER
PRO
ASP
R30
P31
W32
N33
P34
P35
T36
F37
S38
P39
L42
N49
A50
T51
F52
S55
T59
S60
F63
S62
V64
F65
L66
W67
Y68
R69
M70
S71
P72
L79
F82
P83
E84
D85
ARG
SER
GLN
PRO
G90
R94
F95
Q99
F106

V110
V111
D117
T120
Y121
L122
L126
S127
L128
A129
P130
A131
A132
Q133
I134
K135
E136
S137
L138
R139
L142
T145
E146
ARG
GLU
ALA
VAL
PRO
THR
ALA
HIS
PRO
SER
PRO
SER
PRO
ARG
PRO
ALA
GLY
GLN
PHE
THR
LEU
VAL
GLY
LEU
ASN
ASP
ILE
PHE
GLU
ALA

GLN
LYS
ILE
GLU
TRP
HIS
HIS
HIS
HIS
HIS

• Molecule 3: Programmed cell death protein 1



PHE
LEU
ASP
SER
PRO
ASP
R30
P31
W32
N33
P34
P35
T36
F37
S38
P39
L42
N49
A50
T51
F52
S55
E61
S62
F63
V64
L65
W66
W67
Y68
R69
M70
S71
P72
Q75
T76
L79
F82
P83
E84
D85
ARG
SER
GLN
PRO
G91
R94
F95
Q99
L100

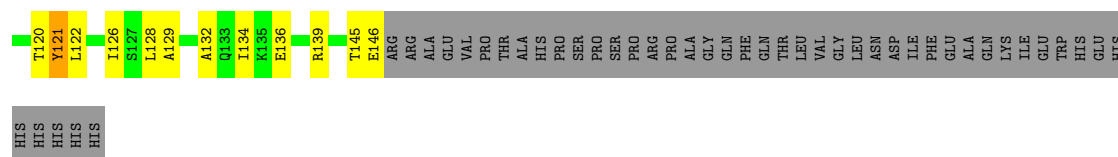
P101
F106
H107
V110
V111
D117
T120
Y121
I126
S127
L128
A129
P130
K131
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Q133
I134
K135
E136
R139
L142
T145
E146
ARG
ALA
GLU
VAL
PRO
THR
ALA
HIS
PRO
SER
PRO
SER
PRO
ARG
PRO
ALA
GLY
GLN
PHE
THR
LEU
VAL
GLY
LEU
ASN
ASP
ILE

PHE
GLU
ALA
GLN
LYS
ILE
GLU
TRP
HIS
HIS
HIS
HIS
HIS

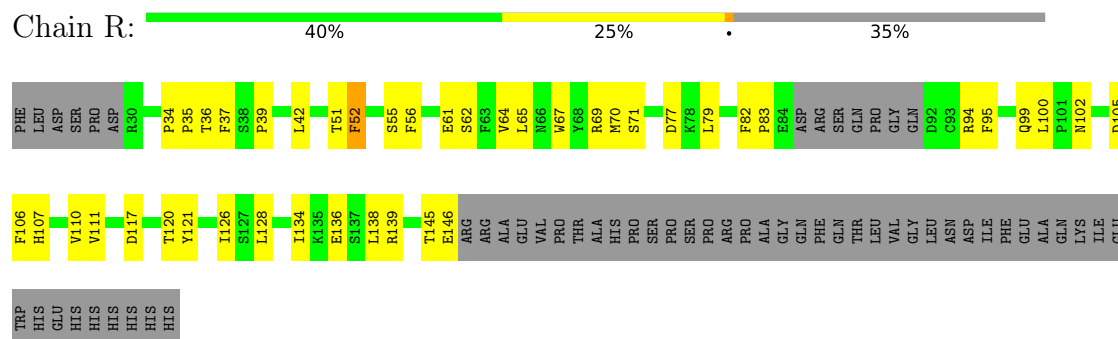
• Molecule 3: Programmed cell death protein 1



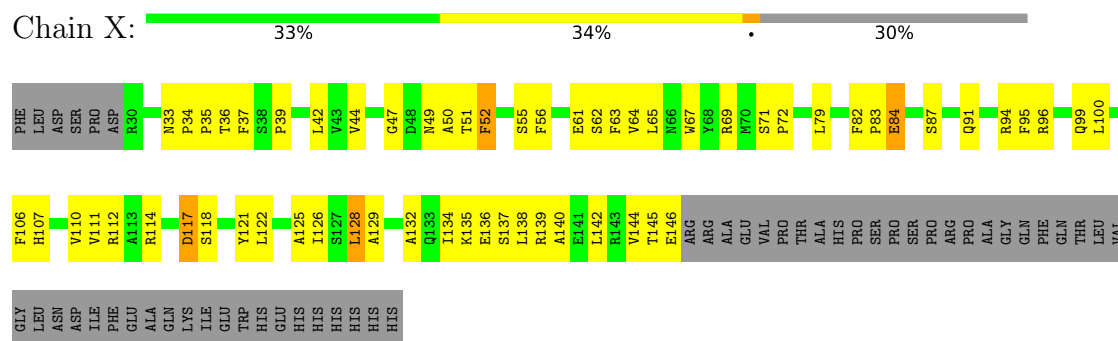
PHE
LEU
ASP
SER
PRO
ASP
R30
P31
W32
N33
P34
P35
T36
F37
S38
P39
L42
N49
A50
T51
F52
S55
F56
E61
S62
F63
V64
L65
W66
W67
Y68
R69
M70
S71
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R94
F95
Q99
L100
F106
H107
V110
V111
D117



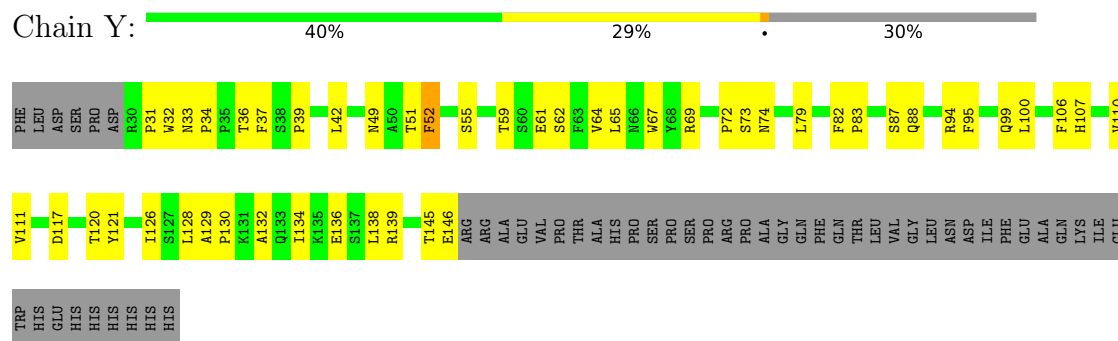
• Molecule 3: Programmed cell death protein 1



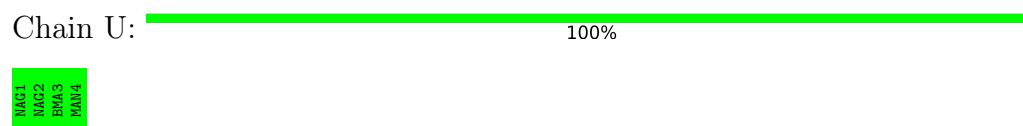
• Molecule 3: Programmed cell death protein 1



• Molecule 3: Programmed cell death protein 1



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

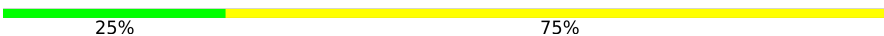


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  25% 75%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  50% 25% 25%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  50% 25% 25%

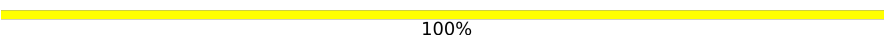


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  33% 67%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%

MAG1
MAG2
FUC3

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2

- Molecule 8: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  25%  75%

MAG1
MAG2
BMA3
FUC4

- Molecule 9: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1
FUC2

- Molecule 9: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  50%  50%

MAG1
FUC2

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

Chain f:  50%  50%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 187.09Å 190.84Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	95.42 – 3.50 95.42 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (95.42-3.50) 95.7 (95.42-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.243 , 0.293 0.243 , 0.293	Depositor DCC
R_{free} test set	3527 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.053 for -h,l,k 0.049 for -h,-l,-k 0.176 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	33524	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: MAN, NAG, BMA, FUC

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	C	0.18	0/1669	0.39	0/2265
1	D	0.12	0/1669	0.35	0/2265
1	G	0.12	0/1669	0.35	0/2265
1	J	0.12	0/1669	0.35	0/2265
1	M	0.12	0/1669	0.34	0/2265
1	P	0.12	0/1669	0.34	0/2265
1	S	0.15	0/1669	0.39	0/2265
1	V	0.12	0/1669	0.35	0/2265
2	B	0.14	0/1632	0.39	0/2221
2	E	0.13	0/1632	0.37	0/2221
2	H	0.15	0/1600	0.39	0/2178
2	K	0.15	0/1617	0.39	0/2202
2	N	0.14	0/1593	0.40	0/2168
2	Q	0.14	0/1600	0.40	0/2178
2	T	0.16	0/1617	0.42	0/2202
2	W	0.14	0/1577	0.39	0/2145
3	A	0.18	0/899	0.43	0/1220
3	F	0.19	0/946	0.42	0/1285
3	I	0.16	0/911	0.42	0/1236
3	L	0.15	0/907	0.39	0/1231
3	O	0.16	0/946	0.41	0/1285
3	R	0.20	0/890	0.48	0/1208
3	X	0.26	0/946	0.60	0/1285
3	Y	0.16	0/946	0.41	0/1285
All	All	0.15	0/33611	0.39	0/45670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	C	1634	0	1586	56	0
1	D	1634	0	1586	53	0
1	G	1634	0	1586	53	0
1	J	1634	0	1586	53	0
1	M	1634	0	1586	55	0
1	P	1634	0	1586	56	0
1	S	1634	0	1586	58	0
1	V	1634	0	1586	52	0
2	B	1593	0	1556	63	0
2	E	1593	0	1556	62	0
2	H	1562	0	1525	60	0
2	K	1578	0	1538	68	0
2	N	1555	0	1516	66	0
2	Q	1562	0	1525	55	0
2	T	1578	0	1538	74	0
2	W	1540	0	1499	66	0
3	A	879	0	849	62	0
3	F	924	0	889	56	0
3	I	891	0	854	51	0
3	L	887	0	852	50	0
3	O	924	0	890	54	0
3	R	870	0	841	47	0
3	X	924	0	889	73	0
3	Y	924	0	889	54	0
4	U	50	0	43	0	0
5	Z	49	0	43	3	0
5	g	49	0	43	5	0
5	h	49	0	43	2	0
5	k	49	0	43	4	0
6	a	38	0	34	2	0
6	e	38	0	34	4	0
6	j	38	0	34	3	0
7	b	28	0	25	5	0
8	c	49	0	43	3	0
9	d	24	0	22	2	0
9	i	24	0	22	2	0
10	f	71	0	61	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	14	0	13	0	0
11	I	14	0	13	0	0
11	L	28	0	26	0	0
11	O	14	0	13	0	0
11	R	14	0	13	0	0
11	Y	28	0	26	0	0
All	All	33524	0	32488	1267	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 19.

