



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 11:05 AM BST

PDB ID : 3TGX
Title : IL-21:IL21R complex
Authors : Hamming, O.J.; Kang, L.; Svenson, A.; Karlsen, J.L.; Rahbek-Nielsen, H.;
Paludan, S.R.; Hjort, S.A.; Bondensgaard, K.; Hartmann, R.
Deposited on : 2011-08-18
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

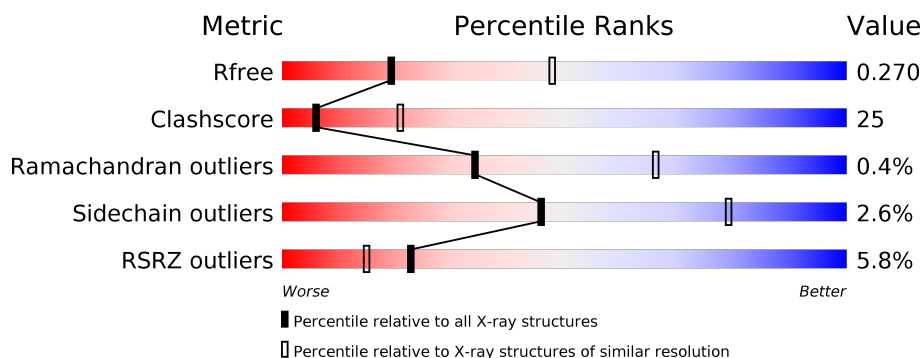
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	219	<div> <div>72%</div> <div>22%</div> <div>• 5%</div> </div>
1	C	219	<div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div>
1	E	219	<div> <div>5%</div> <div>63%</div> <div>31%</div> <div>5%</div> </div>
1	G	219	<div> <div>3%</div> <div>67%</div> <div>26%</div> <div>• 5%</div> </div>
1	I	219	<div> <div>5%</div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div>
1	K	219	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	219	
1	O	219	
2	B	134	
2	D	134	
2	F	134	
2	H	134	
2	J	134	
2	L	134	
2	N	134	
2	P	134	
3	Q	7	
3	R	7	
3	S	7	
3	T	7	
3	U	7	
4	V	6	
4	X	6	
5	W	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	Q	2	-	-	X	-
3	BMA	Q	3	-	-	X	-
3	MAN	Q	5	-	-	X	-
3	MAN	Q	6	-	-	-	X
3	FUL	Q	7	-	-	-	X
3	NAG	R	1	-	-	X	-
3	NAG	R	2	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	R	3	-	-	X	-
3	NAG	S	2	-	-	X	-
3	BMA	S	3	-	-	X	-
3	MAN	S	4	-	-	-	X
3	MAN	S	6	-	-	-	X
3	FUL	S	7	-	-	-	X
3	NAG	T	1	-	-	X	-
3	NAG	T	2	-	-	X	-
3	BMA	T	3	-	-	X	-
3	MAN	T	6	-	-	-	X
3	FUL	T	7	-	-	-	X
3	NAG	U	1	-	-	X	-
3	NAG	U	2	-	-	X	-
3	BMA	U	3	-	-	X	-
3	MAN	U	4	-	-	-	X
3	MAN	U	6	-	-	-	X
4	FUL	V	6	-	-	-	X
4	MAN	X	5	-	-	-	X
5	NAG	W	2	-	-	X	-
5	BMA	W	3	-	-	X	-
6	MAN	A	301	-	-	X	-
8	SO4	A	305	-	-	-	X
8	SO4	I	305	-	-	-	X
8	SO4	O	312	-	-	-	X
8	SO4	O	313	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21830 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 Interleukin-21 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1687	1071	277	328	11			
1	C	209	Total	C	N	O	S	0	0	0
			1696	1076	278	331	11			
1	E	207	Total	C	N	O	S	0	0	0
			1681	1068	276	326	11			
1	G	209	Total	C	N	O	S	0	0	0
			1696	1076	278	331	11			
1	I	209	Total	C	N	O	S	0	0	0
			1696	1076	278	331	11			
1	K	209	Total	C	N	O	S	0	0	0
			1696	1076	278	331	11			
1	M	208	Total	C	N	O	S	0	0	0
			1687	1071	277	328	11			
1	O	208	Total	C	N	O	S	0	0	0
			1687	1071	277	328	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLN	ASN	engineered mutation	UNP Q9HBE5
A	85	GLN	ASN	engineered mutation	UNP Q9HBE5
A	106	ASP	ASN	engineered mutation	UNP Q9HBE5
A	116	GLN	ASN	engineered mutation	UNP Q9HBE5
A	214	HIS	-	expression tag	UNP Q9HBE5
A	215	HIS	-	expression tag	UNP Q9HBE5
A	216	HIS	-	expression tag	UNP Q9HBE5
A	217	HIS	-	expression tag	UNP Q9HBE5
A	218	HIS	-	expression tag	UNP Q9HBE5
A	219	HIS	-	expression tag	UNP Q9HBE5
C	78	GLN	ASN	engineered mutation	UNP Q9HBE5
C	85	GLN	ASN	engineered mutation	UNP Q9HBE5
C	106	ASP	ASN	engineered mutation	UNP Q9HBE5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	116	GLN	ASN	engineered mutation	UNP Q9HBE5
C	214	HIS	-	expression tag	UNP Q9HBE5
C	215	HIS	-	expression tag	UNP Q9HBE5
C	216	HIS	-	expression tag	UNP Q9HBE5
C	217	HIS	-	expression tag	UNP Q9HBE5
C	218	HIS	-	expression tag	UNP Q9HBE5
C	219	HIS	-	expression tag	UNP Q9HBE5
E	78	GLN	ASN	engineered mutation	UNP Q9HBE5
E	85	GLN	ASN	engineered mutation	UNP Q9HBE5
E	106	ASP	ASN	engineered mutation	UNP Q9HBE5
E	116	GLN	ASN	engineered mutation	UNP Q9HBE5
E	214	HIS	-	expression tag	UNP Q9HBE5
E	215	HIS	-	expression tag	UNP Q9HBE5
E	216	HIS	-	expression tag	UNP Q9HBE5
E	217	HIS	-	expression tag	UNP Q9HBE5
E	218	HIS	-	expression tag	UNP Q9HBE5
E	219	HIS	-	expression tag	UNP Q9HBE5
G	78	GLN	ASN	engineered mutation	UNP Q9HBE5
G	85	GLN	ASN	engineered mutation	UNP Q9HBE5
G	106	ASP	ASN	engineered mutation	UNP Q9HBE5
G	116	GLN	ASN	engineered mutation	UNP Q9HBE5
G	214	HIS	-	expression tag	UNP Q9HBE5
G	215	HIS	-	expression tag	UNP Q9HBE5
G	216	HIS	-	expression tag	UNP Q9HBE5
G	217	HIS	-	expression tag	UNP Q9HBE5
G	218	HIS	-	expression tag	UNP Q9HBE5
G	219	HIS	-	expression tag	UNP Q9HBE5
I	78	GLN	ASN	engineered mutation	UNP Q9HBE5
I	85	GLN	ASN	engineered mutation	UNP Q9HBE5
I	106	ASP	ASN	engineered mutation	UNP Q9HBE5
I	116	GLN	ASN	engineered mutation	UNP Q9HBE5
I	214	HIS	-	expression tag	UNP Q9HBE5
I	215	HIS	-	expression tag	UNP Q9HBE5
I	216	HIS	-	expression tag	UNP Q9HBE5
I	217	HIS	-	expression tag	UNP Q9HBE5
I	218	HIS	-	expression tag	UNP Q9HBE5
I	219	HIS	-	expression tag	UNP Q9HBE5
K	78	GLN	ASN	engineered mutation	UNP Q9HBE5
K	85	GLN	ASN	engineered mutation	UNP Q9HBE5
K	106	ASP	ASN	engineered mutation	UNP Q9HBE5
K	116	GLN	ASN	engineered mutation	UNP Q9HBE5
K	214	HIS	-	expression tag	UNP Q9HBE5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	215	HIS	-	expression tag	UNP Q9HBE5
K	216	HIS	-	expression tag	UNP Q9HBE5
K	217	HIS	-	expression tag	UNP Q9HBE5
K	218	HIS	-	expression tag	UNP Q9HBE5
K	219	HIS	-	expression tag	UNP Q9HBE5
M	78	GLN	ASN	engineered mutation	UNP Q9HBE5
M	85	GLN	ASN	engineered mutation	UNP Q9HBE5
M	106	ASP	ASN	engineered mutation	UNP Q9HBE5
M	116	GLN	ASN	engineered mutation	UNP Q9HBE5
M	214	HIS	-	expression tag	UNP Q9HBE5
M	215	HIS	-	expression tag	UNP Q9HBE5
M	216	HIS	-	expression tag	UNP Q9HBE5
M	217	HIS	-	expression tag	UNP Q9HBE5
M	218	HIS	-	expression tag	UNP Q9HBE5
M	219	HIS	-	expression tag	UNP Q9HBE5
O	78	GLN	ASN	engineered mutation	UNP Q9HBE5
O	85	GLN	ASN	engineered mutation	UNP Q9HBE5
O	106	ASP	ASN	engineered mutation	UNP Q9HBE5
O	116	GLN	ASN	engineered mutation	UNP Q9HBE5
O	214	HIS	-	expression tag	UNP Q9HBE5
O	215	HIS	-	expression tag	UNP Q9HBE5
O	216	HIS	-	expression tag	UNP Q9HBE5
O	217	HIS	-	expression tag	UNP Q9HBE5
O	218	HIS	-	expression tag	UNP Q9HBE5
O	219	HIS	-	expression tag	UNP Q9HBE5