The worst 5 of 1267 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:S:140:TYR:HD1	1:S:141:PRO:HA	1.23	1.01
1:P:115:VAL:HG21	1:P:196:VAL:HG11	1.55	0.88
1:S:140:TYR:CD1	1:S:141:PRO:HA	2.09	0.86
3:A:82:PHE:HE2	3:A:99:GLN:HB2	1.39	0.85
1:M:115:VAL:HG21	1:M:196:VAL:HG11	1.59	0.85

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	C	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	D	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	G	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	J	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	M	211/214 (99%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	S	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	V	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	B	210/225 (93%)	200 (95%)	9 (4%)	1 (0%)	24	57
2	E	210/225 (93%)	201 (96%)	8 (4%)	1 (0%)	24	57
2	H	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	24	57
2	K	208/225 (92%)	200 (96%)	7 (3%)	1 (0%)	24	57
2	N	205/225 (91%)	197 (96%)	7 (3%)	1 (0%)	24	57
2	Q	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	24	57
2	T	208/225 (92%)	197 (95%)	10 (5%)	1 (0%)	24	57
2	W	200/225 (89%)	193 (96%)	6 (3%)	1 (0%)	24	57
3	A	107/168 (64%)	102 (95%)	5 (5%)	0	100	100
3	F	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
3	I	109/168 (65%)	102 (94%)	7 (6%)	0	100	100
3	L	108/168 (64%)	103 (95%)	5 (5%)	0	100	100
3	O	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
3	R	106/168 (63%)	100 (94%)	6 (6%)	0	100	100
3	X	115/168 (68%)	107 (93%)	7 (6%)	1 (1%)	14	47
3	Y	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
All	All	4231/4856 (87%)	4049 (96%)	173 (4%)	9 (0%)	43	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	X	84	GLU
2	B	103	PRO
2	H	103	PRO
2	Q	103	PRO
2	N	103	PRO

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	C	136/188 (72%)	133 (98%)	3 (2%)	45	65
1	D	187/188 (100%)	184 (98%)	3 (2%)	55	70
1	G	187/188 (100%)	184 (98%)	3 (2%)	55	70
1	J	187/188 (100%)	184 (98%)	3 (2%)	55	70
1	M	187/188 (100%)	184 (98%)	3 (2%)	55	70
1	P	187/188 (100%)	183 (98%)	4 (2%)	47	66
1	S	187/188 (100%)	183 (98%)	4 (2%)	47	66
1	V	187/188 (100%)	183 (98%)	4 (2%)	47	66
2	B	178/188 (95%)	174 (98%)	4 (2%)	45	65
2	E	178/188 (95%)	174 (98%)	4 (2%)	45	65
2	H	174/188 (93%)	168 (97%)	6 (3%)	32	57
2	K	176/188 (94%)	170 (97%)	6 (3%)	32	57
2	N	173/188 (92%)	168 (97%)	5 (3%)	37	60
2	Q	174/188 (93%)	169 (97%)	5 (3%)	37	60
2	T	176/188 (94%)	171 (97%)	5 (3%)	38	61
2	W	171/188 (91%)	166 (97%)	5 (3%)	37	60
3	A	98/148 (66%)	95 (97%)	3 (3%)	35	59
3	F	103/148 (70%)	102 (99%)	1 (1%)	68	75
3	I	99/148 (67%)	98 (99%)	1 (1%)	68	75
3	L	99/148 (67%)	98 (99%)	1 (1%)	68	75
3	O	103/148 (70%)	102 (99%)	1 (1%)	68	75
3	R	97/148 (66%)	96 (99%)	1 (1%)	68	75
3	X	103/148 (70%)	100 (97%)	3 (3%)	37	60
3	Y	103/148 (70%)	102 (99%)	1 (1%)	68	75
All	All	3650/4192 (87%)	3571 (98%)	79 (2%)	45	65

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	71	PHE
1	S	140	TYR
1	V	116	PHE

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Mol	Chain	Res	Type
2	W	199	TYR
2	T	95	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	74	ASN
1	P	160	GLN
2	N	176	GLN
1	P	124	GLN
2	Q	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	U	1	3,4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.57	0
4	BMA	U	3	4	11,11,12	0.25	0	15,15,17	0.61	0
4	MAN	U	4	4	11,11,12	0.23	0	15,15,17	0.53	0
5	NAG	Z	1	3,5	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	Z	2	5	14,14,15	0.28	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	Z	3	5	11,11,12	0.62	0	15,15,17	0.68	0
5	FUC	Z	4	5	10,10,11	0.34	0	14,14,16	0.62	0
6	NAG	a	1	3,6	14,14,15	0.42	0	17,19,21	0.80	0
6	NAG	a	2	6	14,14,15	0.24	0	17,19,21	0.50	0
6	FUC	a	3	6	10,10,11	0.23	0	14,14,16	0.59	0
7	NAG	b	1	7,3	14,14,15	0.20	0	17,19,21	0.62	0
7	NAG	b	2	7	14,14,15	0.34	0	17,19,21	0.43	0
8	NAG	c	1	3,8	14,14,15	0.40	0	17,19,21	0.68	0
8	NAG	c	2	8	14,14,15	0.38	0	17,19,21	0.50	0
8	BMA	c	3	8	11,11,12	0.53	0	15,15,17	0.77	0
8	FUC	c	4	8	10,10,11	0.26	0	14,14,16	0.56	0
9	NAG	d	1	3,9	14,14,15	0.28	0	17,19,21	0.57	0
9	FUC	d	2	9	10,10,11	0.25	0	14,14,16	0.86	0
6	NAG	e	1	3,6	14,14,15	0.39	0	17,19,21	0.66	0
6	NAG	e	2	6	14,14,15	0.25	0	17,19,21	0.48	0
6	FUC	e	3	6	10,10,11	0.26	0	14,14,16	0.59	0
10	NAG	f	1	3,10	14,14,15	0.41	0	17,19,21	0.55	0
10	NAG	f	2	10	14,14,15	0.30	0	17,19,21	0.81	1 (5%)
10	BMA	f	3	10	11,11,12	0.26	0	15,15,17	0.61	0
10	MAN	f	4	10	11,11,12	0.23	0	15,15,17	0.81	0
10	MAN	f	5	10	11,11,12	0.21	0	15,15,17	0.53	0
10	FUC	f	6	10	10,10,11	0.24	0	14,14,16	0.60	0
5	NAG	g	1	3,5	14,14,15	0.42	0	17,19,21	0.80	0
5	NAG	g	2	5	14,14,15	0.29	0	17,19,21	0.71	0
5	BMA	g	3	5	11,11,12	0.23	0	15,15,17	0.58	0
5	FUC	g	4	5	10,10,11	0.25	0	14,14,16	0.62	0
5	NAG	h	1	3,5	14,14,15	0.43	0	17,19,21	0.88	1 (5%)
5	NAG	h	2	5	14,14,15	0.22	0	17,19,21	0.48	0
5	BMA	h	3	5	11,11,12	0.50	0	15,15,17	0.68	0
5	FUC	h	4	5	10,10,11	0.24	0	14,14,16	0.59	0
9	NAG	i	1	3,9	14,14,15	0.29	0	17,19,21	0.57	0
9	FUC	i	2	9	10,10,11	0.25	0	14,14,16	0.53	0
6	NAG	j	1	3,6	14,14,15	0.42	0	17,19,21	0.49	0
6	NAG	j	2	6	14,14,15	0.31	0	17,19,21	0.51	0
6	FUC	j	3	6	10,10,11	0.25	0	14,14,16	0.55	0
5	NAG	k	1	3,5	14,14,15	0.42	0	17,19,21	0.67	0
5	NAG	k	2	5	14,14,15	0.32	0	17,19,21	0.84	1 (5%)
5	BMA	k	3	5	11,11,12	0.54	0	15,15,17	0.67	0
5	FUC	k	4	5	10,10,11	0.25	0	14,14,16	0.59	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	U	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
4	MAN	U	4	4	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
5	FUC	Z	4	5	-	-	0/1/1/1
6	NAG	a	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
6	FUC	a	3	6	-	-	0/1/1/1
7	NAG	b	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
8	NAG	c	1	3,8	-	4/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
8	FUC	c	4	8	-	-	0/1/1/1
9	NAG	d	1	3,9	-	0/6/23/26	0/1/1/1
9	FUC	d	2	9	-	-	0/1/1/1
6	NAG	e	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	FUC	e	3	6	-	-	0/1/1/1
10	NAG	f	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	BMA	f	3	10	-	0/2/19/22	0/1/1/1
10	MAN	f	4	10	-	0/2/19/22	0/1/1/1
10	MAN	f	5	10	-	0/2/19/22	0/1/1/1
10	FUC	f	6	10	-	-	0/1/1/1
5	NAG	g	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	BMA	g	3	5	-	0/2/19/22	0/1/1/1
5	FUC	g	4	5	-	-	0/1/1/1
5	NAG	h	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	h	2	5	-	0/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	FUC	h	4	5	-	-	0/1/1/1
9	NAG	i	1	3,9	-	4/6/23/26	0/1/1/1
9	FUC	i	2	9	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	j	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	FUC	j	3	6	-	-	0/1/1/1
5	NAG	k	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	BMA	k	3	5	-	0/2/19/22	0/1/1/1
5	FUC	k	4	5	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	2	NAG	C4-C3-C2	-2.52	107.32	111.02
5	h	1	NAG	C1-O5-C5	2.36	115.35	112.19
10	f	2	NAG	O3-C3-C2	-2.24	104.74	109.40

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
9	i	1	NAG	C8-C7-N2-C2

There are no ring outliers.

27 monomers are involved in 38 short contacts:

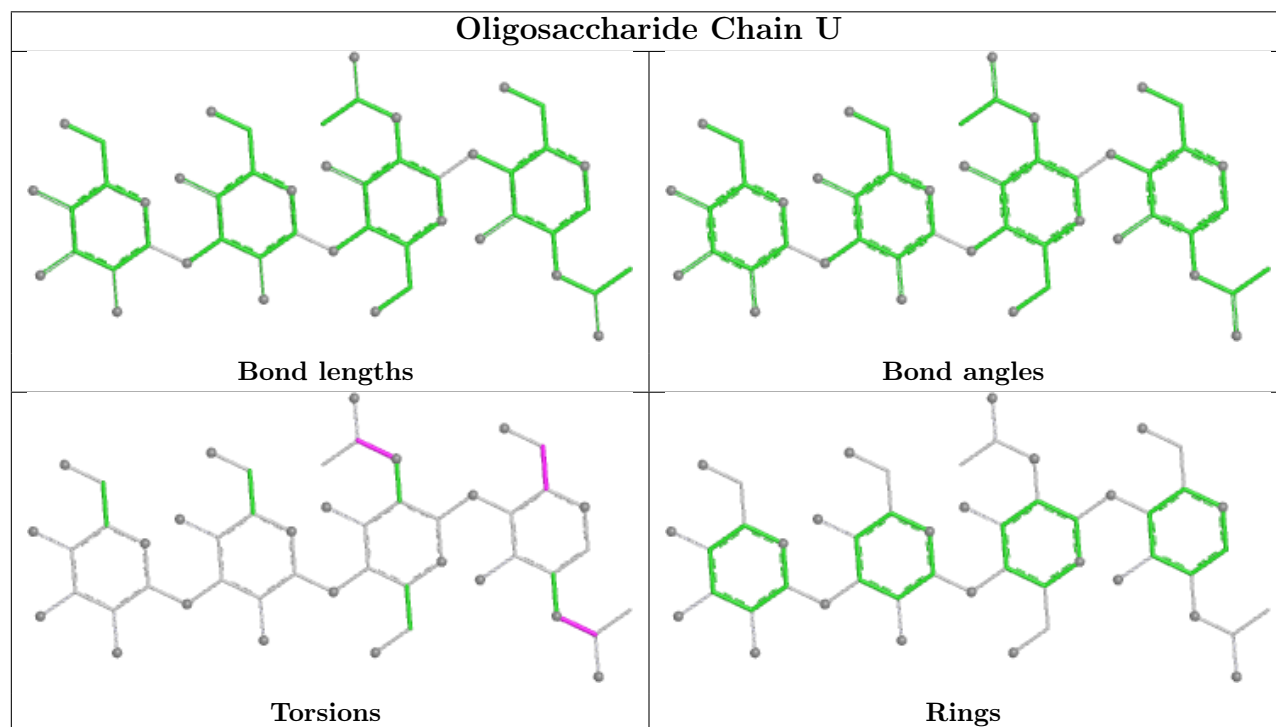
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	k	1	NAG	4	0
6	a	1	NAG	2	0
5	h	2	NAG	1	0
5	g	4	FUC	2	0
9	d	2	FUC	2	0
5	k	2	NAG	2	0
5	g	1	NAG	4	0
8	c	4	FUC	1	0
8	c	1	NAG	2	0
9	d	1	NAG	2	0