- Molecule 2 is a protein called Interleukin-21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			944	595	171	171	7			
2	D	117	Total	C	N	O	S	0	0	0
			951	598	172	174	7			
2	F	113	Total	C	N	O	S	0	0	0
			923	581	165	170	7			
2	H	116	Total	C	N	O	S	0	0	0
			957	603	174	173	7			
2	J	116	Total	C	N	O	S	0	0	0
			940	592	167	174	7			
2	L	110	Total	C	N	O	S	0	0	0
			902	570	160	165	7			
2	N	107	Total	C	N	O	S	0	0	0
			875	553	154	161	7			

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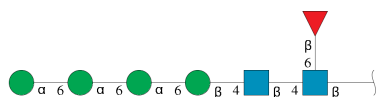
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	110	Total	C	N	O	S	0	0	0
			902	570	160	165	7			

There are 8 discrepancies between the modelled and reference sequences:

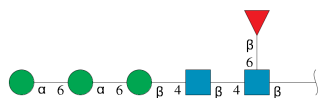
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP Q9HBE4
D	0	MET	-	expression tag	UNP Q9HBE4
F	0	MET	-	expression tag	UNP Q9HBE4
H	0	MET	-	expression tag	UNP Q9HBE4
J	0	MET	-	expression tag	UNP Q9HBE4
L	0	MET	-	expression tag	UNP Q9HBE4
N	0	MET	-	expression tag	UNP Q9HBE4
P	0	MET	-	expression tag	UNP Q9HBE4

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



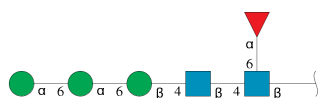
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	7	Total	C	N	O		0	0	0
			82	46	2	34				
3	R	7	Total	C	N	O		0	0	0
			82	46	2	34				
3	S	7	Total	C	N	O		0	0	0
			82	46	2	34				
3	T	7	Total	C	N	O		0	0	0
			82	46	2	34				
3	U	7	Total	C	N	O		0	0	0
			82	46	2	34				

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



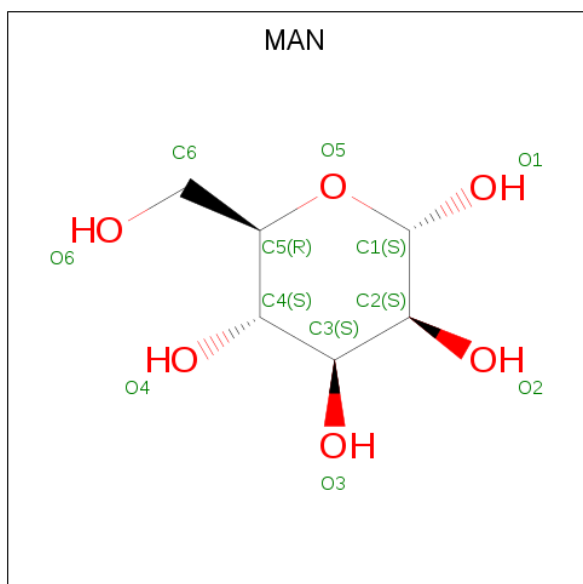
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	V	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	X	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-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.



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

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

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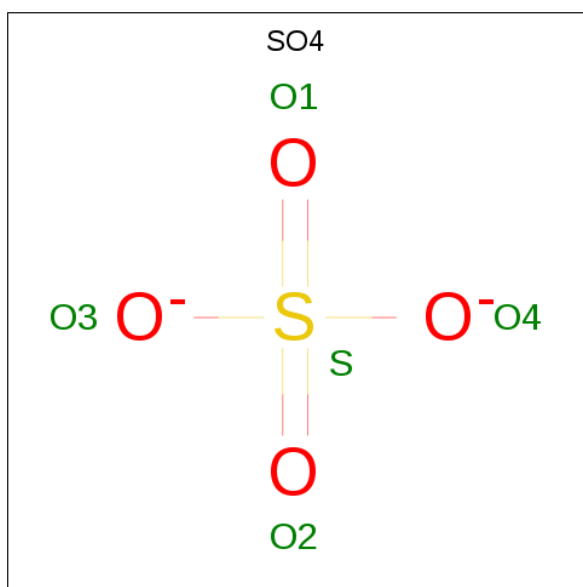
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		
6	O	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ni	0	0
			1	1		
7	O	1	Total	Ni	0	0
			1	1		
7	A	1	Total	Ni	0	0
			1	1		
7	E	1	Total	Ni	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	K	1	Total	O	S	0	0
			5	4	1		
8	K	1	Total	O	S	0	0
			5	4	1		
8	K	1	Total	O	S	0	0
			5	4	1		
8	K	1	Total	O	S	0	0
			5	4	1		
8	K	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		

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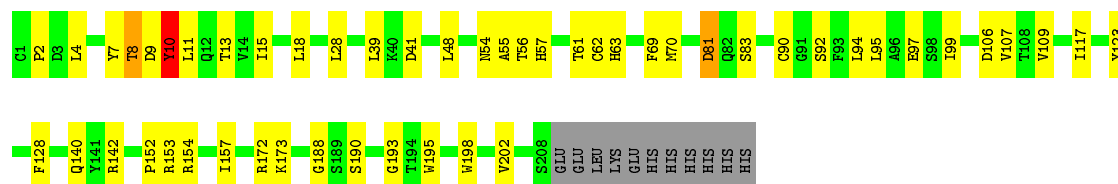
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	O	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		

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.

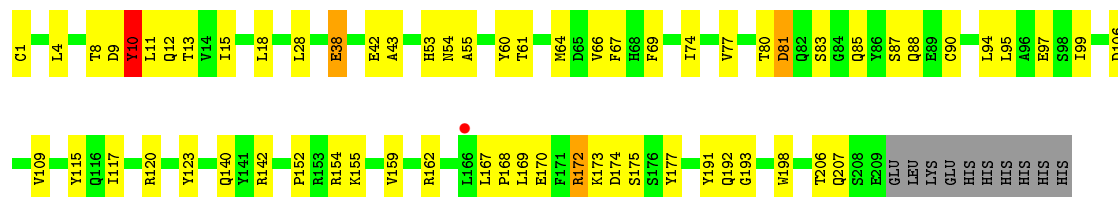
• Molecule 1: Interleukin-21 receptor

Chain A: 



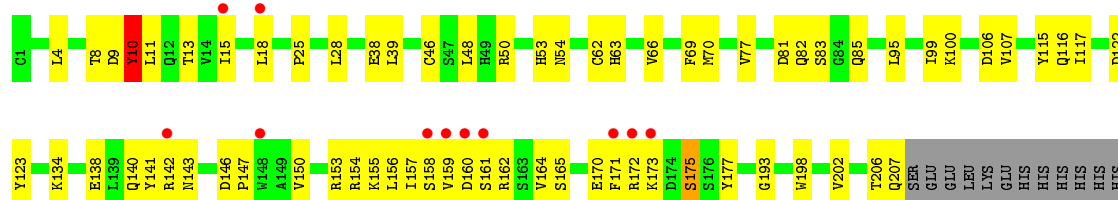
• Molecule 1: Interleukin-21 receptor

Chain C: 



• Molecule 1: Interleukin-21 receptor

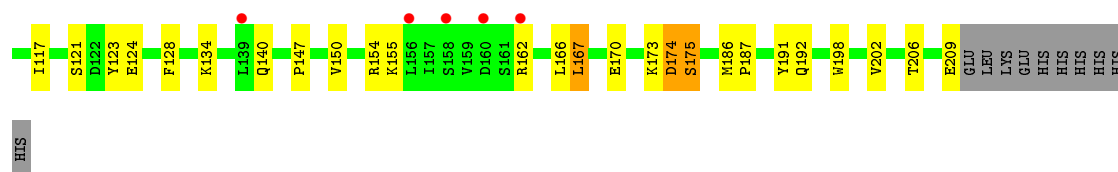
Chain E: 