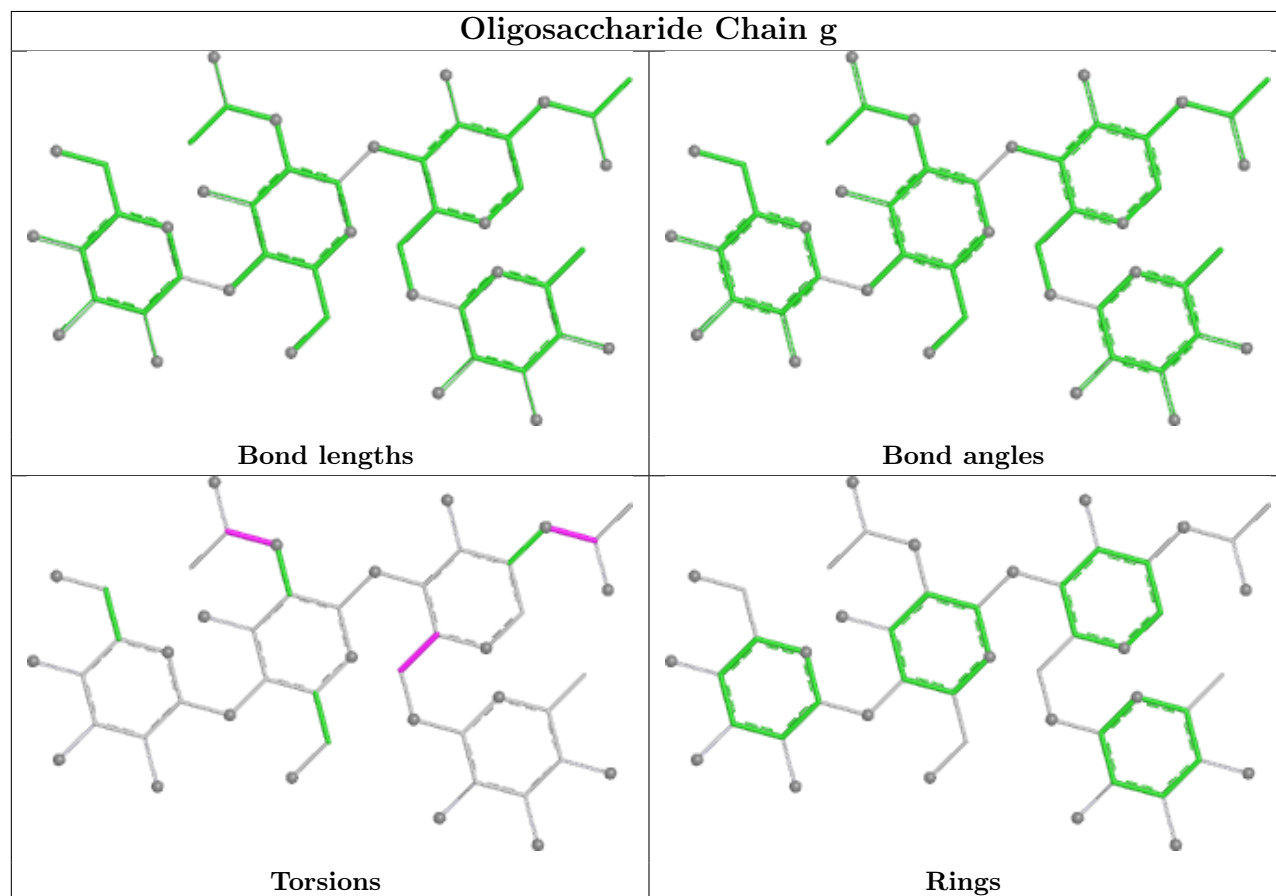
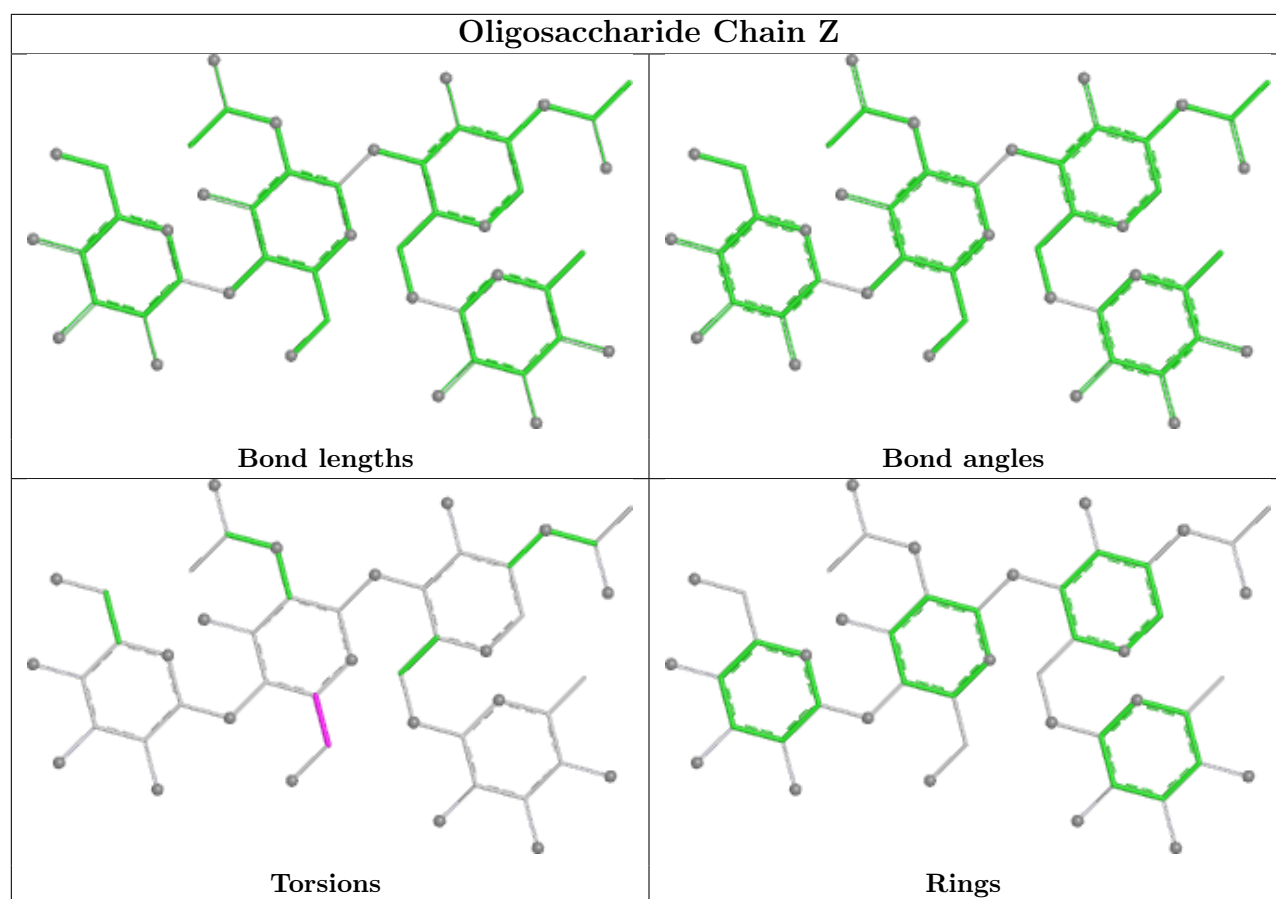
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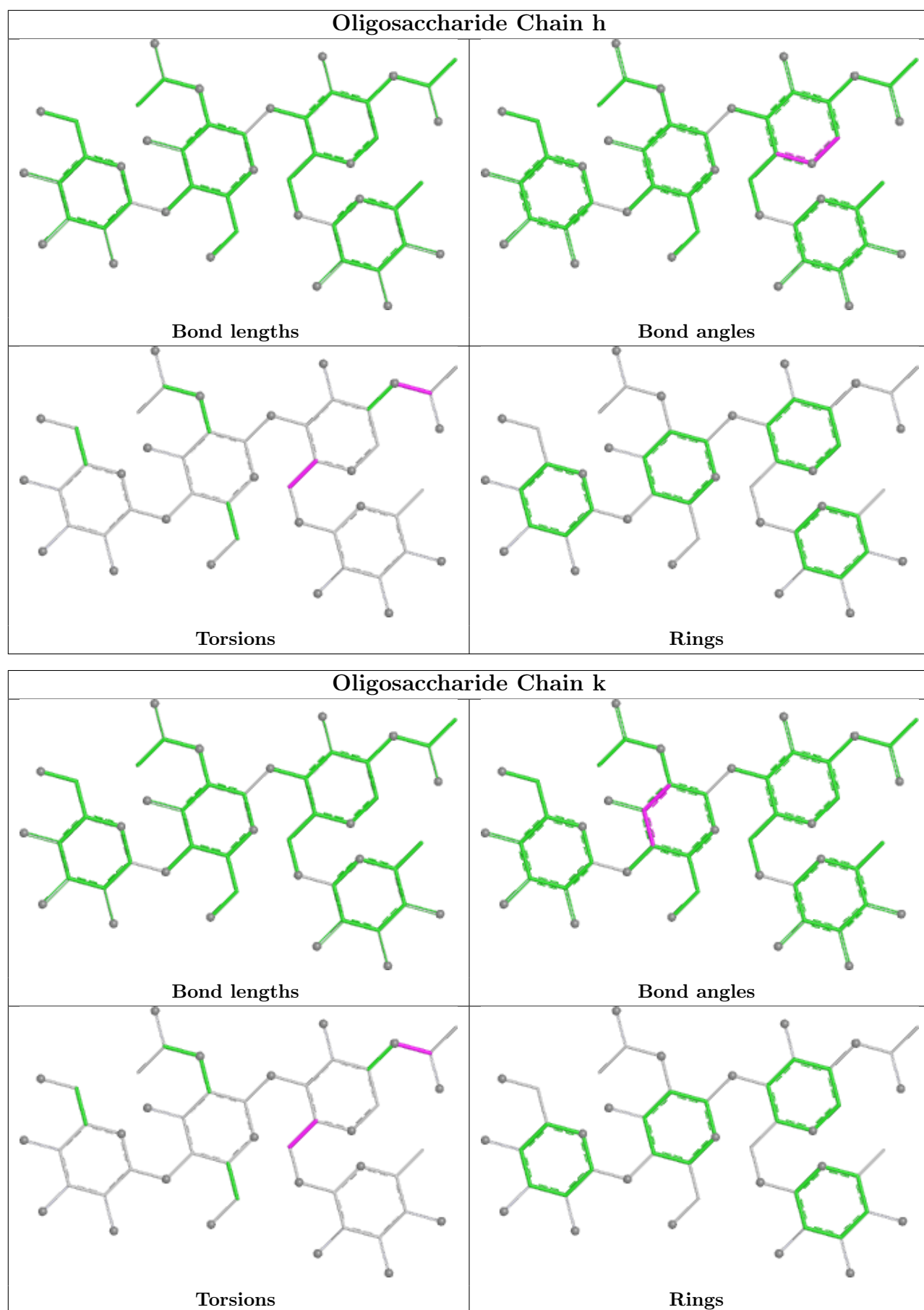
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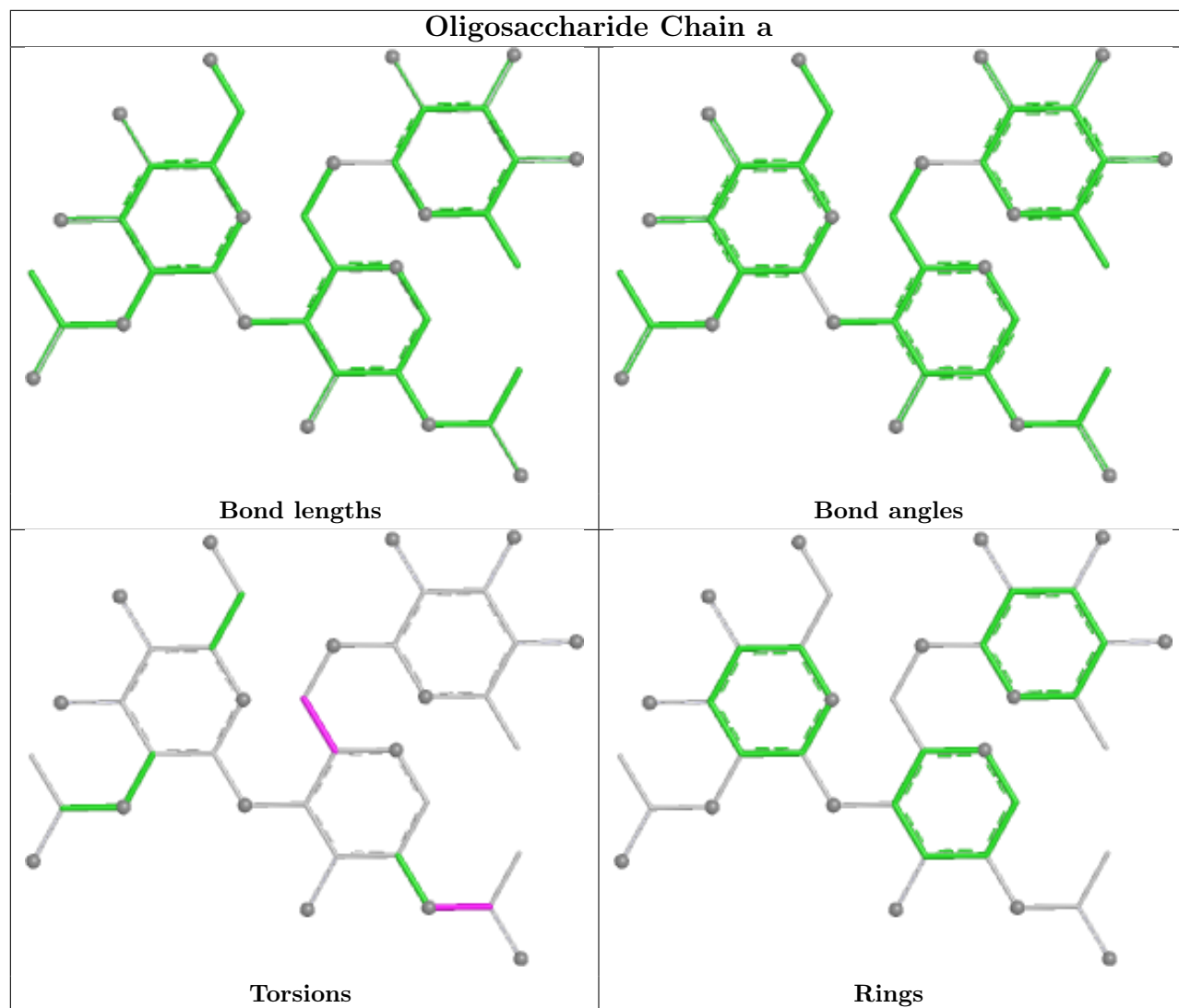
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	2	NAG	1	0
6	j	3	FUC	1	0
5	g	2	NAG	1	0
5	Z	1	NAG	3	0
6	j	2	NAG	1	0
5	h	1	NAG	2	0
9	i	2	FUC	2	0
7	b	1	NAG	3	0
7	b	2	NAG	3	0
6	e	2	NAG	1	0
6	j	1	NAG	2	0
8	c	2	NAG	1	0
10	f	1	NAG	1	0
6	e	3	FUC	1	0
10	f	4	MAN	2	0
6	e	1	NAG	3	0
5	Z	4	FUC	3	0