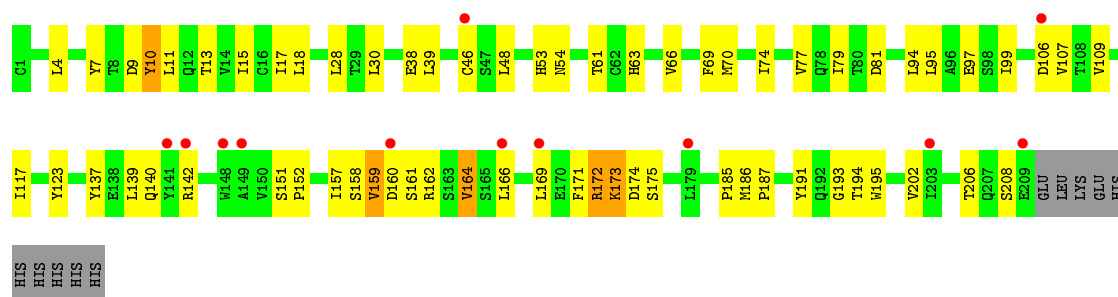
• Molecule 1: Interleukin-21 receptor

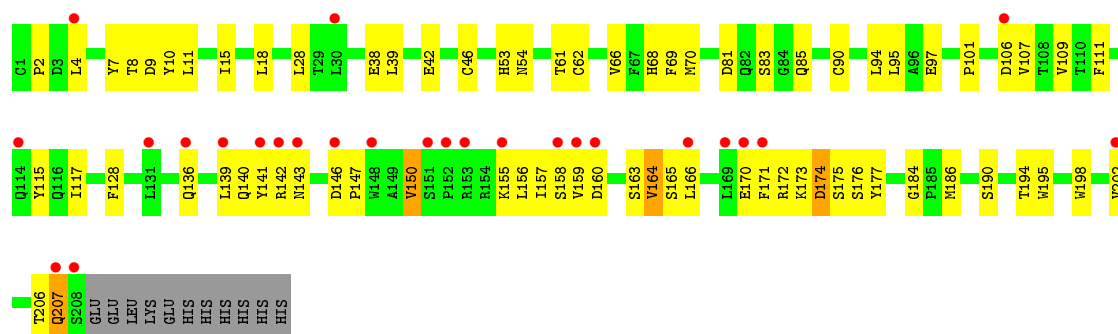
Chain G: 



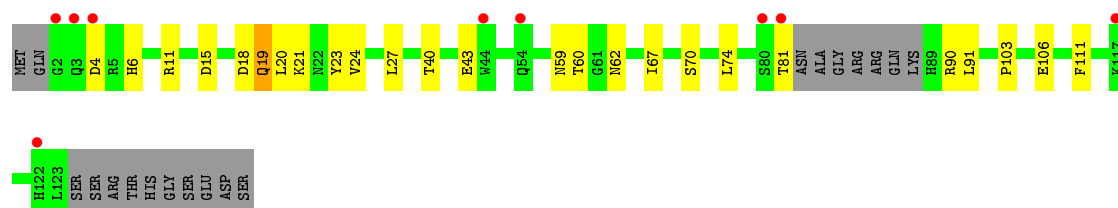


- Molecule 1: Interleukin-21 receptor

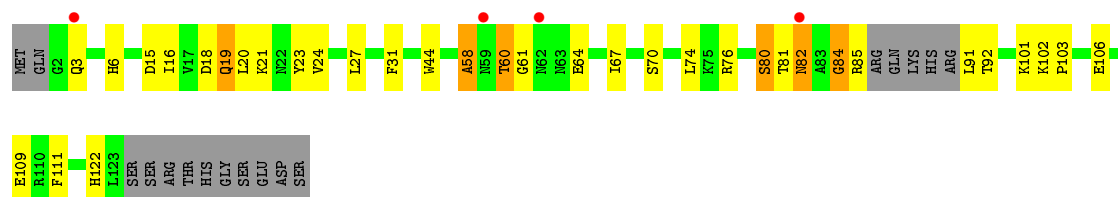




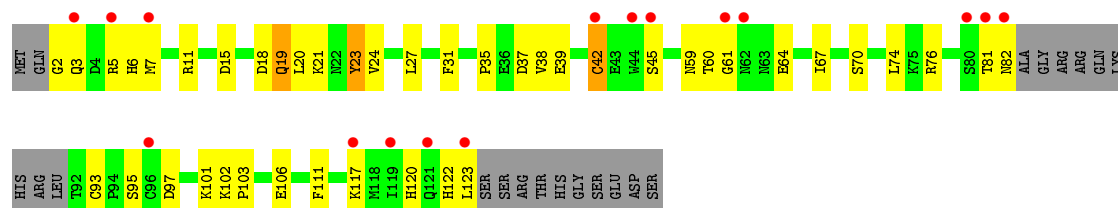
• Molecule 2: Interleukin-21



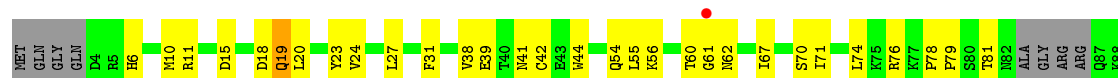
• Molecule 2: Interleukin-21



• Molecule 2: Interleukin-21



• Molecule 2: Interleukin-21

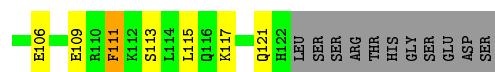




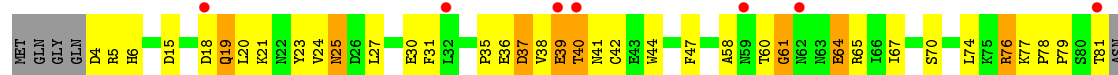
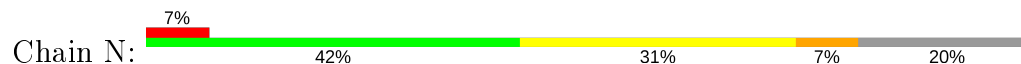
• Molecule 2: Interleukin-21



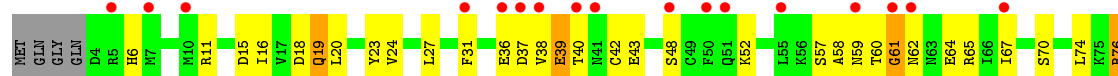
• Molecule 2: Interleukin-21



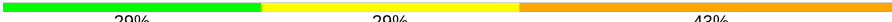
• Molecule 2: Interleukin-21

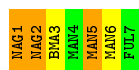


• Molecule 2: Interleukin-21



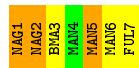
• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  29% 29% 43%



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

Chain R:  14% 43% 43%

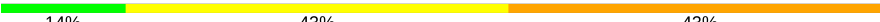


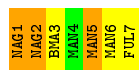
- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  14% 43% 43%



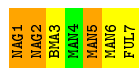
- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  14% 43% 43%



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

Chain U:  14% 43% 43%



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

Chain V:  17% 17% 67%



- Molecule 4: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[β -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  17% 17% 67%