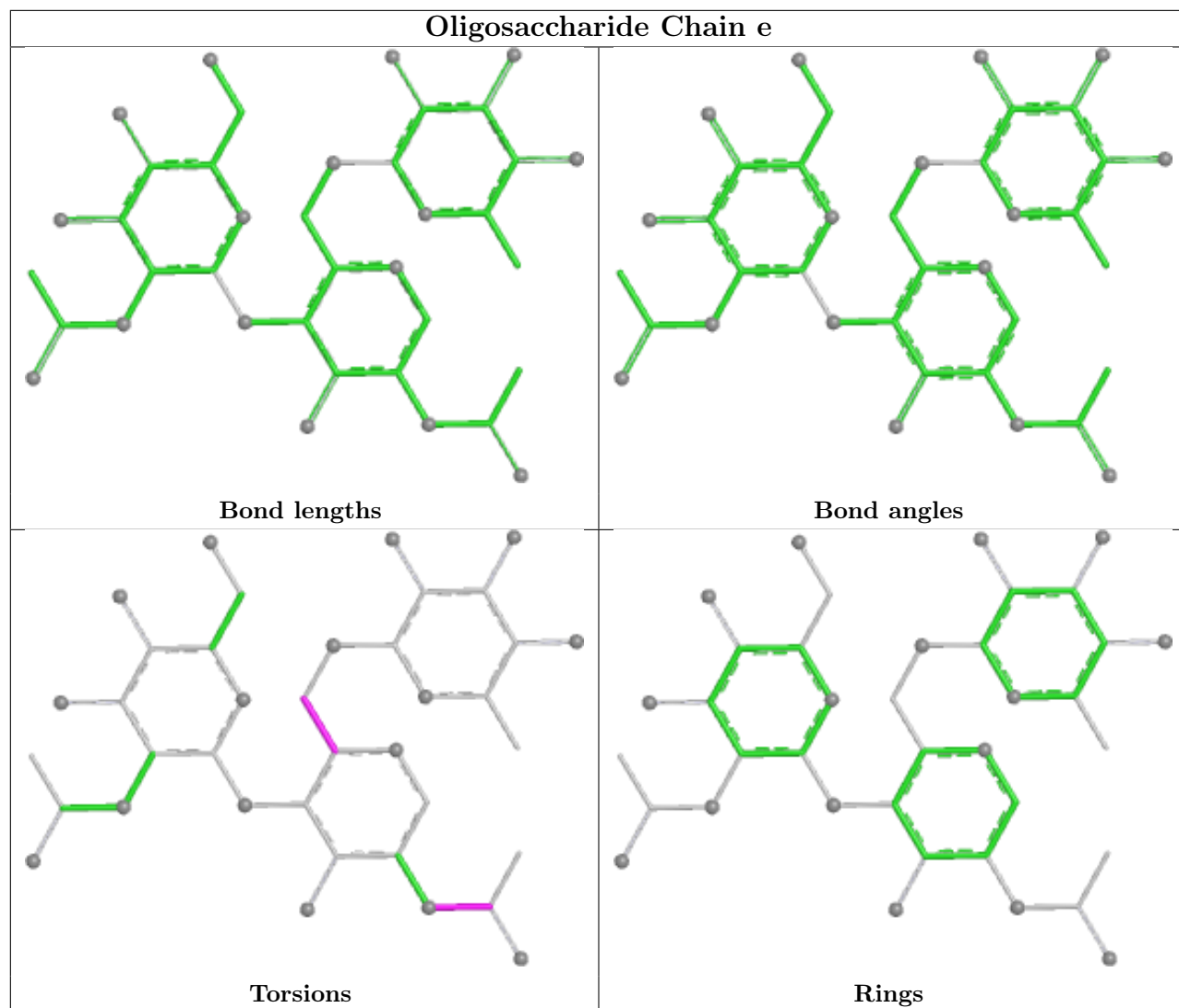
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