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

Chain W:  17% 83%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.23Å 151.12Å 364.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.22 – 2.80 80.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (80.22-2.80) 99.7 (80.22-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.242 , 0.273 0.242 , 0.270	Depositor DCC
R_{free} test set	5633 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21830	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.03% 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: NI, BMA, NAG, FUC, FUL, MAN, SO4

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	0.70	1/1737 (0.1%)	0.62	3/2367 (0.1%)
1	C	0.85	7/1746 (0.4%)	0.68	3/2379 (0.1%)
1	E	0.57	2/1731 (0.1%)	0.64	2/2359 (0.1%)
1	G	0.65	4/1746 (0.2%)	0.64	4/2379 (0.2%)
1	I	0.41	1/1746 (0.1%)	0.58	4/2379 (0.2%)
1	K	0.61	1/1746 (0.1%)	0.64	6/2379 (0.3%)
1	M	0.38	0/1737	0.59	2/2367 (0.1%)
1	O	0.40	2/1737 (0.1%)	0.62	1/2367 (0.0%)
2	B	0.47	0/963	0.49	0/1294
2	D	0.53	0/969	0.62	1/1302 (0.1%)
2	F	0.85	6/941 (0.6%)	0.58	0/1265
2	H	0.30	0/976	0.45	0/1311
2	J	0.46	0/958	0.54	1/1288 (0.1%)
2	L	0.29	0/920	0.45	0/1237
2	N	0.44	0/892	0.55	1/1199 (0.1%)
2	P	0.48	0/920	0.62	1/1237 (0.1%)
All	All	0.56	24/21465 (0.1%)	0.60	29/29109 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	K	0	1
1	O	0	1
2	D	0	2
2	N	0	1
2	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	8

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	42	CYS	CB-SG	-10.35	1.64	1.82
2	F	23	TYR	CD1-CE1	-7.96	1.27	1.39
1	C	191	TYR	CD2-CE2	-7.56	1.28	1.39
2	F	23	TYR	CD2-CE2	-7.16	1.28	1.39
1	C	10	TYR	CE1-CZ	-6.90	1.29	1.38

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	10	TYR	CA-CB-CG	7.84	128.30	113.40
1	K	11	LEU	CA-CB-CG	7.80	133.25	115.30
1	C	10	TYR	CA-CB-CG	6.72	126.16	113.40
1	E	10	TYR	CA-CB-CG	6.70	126.13	113.40
1	G	10	TYR	N-CA-CB	-6.51	98.88	110.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	THR	Peptide
1	C	172	ARG	Peptide
2	D	58	ALA	Peptide
2	D	60	THR	Peptide
1	K	13	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1582	56	0
1	C	1696	0	1588	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1681	0	1575	98	0
1	G	1696	0	1590	74	0
1	I	1696	0	1590	69	0
1	K	1696	0	1590	51	0
1	M	1687	0	1584	124	1
1	O	1687	0	1584	87	0
2	B	944	0	952	30	0
2	D	951	0	959	57	0
2	F	923	0	926	45	0
2	H	957	0	968	38	0
2	J	940	0	944	23	0
2	L	902	0	910	24	0
2	N	875	0	884	54	1
2	P	902	0	910	63	0
3	Q	82	0	71	20	0
3	R	82	0	71	19	0
3	S	82	0	71	14	0
3	T	82	0	71	20	0
3	U	82	0	71	21	0
4	V	71	0	61	11	0
4	X	71	0	61	8	0
5	W	71	0	62	19	0
6	A	11	0	10	7	0
6	C	11	0	10	0	0
6	E	11	0	10	0	0
6	G	11	0	10	1	0
6	I	11	0	10	4	0
6	K	11	0	10	0	0
6	M	11	0	10	0	0
6	O	11	0	10	1	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	O	1	0	0	0	0
8	A	20	0	0	0	0
8	C	30	0	0	1	0
8	E	20	0	0	0	0
8	G	20	0	0	0	0
8	H	10	0	0	0	0
8	I	20	0	0	0	0
8	K	25	0	0	1	0
8	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	20	0	0	0	0
8	O	25	0	0	0	0
All	All	21830	0	20755	1041	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 1041 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:I:195:TRP:CD1	6:I:301:MAN:C1	1.77	1.64
1:E:172:ARG:HB3	1:E:173:LYS:CG	1.30	1.55
1:E:172:ARG:HD3	1:E:173:LYS:CE	1.39	1.52
1:I:195:TRP:HD1	6:I:301:MAN:C1	0.90	1.51
1:M:54:ASN:HD21	5:W:1:NAG:C1	1.24	1.49

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:156:LEU:O	2:N:39:GLU:CG[4_455]	2.07	0.13

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	206/219 (94%)	202 (98%)	4 (2%)	0	100	100
1	C	207/219 (94%)	198 (96%)	9 (4%)	0	100	100
1	E	205/219 (94%)	200 (98%)	5 (2%)	0	100	100
1	G	207/219 (94%)	199 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	207/219 (94%)	199 (96%)	7 (3%)	1 (0%)	29	61
1	K	207/219 (94%)	197 (95%)	10 (5%)	0	100	100
1	M	206/219 (94%)	197 (96%)	8 (4%)	1 (0%)	29	61
1	O	206/219 (94%)	196 (95%)	10 (5%)	0	100	100
2	B	111/134 (83%)	107 (96%)	3 (3%)	1 (1%)	17	46
2	D	113/134 (84%)	109 (96%)	3 (3%)	1 (1%)	17	46
2	F	109/134 (81%)	102 (94%)	6 (6%)	1 (1%)	17	46
2	H	112/134 (84%)	107 (96%)	4 (4%)	1 (1%)	17	46
2	J	112/134 (84%)	108 (96%)	4 (4%)	0	100	100
2	L	106/134 (79%)	99 (93%)	6 (6%)	1 (1%)	17	46
2	N	103/134 (77%)	96 (93%)	5 (5%)	2 (2%)	8	26
2	P	106/134 (79%)	97 (92%)	9 (8%)	0	100	100
All	All	2523/2824 (89%)	2413 (96%)	101 (4%)	9 (0%)	34	66

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	84	GLY
2	L	40	THR
1	M	170	GLU
2	H	62	ASN
1	I	159	VAL

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	190/201 (94%)	187 (98%)	3 (2%)	62	88
1	C	191/201 (95%)	188 (98%)	3 (2%)	62	88
1	E	189/201 (94%)	185 (98%)	4 (2%)	53	84
1	G	191/201 (95%)	184 (96%)	7 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	191/201 (95%)	183 (96%)	8 (4%)	30	63
1	K	191/201 (95%)	188 (98%)	3 (2%)	62	88
1	M	190/201 (94%)	187 (98%)	3 (2%)	62	88
1	O	190/201 (94%)	186 (98%)	4 (2%)	53	84
2	B	109/125 (87%)	107 (98%)	2 (2%)	59	86
2	D	109/125 (87%)	106 (97%)	3 (3%)	43	77
2	F	107/125 (86%)	105 (98%)	2 (2%)	57	85
2	H	111/125 (89%)	107 (96%)	4 (4%)	35	69
2	J	109/125 (87%)	107 (98%)	2 (2%)	59	86
2	L	105/125 (84%)	102 (97%)	3 (3%)	42	76
2	N	102/125 (82%)	93 (91%)	9 (9%)	10	29
2	P	105/125 (84%)	102 (97%)	3 (3%)	42	76
All	All	2380/2608 (91%)	2317 (97%)	63 (3%)	46	79

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	10	TYR
1	I	194	THR
1	O	150	VAL
1	I	81	ASP
1	I	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	57	HIS
2	H	62	ASN
2	N	19	GLN
1	G	136	GLN
2	H	19	GLN

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 ⓘ

53 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	Q	1	3	14,14,15	0.51	0	17,19,21	1.20	2 (11%)
3	NAG	Q	2	3	14,14,15	0.54	0	17,19,21	1.38	4 (23%)
3	BMA	Q	3	3	11,11,12	0.28	0	15,15,17	0.63	0
3	MAN	Q	4	3	11,11,12	0.64	0	15,15,17	0.94	0
3	MAN	Q	5	3	11,11,12	0.67	0	15,15,17	1.87	4 (26%)
3	MAN	Q	6	3	11,11,12	0.57	0	15,15,17	0.71	0
3	FUL	Q	7	3	10,10,11	0.27	0	14,14,16	0.63	0
3	NAG	R	1	3	14,14,15	0.51	0	17,19,21	1.20	2 (11%)
3	NAG	R	2	3	14,14,15	0.53	0	17,19,21	1.38	4 (23%)
3	BMA	R	3	3	11,11,12	0.27	0	15,15,17	0.62	0
3	MAN	R	4	3	11,11,12	0.64	0	15,15,17	0.94	0
3	MAN	R	5	3	11,11,12	0.66	0	15,15,17	1.87	4 (26%)
3	MAN	R	6	3	11,11,12	0.57	0	15,15,17	0.71	0
3	FUL	R	7	3	10,10,11	0.29	0	14,14,16	0.62	0
3	NAG	S	1	1,3	14,14,15	0.51	0	17,19,21	1.19	2 (11%)
3	NAG	S	2	3	14,14,15	0.54	0	17,19,21	1.38	4 (23%)
3	BMA	S	3	3	11,11,12	0.29	0	15,15,17	0.63	0
3	MAN	S	4	3	11,11,12	0.65	0	15,15,17	0.94	0
3	MAN	S	5	3	11,11,12	0.67	0	15,15,17	1.87	4 (26%)
3	MAN	S	6	3	11,11,12	0.57	0	15,15,17	0.70	0
3	FUL	S	7	3	10,10,11	0.59	0	14,14,16	1.48	2 (14%)
3	NAG	T	1	3	14,14,15	0.50	0	17,19,21	1.19	2 (11%)
3	NAG	T	2	3	14,14,15	0.54	0	17,19,21	1.37	4 (23%)
3	BMA	T	3	3	11,11,12	0.28	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	T	4	3	11,11,12	0.64	0	15,15,17	0.94	0
3	MAN	T	5	3	11,11,12	0.67	0	15,15,17	1.87	4 (26%)
3	MAN	T	6	3	11,11,12	0.58	0	15,15,17	0.71	0
3	FUL	T	7	3	10,10,11	0.28	0	14,14,16	0.62	0
3	NAG	U	1	3	14,14,15	0.50	0	17,19,21	1.19	2 (11%)
3	NAG	U	2	3	14,14,15	0.55	0	17,19,21	1.37	4 (23%)
3	BMA	U	3	3	11,11,12	0.28	0	15,15,17	0.63	0
3	MAN	U	4	3	11,11,12	0.64	0	15,15,17	0.95	0
3	MAN	U	5	3	11,11,12	0.67	0	15,15,17	1.87	4 (26%)
3	MAN	U	6	3	11,11,12	0.58	0	15,15,17	0.70	0
3	FUL	U	7	3	10,10,11	0.30	0	14,14,16	0.62	0
4	NAG	V	1	4	14,14,15	0.61	0	17,19,21	1.20	2 (11%)
4	NAG	V	2	4	14,14,15	0.50	0	17,19,21	1.52	4 (23%)
4	BMA	V	3	4	11,11,12	0.27	0	15,15,17	0.65	0
4	MAN	V	4	4	11,11,12	0.65	0	15,15,17	0.83	1 (6%)
4	MAN	V	5	4	11,11,12	0.69	0	15,15,17	2.55	5 (33%)
4	FUL	V	6	4	10,10,11	0.29	0	14,14,16	0.63	0
5	NAG	W	1	5	14,14,15	0.54	0	17,19,21	1.08	2 (11%)
5	NAG	W	2	5	14,14,15	0.59	0	17,19,21	1.50	5 (29%)
5	BMA	W	3	5	11,11,12	0.27	0	15,15,17	0.65	0
5	MAN	W	4	5	11,11,12	0.68	0	15,15,17	1.03	1 (6%)
5	MAN	W	5	5	11,11,12	0.59	0	15,15,17	2.70	4 (26%)
5	FUC	W	6	5	10,10,11	0.88	0	14,14,16	3.12	8 (57%)
4	NAG	X	1	4	14,14,15	0.54	0	17,19,21	1.17	3 (17%)
4	NAG	X	2	4	14,14,15	0.56	0	17,19,21	1.44	2 (11%)
4	BMA	X	3	4	11,11,12	0.26	0	15,15,17	0.64	0
4	MAN	X	4	4	11,11,12	0.68	0	15,15,17	1.00	1 (6%)
4	MAN	X	5	4	11,11,12	0.62	0	15,15,17	2.17	3 (20%)
4	FUL	X	6	4	10,10,11	0.29	0	14,14,16	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	2/2/19/22	1/1/1/1
3	MAN	Q	5	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	6	3	-	0/2/19/22	0/1/1/1
3	FUL	Q	7	3	-	-	0/1/1/1
3	NAG	R	1	3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	BMA	R	3	3	-	2/2/19/22	0/1/1/1
3	MAN	R	4	3	-	2/2/19/22	1/1/1/1
3	MAN	R	5	3	-	1/2/19/22	0/1/1/1
3	MAN	R	6	3	-	0/2/19/22	0/1/1/1
3	FUL	R	7	3	-	-	0/1/1/1
3	NAG	S	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
3	MAN	S	4	3	-	2/2/19/22	1/1/1/1
3	MAN	S	5	3	-	1/2/19/22	0/1/1/1
3	MAN	S	6	3	-	0/2/19/22	0/1/1/1
3	FUL	S	7	3	-	-	0/1/1/1
3	NAG	T	1	3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	BMA	T	3	3	-	2/2/19/22	0/1/1/1
3	MAN	T	4	3	-	2/2/19/22	1/1/1/1
3	MAN	T	5	3	-	1/2/19/22	0/1/1/1
3	MAN	T	6	3	-	0/2/19/22	0/1/1/1
3	FUL	T	7	3	-	-	0/1/1/1
3	NAG	U	1	3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	MAN	U	4	3	-	2/2/19/22	1/1/1/1
3	MAN	U	5	3	-	1/2/19/22	0/1/1/1
3	MAN	U	6	3	-	0/2/19/22	0/1/1/1
3	FUL	U	7	3	-	-	0/1/1/1
4	NAG	V	1	4	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	3/6/23/26	0/1/1/1
4	BMA	V	3	4	-	2/2/19/22	0/1/1/1
4	MAN	V	4	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	V	5	4	-	1/2/19/22	0/1/1/1
4	FUL	V	6	4	-	-	0/1/1/1
5	NAG	W	1	5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	1/1/1/1
5	MAN	W	5	5	-	1/2/19/22	0/1/1/1
5	FUC	W	6	5	-	-	0/1/1/1
4	NAG	X	1	4	-	3/6/23/26	0/1/1/1
4	NAG	X	2	4	-	3/6/23/26	0/1/1/1
4	BMA	X	3	4	-	2/2/19/22	0/1/1/1
4	MAN	X	4	4	-	2/2/19/22	0/1/1/1
4	MAN	X	5	4	-	2/2/19/22	0/1/1/1
4	FUL	X	6	4	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	6	FUC	C1-C2-C3	7.49	118.88	109.67
4	X	5	MAN	C1-O5-C5	6.30	120.73	112.19
5	W	5	MAN	C1-C2-C3	6.16	117.24	109.67
4	V	5	MAN	C1-C2-C3	5.97	117.00	109.67
5	W	5	MAN	C1-O5-C5	5.94	120.25	112.19