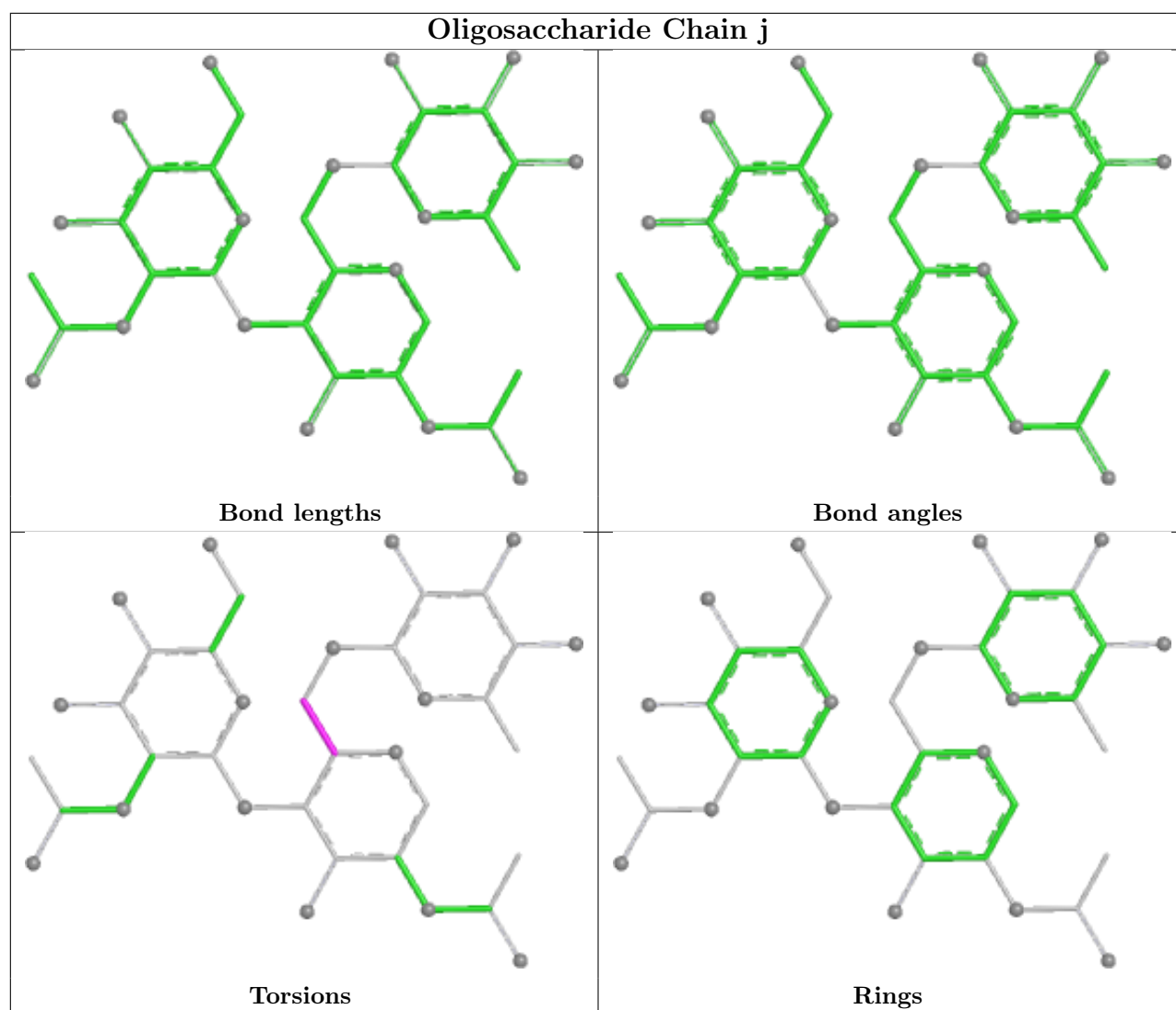


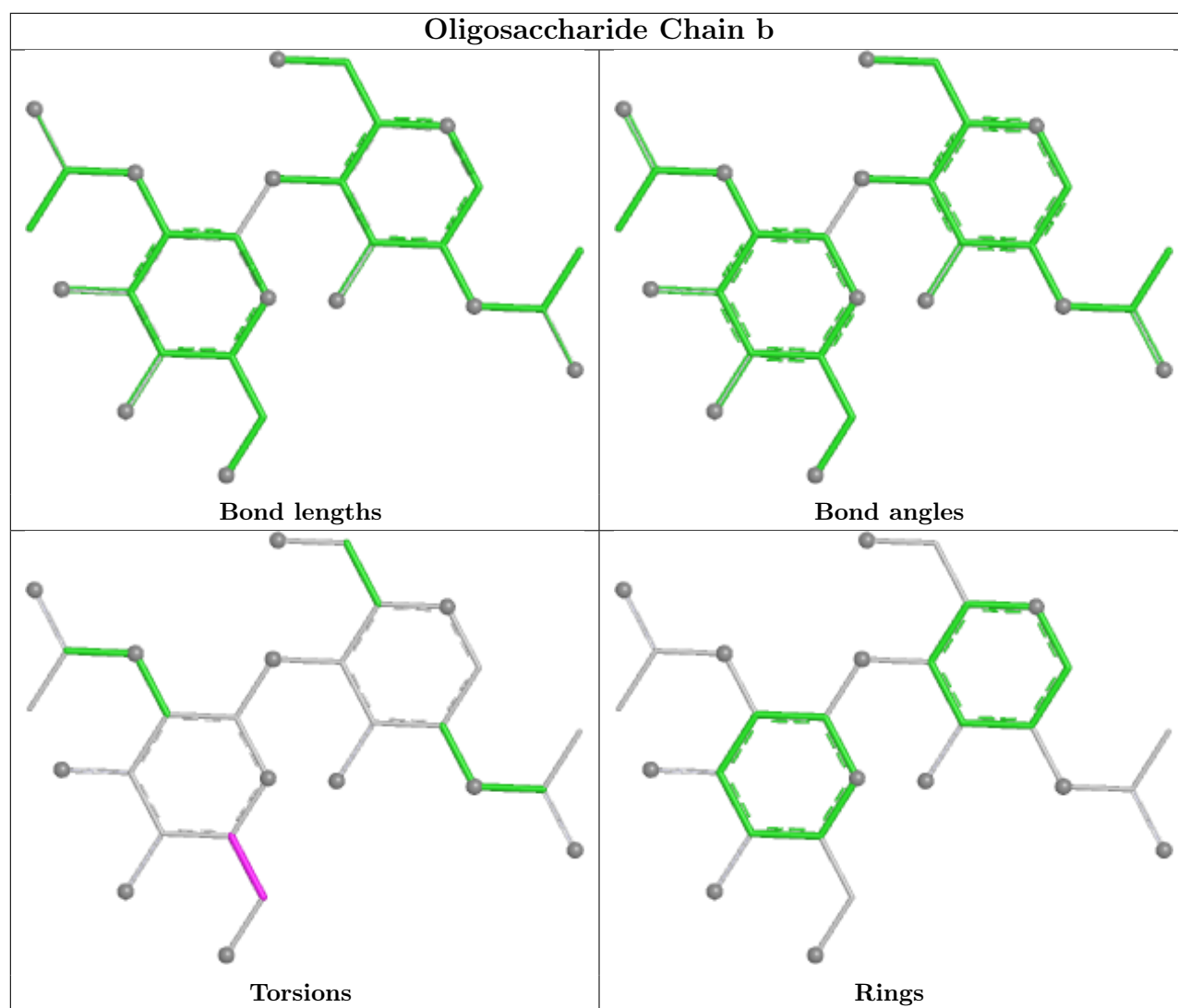


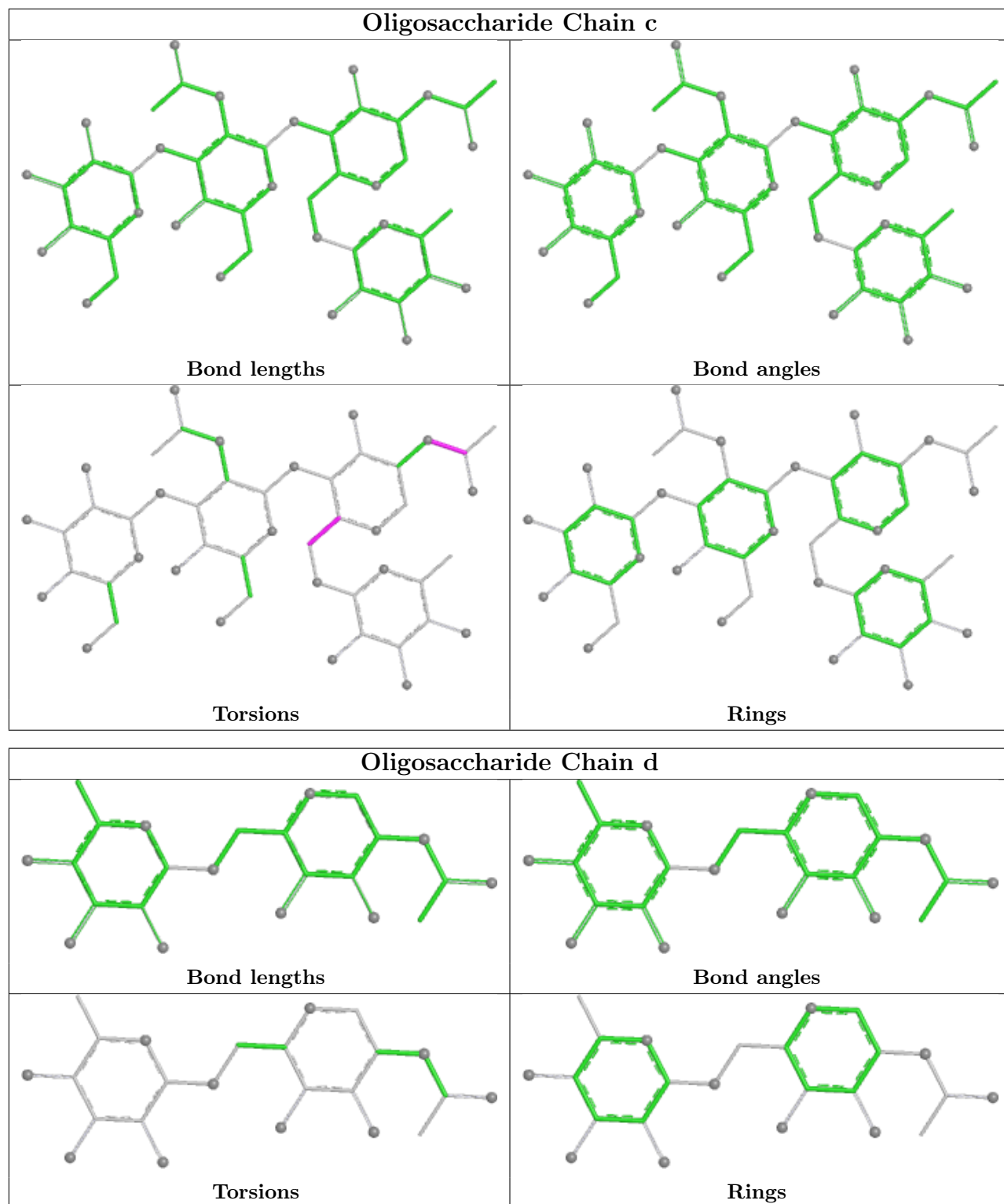


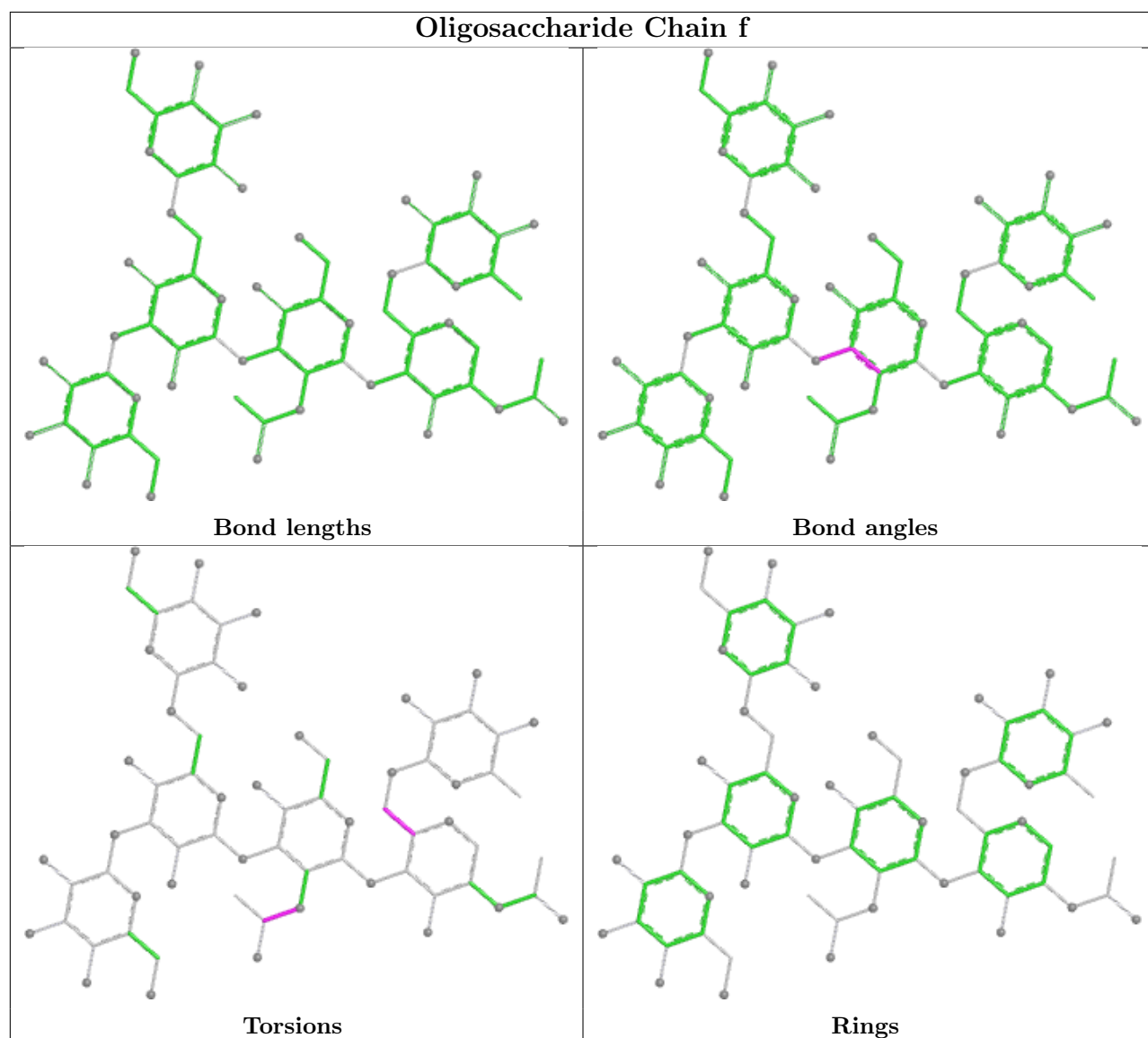
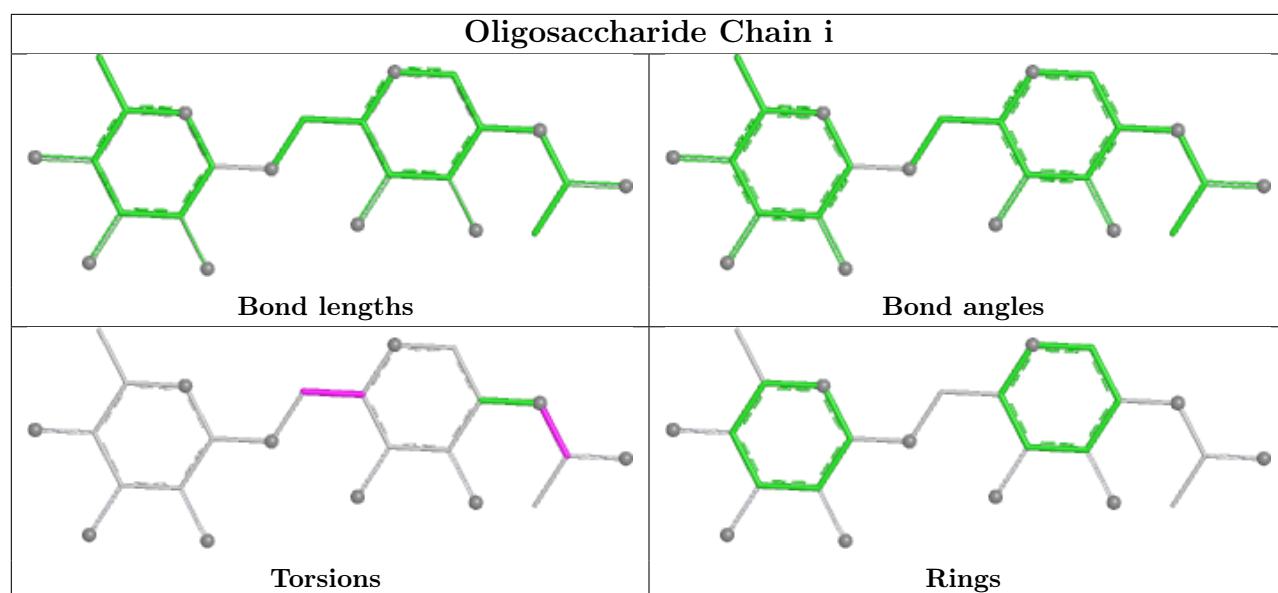