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	2	NAG	C8-C7-N2-C2
4	X	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2

5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	W	4	MAN	C1-C2-C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
3	U	4	MAN	C1-C2-C3-C4-C5-O5
3	T	4	MAN	C1-C2-C3-C4-C5-O5
3	S	4	MAN	C1-C2-C3-C4-C5-O5
3	Q	4	MAN	C1-C2-C3-C4-C5-O5

44 monomers are involved in 132 short contacts:

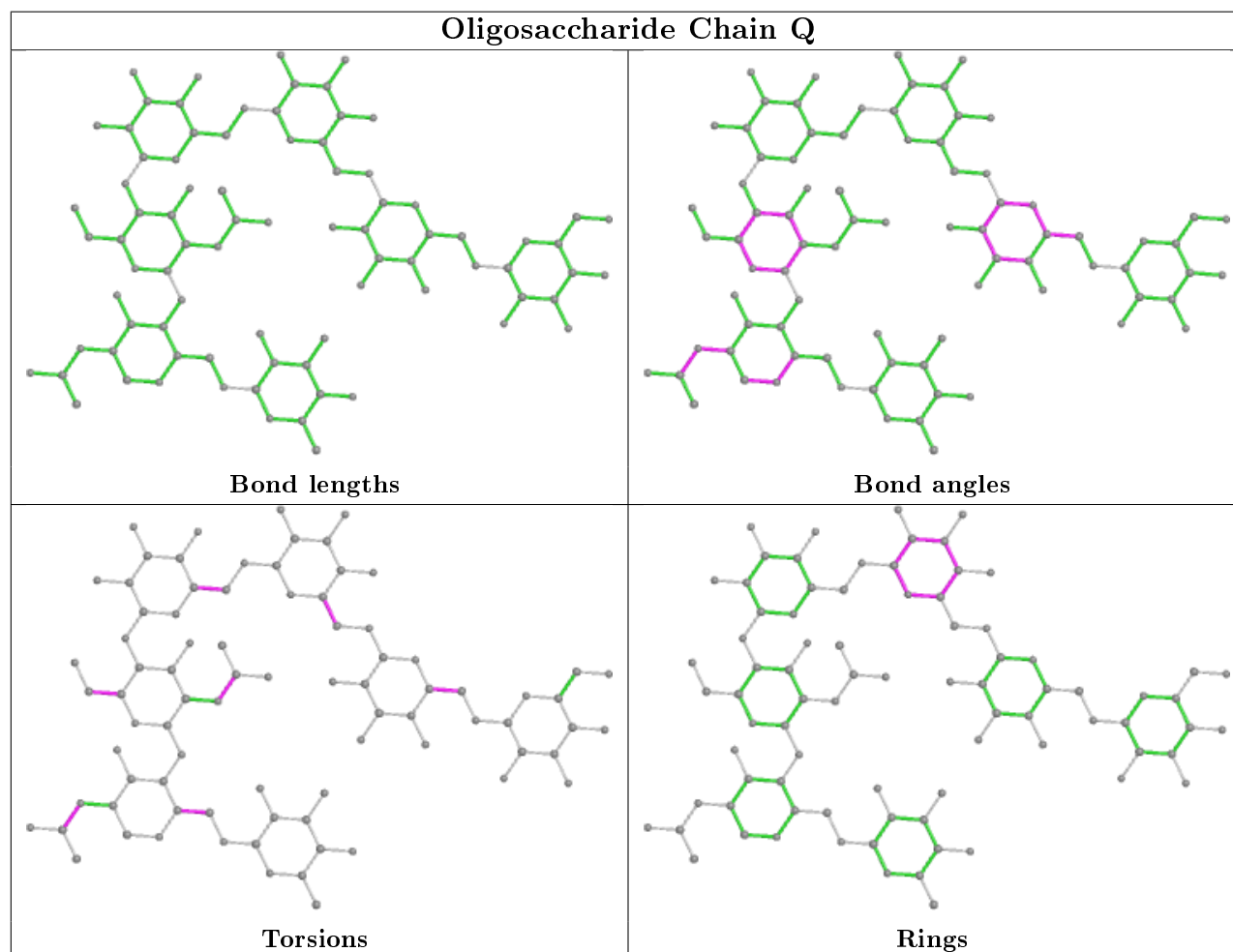
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	2	NAG	8	0
3	Q	3	BMA	6	0
4	X	3	BMA	2	0
3	S	1	NAG	1	0
3	R	7	FUL	4	0
3	R	6	MAN	1	0
4	V	5	MAN	2	0
3	T	2	NAG	11	0
4	X	4	MAN	1	0
4	V	4	MAN	1	0
3	T	3	BMA	9	0
3	S	3	BMA	9	0
3	R	3	BMA	7	0
3	U	3	BMA	8	0
3	U	7	FUL	4	0
3	Q	5	MAN	8	0
3	T	6	MAN	1	0
4	V	1	NAG	4	0
3	Q	6	MAN	1	0
3	S	6	MAN	1	0
3	T	5	MAN	3	0
4	X	5	MAN	1	0
4	V	2	NAG	5	0
5	W	1	NAG	6	0
3	R	1	NAG	8	0
4	X	1	NAG	5	0
3	S	5	MAN	4	0
5	W	2	NAG	8	0
4	X	2	NAG	4	0
3	U	6	MAN	3	0
4	V	3	BMA	5	0
3	R	5	MAN	4	0
5	W	3	BMA	8	0
3	Q	1	NAG	6	0
5	W	5	MAN	4	0