5.6 Ligand geometry

8 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	$\# Z > 2$
11	NAG	L	201	3	14,14,15	0.22	0	17,19,21	0.50	0
11	NAG	R	201	3	14,14,15	0.25	0	17,19,21	0.57	0
11	NAG	I	206	3	14,14,15	0.70	1 (7%)	17,19,21	0.74	0
11	NAG	F	207	3	14,14,15	0.29	0	17,19,21	0.50	0
11	NAG	O	201	3	14,14,15	0.22	0	17,19,21	0.51	0
11	NAG	L	208	3	14,14,15	0.32	0	17,19,21	0.50	0
11	NAG	Y	201	3	14,14,15	0.23	0	17,19,21	0.49	0
11	NAG	Y	206	3	14,14,15	0.30	0	17,19,21	0.51	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
11	NAG	L	201	3	-	0/6/23/26	0/1/1/1
11	NAG	R	201	3	-	2/6/23/26	0/1/1/1
11	NAG	I	206	3	-	2/6/23/26	0/1/1/1
11	NAG	F	207	3	-	2/6/23/26	0/1/1/1
11	NAG	O	201	3	-	2/6/23/26	0/1/1/1
11	NAG	L	208	3	-	1/6/23/26	0/1/1/1
11	NAG	Y	201	3	-	2/6/23/26	0/1/1/1
11	NAG	Y	206	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	206	NAG	O5-C1	-2.14	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	201	NAG	O5-C5-C6-O6
11	I	206	NAG	O5-C5-C6-O6
11	R	201	NAG	C4-C5-C6-O6
11	I	206	NAG	C4-C5-C6-O6
11	F	207	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	C	213/214 (99%)	0.07	0 100 100	57, 84, 123, 174	0
1	D	213/214 (99%)	0.12	1 (0%) 87 68	59, 96, 132, 165	0
1	G	213/214 (99%)	0.08	0 100 100	64, 90, 118, 152	0
1	J	213/214 (99%)	0.12	0 100 100	61, 82, 116, 145	0
1	M	213/214 (99%)	0.07	1 (0%) 87 68	59, 94, 135, 177	0
1	P	213/214 (99%)	0.04	0 100 100	59, 93, 146, 174	0
1	S	213/214 (99%)	0.06	0 100 100	77, 109, 155, 189	0
1	V	213/214 (99%)	0.14	1 (0%) 87 68	62, 102, 154, 190	0
2	B	214/225 (95%)	0.05	2 (0%) 81 58	46, 73, 112, 140	0
2	E	214/225 (95%)	0.10	1 (0%) 87 68	51, 78, 119, 154	0
2	H	210/225 (93%)	0.20	1 (0%) 87 68	57, 79, 111, 137	0
2	K	212/225 (94%)	0.11	0 100 100	58, 81, 113, 150	0
2	N	209/225 (92%)	0.12	0 100 100	61, 86, 131, 204	0
2	Q	210/225 (93%)	0.16	0 100 100	62, 90, 146, 221	0
2	T	212/225 (94%)	0.16	1 (0%) 87 68	80, 107, 159, 252	0
2	W	206/225 (91%)	0.17	0 100 100	87, 115, 151, 209	0
3	A	111/168 (66%)	0.08	1 (0%) 81 58	68, 98, 134, 173	0
3	F	117/168 (69%)	0.23	1 (0%) 81 58	59, 90, 152, 203	0
3	I	113/168 (67%)	0.24	1 (0%) 81 58	69, 112, 164, 190	0
3	L	112/168 (66%)	0.20	1 (0%) 81 58	75, 123, 161, 195	0
3	O	117/168 (69%)	0.17	2 (1%) 69 43	73, 100, 199, 287	0
3	R	110/168 (65%)	0.17	0 100 100	69, 102, 147, 200	0
3	X	117/168 (69%)	0.14	0 100 100	87, 136, 185, 266	0
3	Y	117/168 (69%)	0.24	0 100 100	87, 123, 206, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4305/4856 (88%)	0.13	14 (0%) 90 76	46, 95, 149, 287	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	33	ASN	3.2
3	F	76	THR	2.8
2	B	17	SER	2.5
3	I	33	ASN	2.4
1	M	194	CYS	2.4

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	U	1	14/15	-	-	109,131,136,138	0
4	NAG	U	2	14/15	-	-	91,114,123,125	0
4	BMA	U	3	11/12	-	-	98,103,108,112	0
4	MAN	U	4	11/12	-	-	94,102,106,109	0
5	NAG	Z	2	14/15	0.50	0.12	93,103,106,109	0
5	BMA	Z	3	11/12	0.55	0.11	89,95,102,103	0
5	NAG	Z	1	14/15	0.71	0.11	102,110,113,114	0
5	FUC	Z	4	10/11	0.72	0.15	93,103,106,111	0
5	NAG	g	1	14/15	-	-	75,88,94,98	0
5	NAG	g	2	14/15	-	-	89,101,112,122	0
5	BMA	g	3	11/12	-	-	92,103,111,113	0
5	FUC	g	4	10/11	-	-	92,95,100,102	0
5	NAG	h	1	14/15	-	-	75,90,97,99	0
5	NAG	h	2	14/15	-	-	84,91,101,102	0
5	BMA	h	3	11/12	-	-	92,97,100,101	0
5	FUC	h	4	10/11	-	-	93,97,101,101	0
5	NAG	k	1	14/15	-	-	114,122,130,131	0

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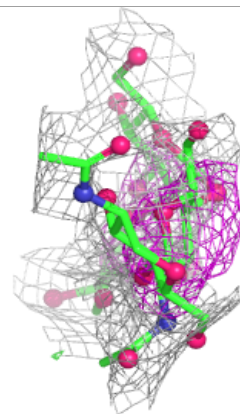
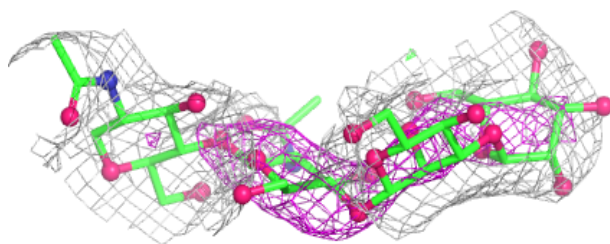
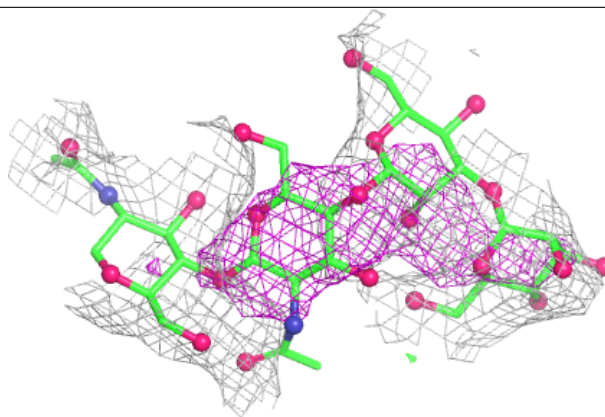
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	k	2	14/15	-	-	108,116,123,126	0
5	BMA	k	3	11/12	-	-	101,106,113,115	0
5	FUC	k	4	10/11	-	-	112,121,122,128	0
6	NAG	a	1	14/15	-	-	102,107,116,116	0
6	NAG	a	2	14/15	-	-	95,103,111,111	0
6	FUC	a	3	10/11	-	-	90,97,102,105	0
6	NAG	e	1	14/15	-	-	109,118,126,132	0
6	NAG	e	2	14/15	-	-	105,119,123,123	0
6	FUC	e	3	10/11	-	-	105,109,113,115	0
6	NAG	j	1	14/15	-	-	106,120,132,133	0
6	NAG	j	2	14/15	-	-	102,109,115,115	0
6	FUC	j	3	10/11	-	-	113,119,123,123	0
7	NAG	b	1	14/15	-	-	105,112,114,117	0
7	NAG	b	2	14/15	-	-	100,107,111,112	0
8	NAG	c	1	14/15	-	-	78,85,91,99	0
8	NAG	c	2	14/15	-	-	81,90,98,107	0
8	BMA	c	3	11/12	-	-	78,93,97,98	0
8	FUC	c	4	10/11	-	-	79,82,83,84	0
9	NAG	d	1	14/15	-	-	123,130,133,134	0
9	FUC	d	2	10/11	-	-	108,122,124,125	0
9	NAG	i	1	14/15	-	-	113,121,128,130	0
9	FUC	i	2	10/11	-	-	125,131,135,137	0
10	NAG	f	1	14/15	-	-	110,116,127,136	0
10	NAG	f	2	14/15	-	-	93,108,112,114	0
10	BMA	f	3	11/12	-	-	96,111,115,117	0
10	MAN	f	4	11/12	-	-	97,108,110,110	0
10	MAN	f	5	11/12	-	-	88,99,103,105	0
10	FUC	f	6	10/11	-	-	102,106,110,111	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.

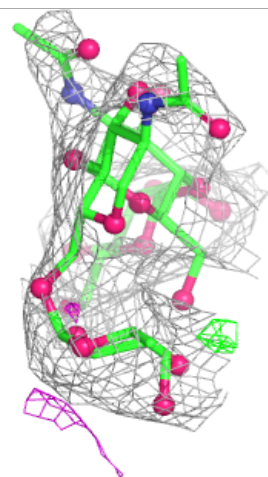
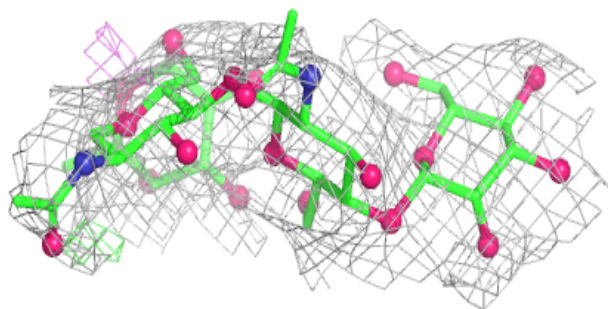
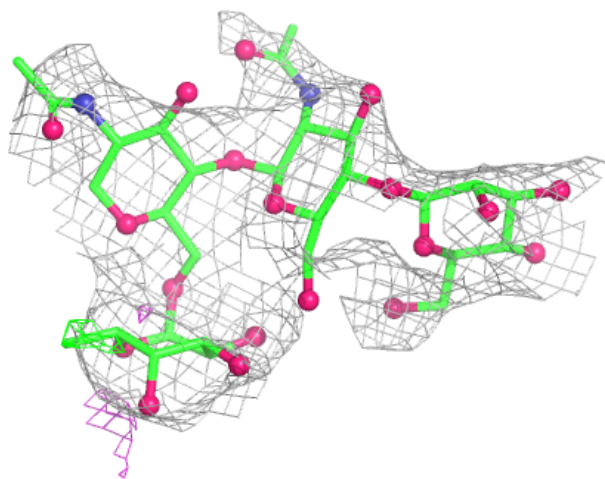
Electron density around Chain U:

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



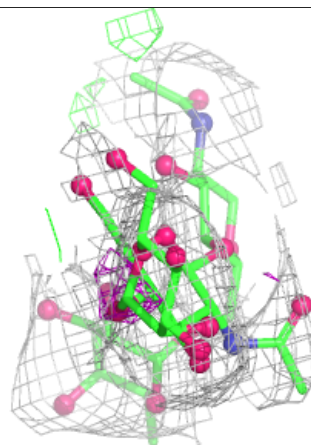
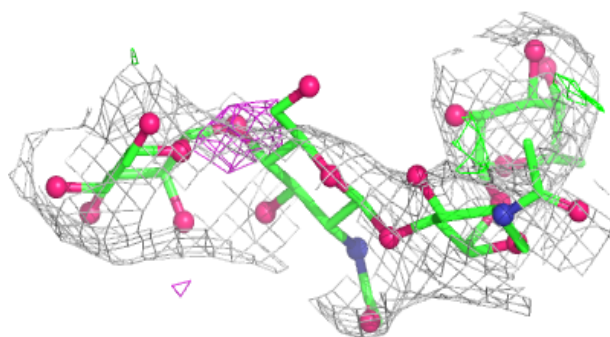
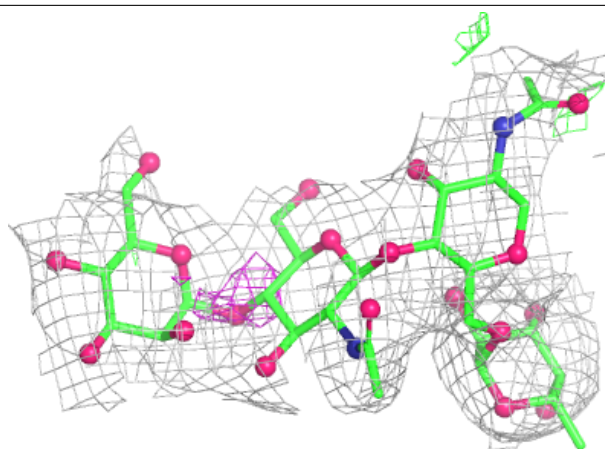
Electron density around Chain Z:

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



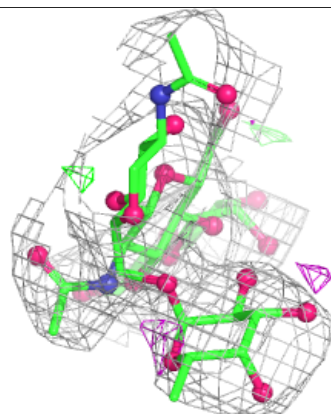
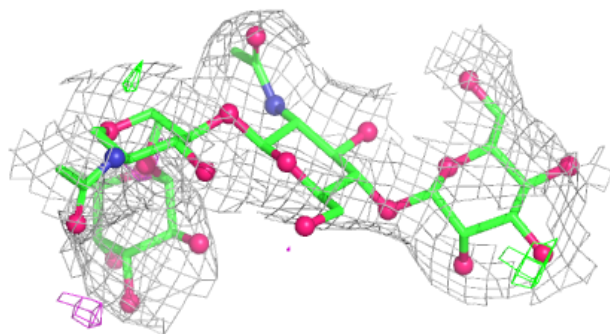
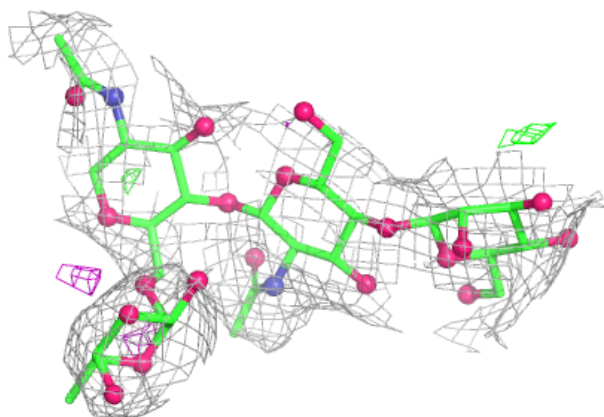
Electron density around Chain g:

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



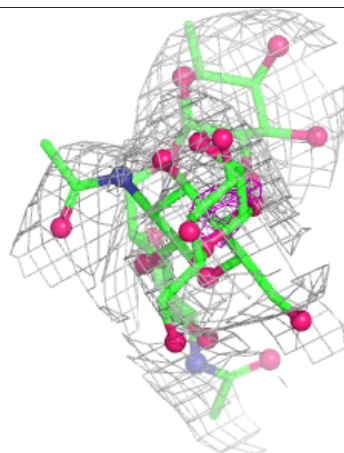
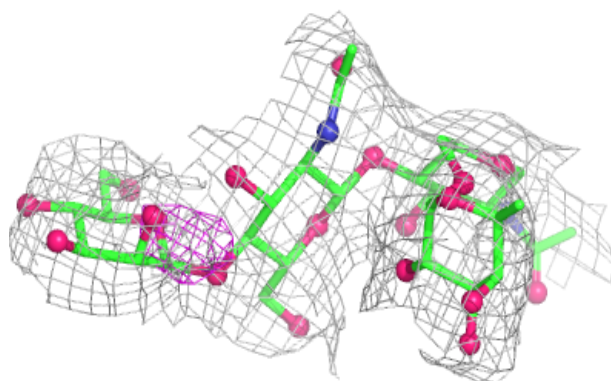
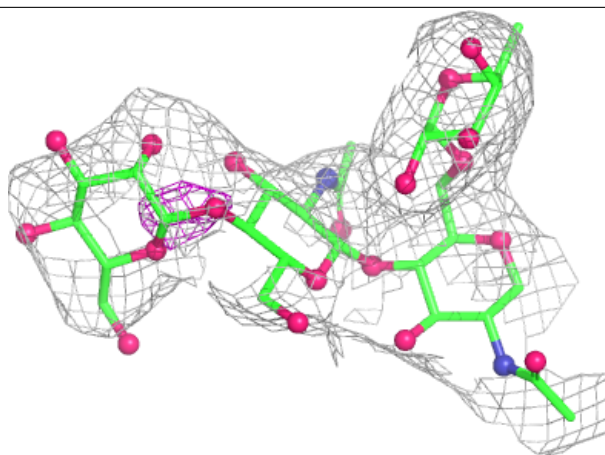
Electron density around Chain h:

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



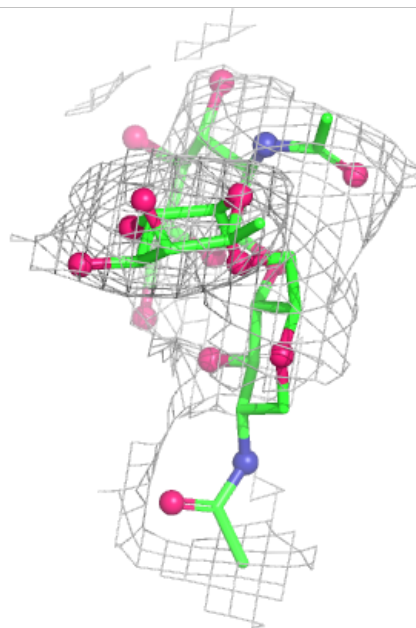
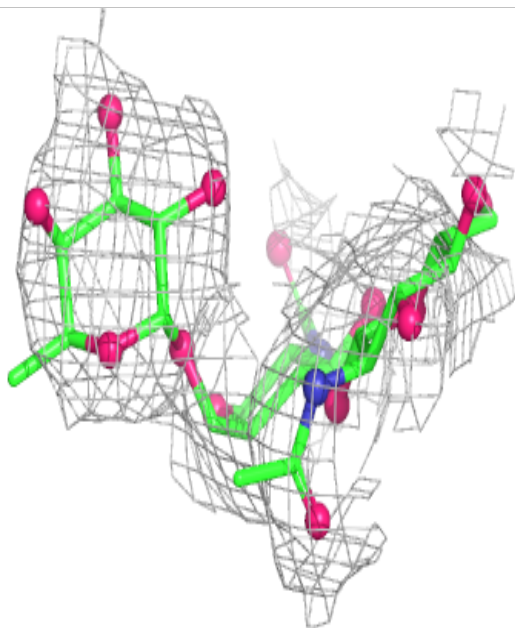
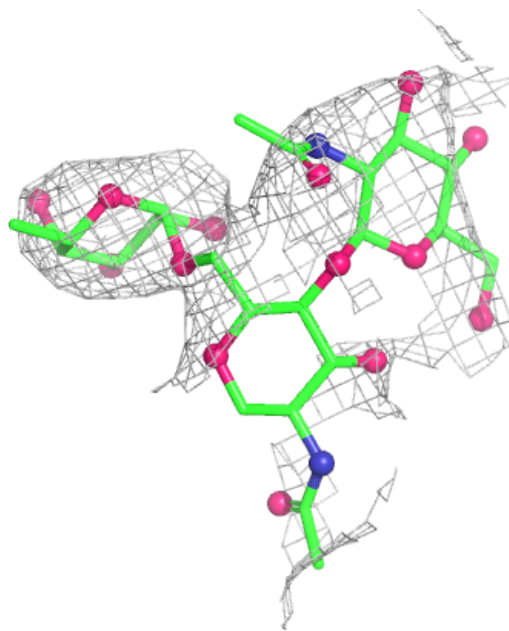
Electron density around Chain k:

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



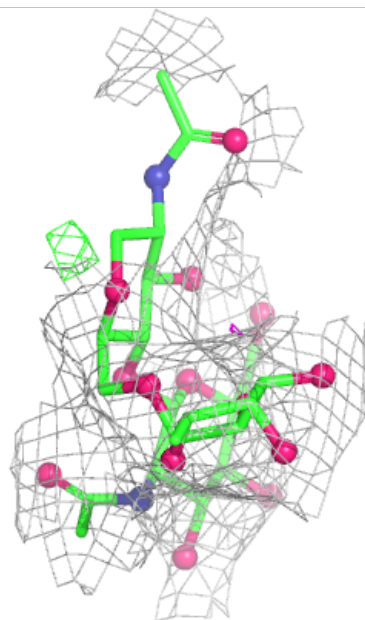
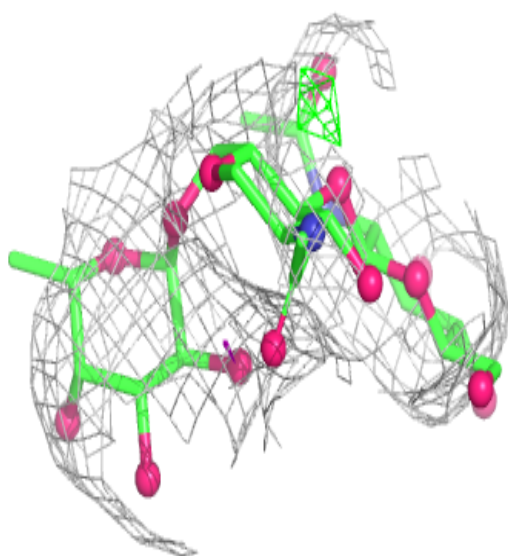
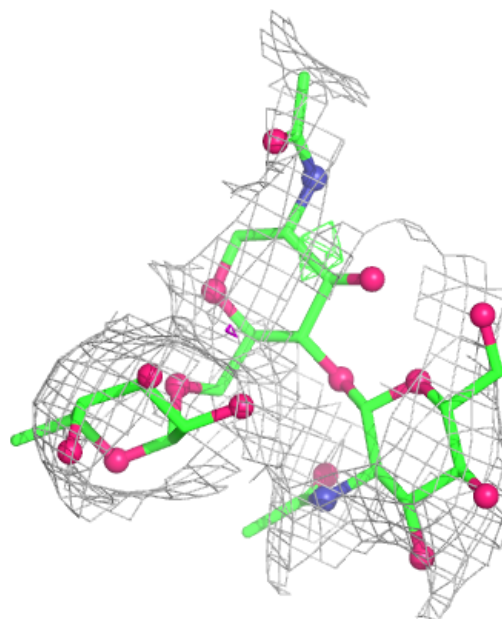
Electron density around Chain a:

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



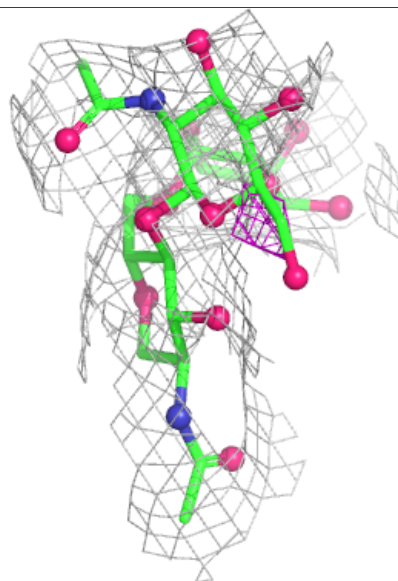
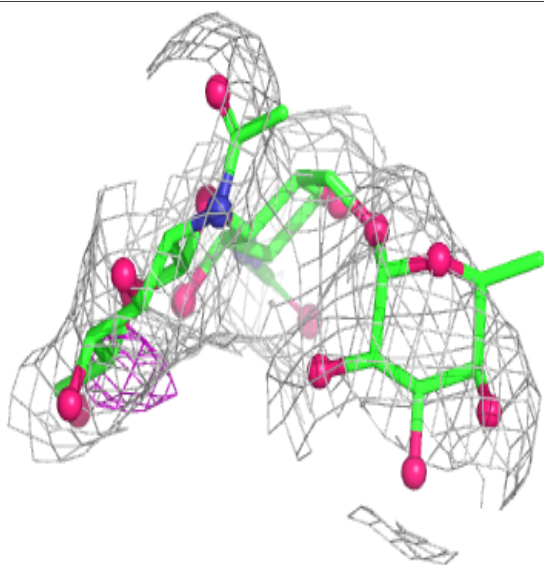
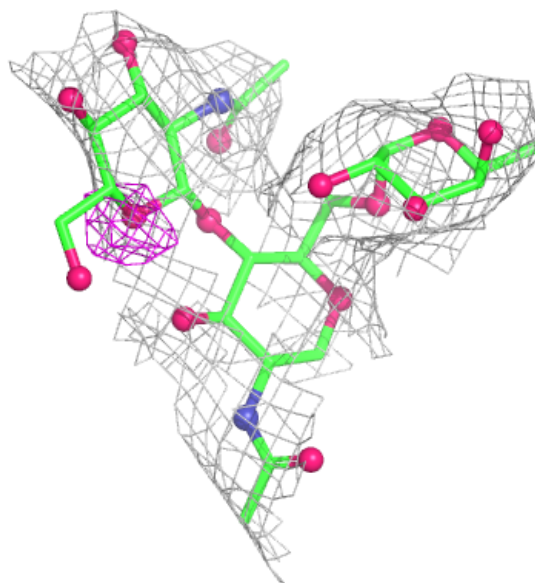
Electron density around Chain e:

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and green (positive)



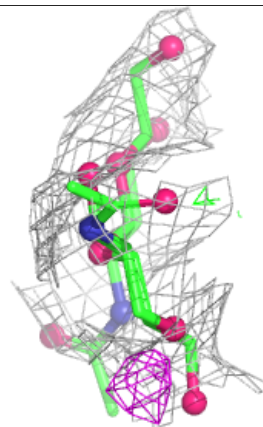
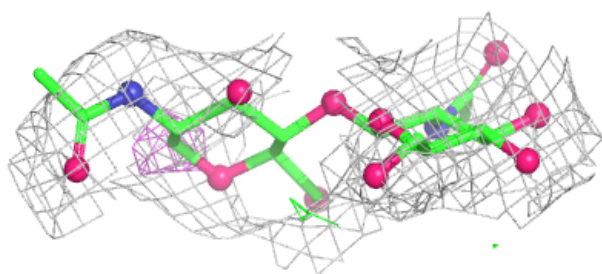
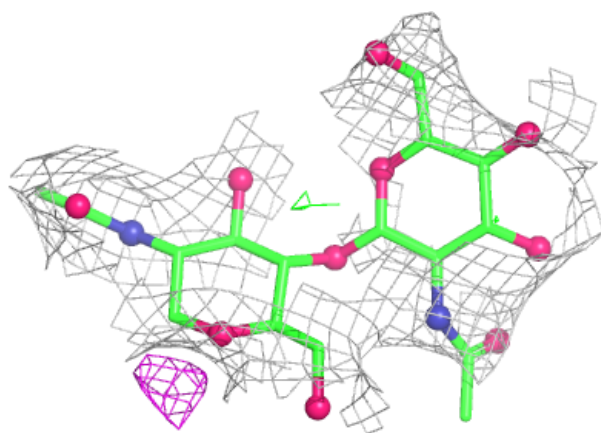
Electron density around Chain j:

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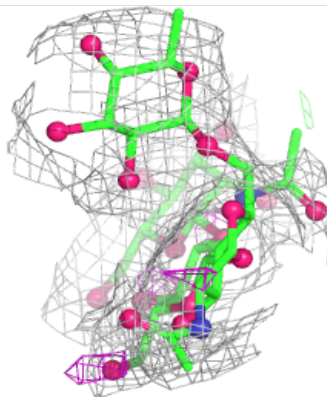
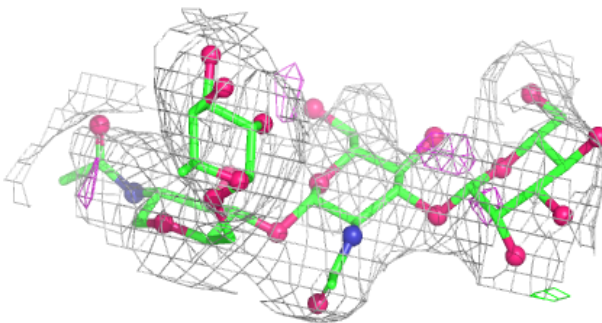
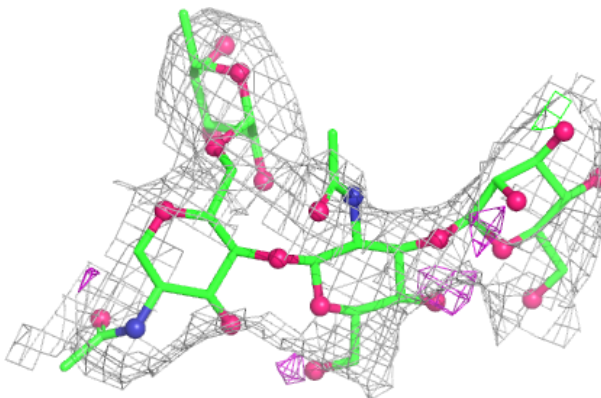


Electron density around Chain b:

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and green (positive)

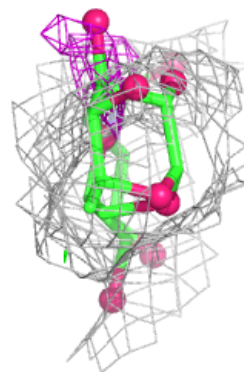
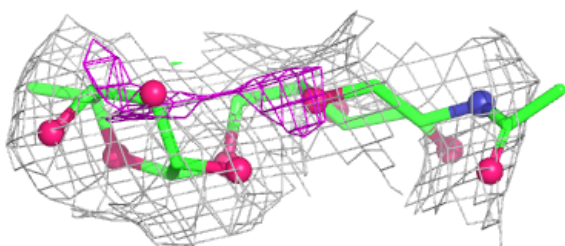
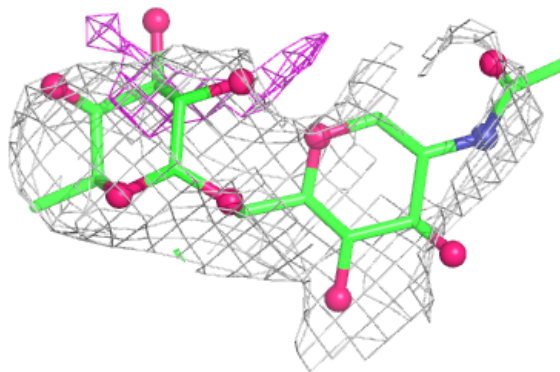
**Electron density around Chain c:**

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

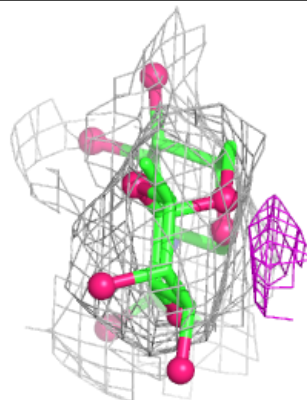
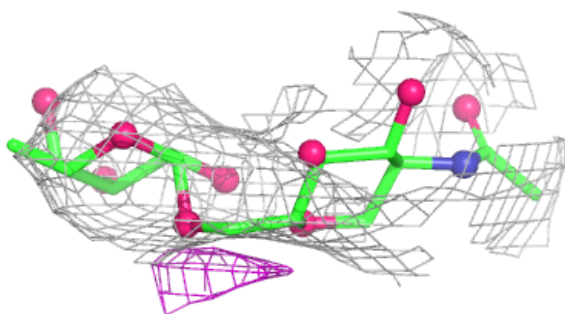
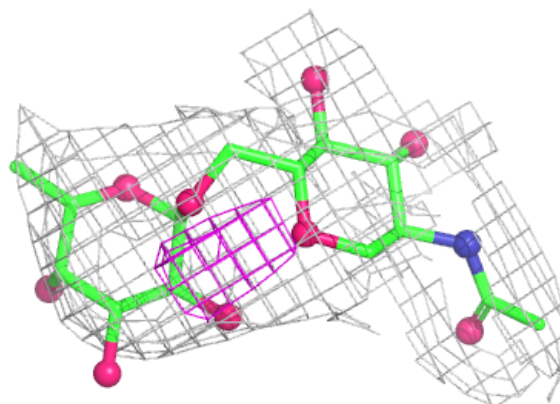


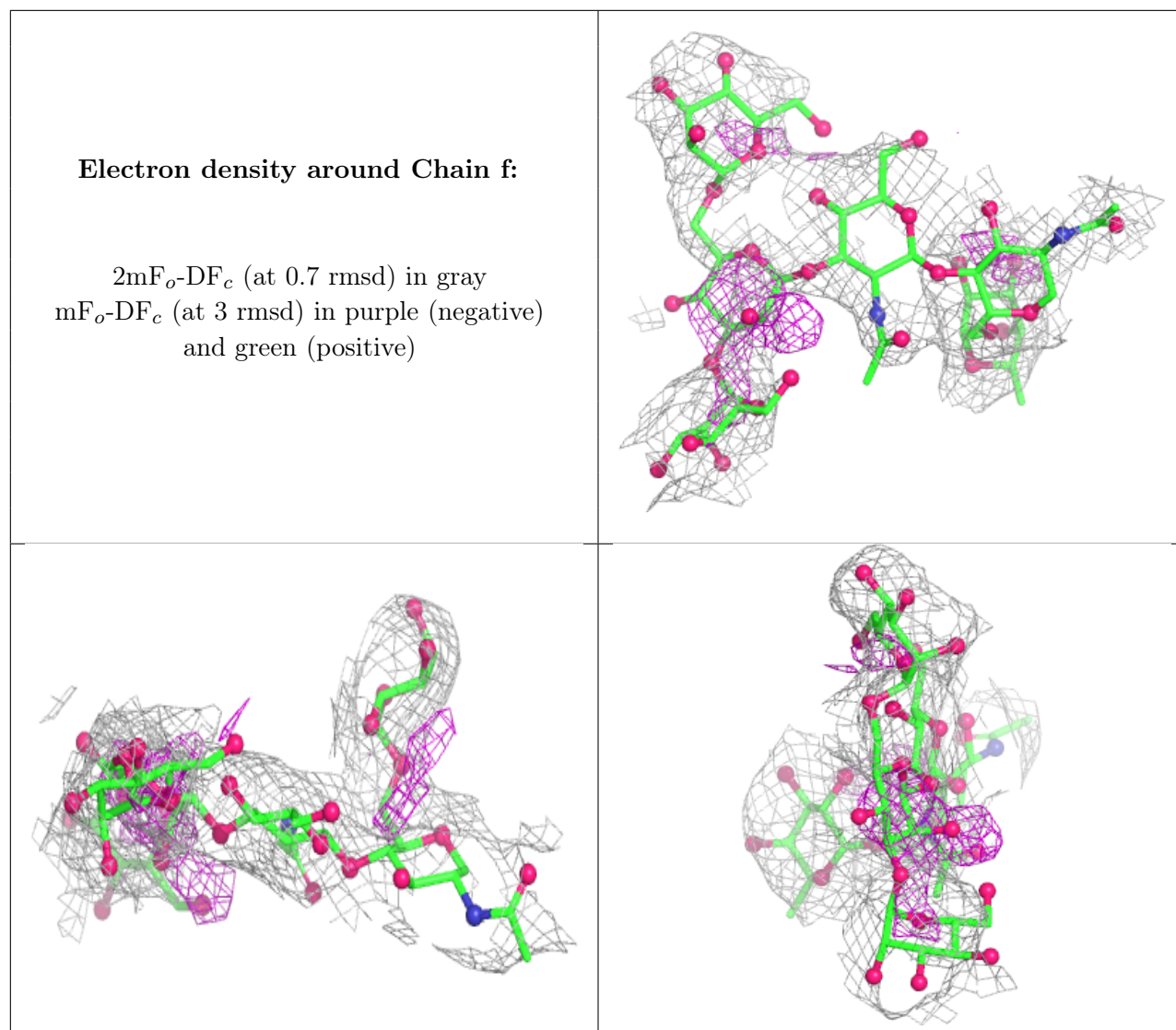
Electron density around Chain d:

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

**Electron density around Chain i:**

$2mF_o - DF_c$ (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(Å ²)	Q<0.9
11	NAG	R	201	14/15	0.27	0.13	109,113,120,121	0
11	NAG	Y	206	14/15	0.30	0.15	122,137,141,143	0
11	NAG	F	207	14/15	0.32	0.16	98,113,121,122	0
11	NAG	L	208	14/15	0.46	0.13	115,122,125,127	0
11	NAG	Y	201	14/15	0.55	0.10	106,112,118,118	0
11	NAG	I	206	14/15	0.58	0.12	104,108,111,111	0
11	NAG	O	201	14/15	0.60	0.12	84,93,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	L	201	14/15	0.63	0.11	122,138,141,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.