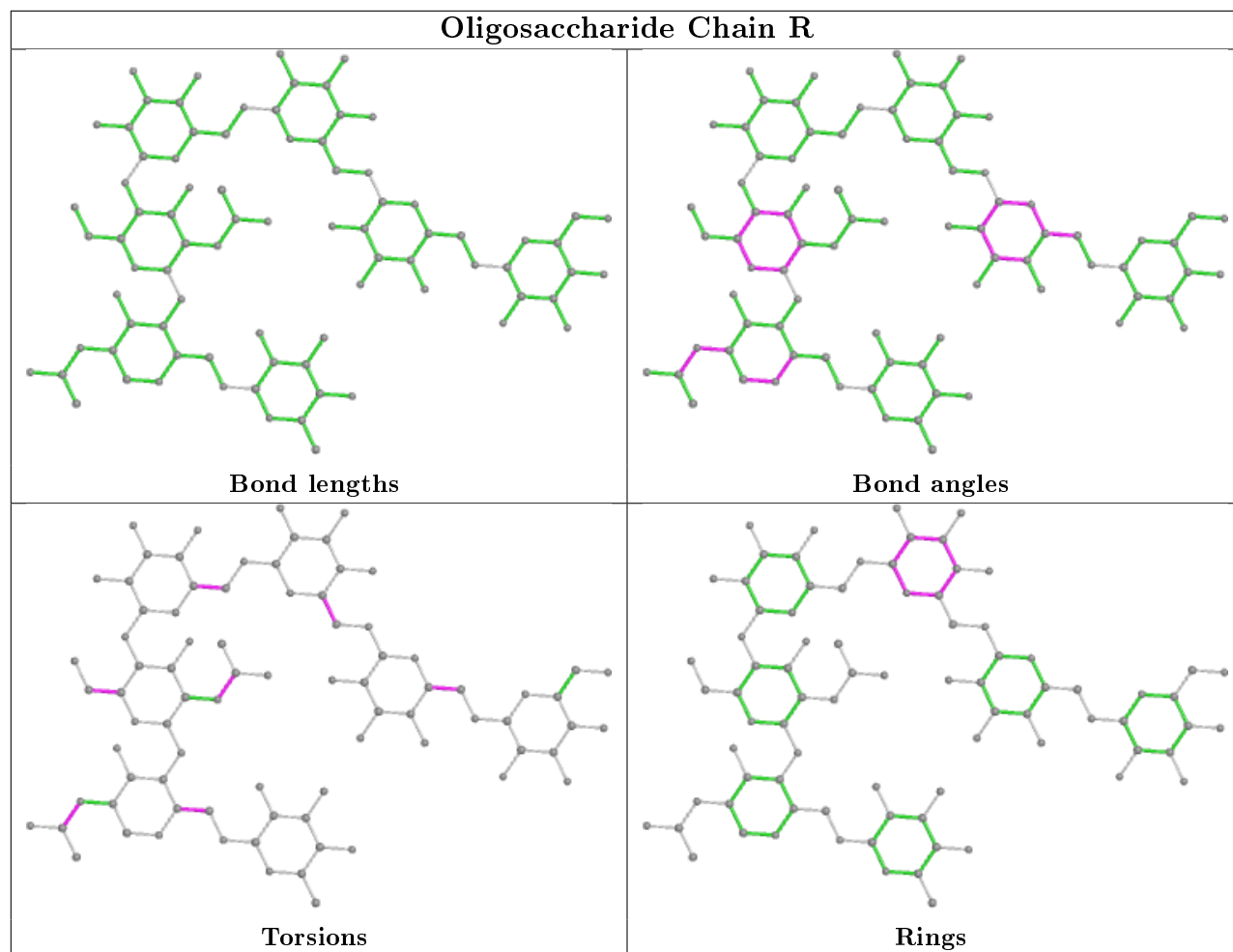
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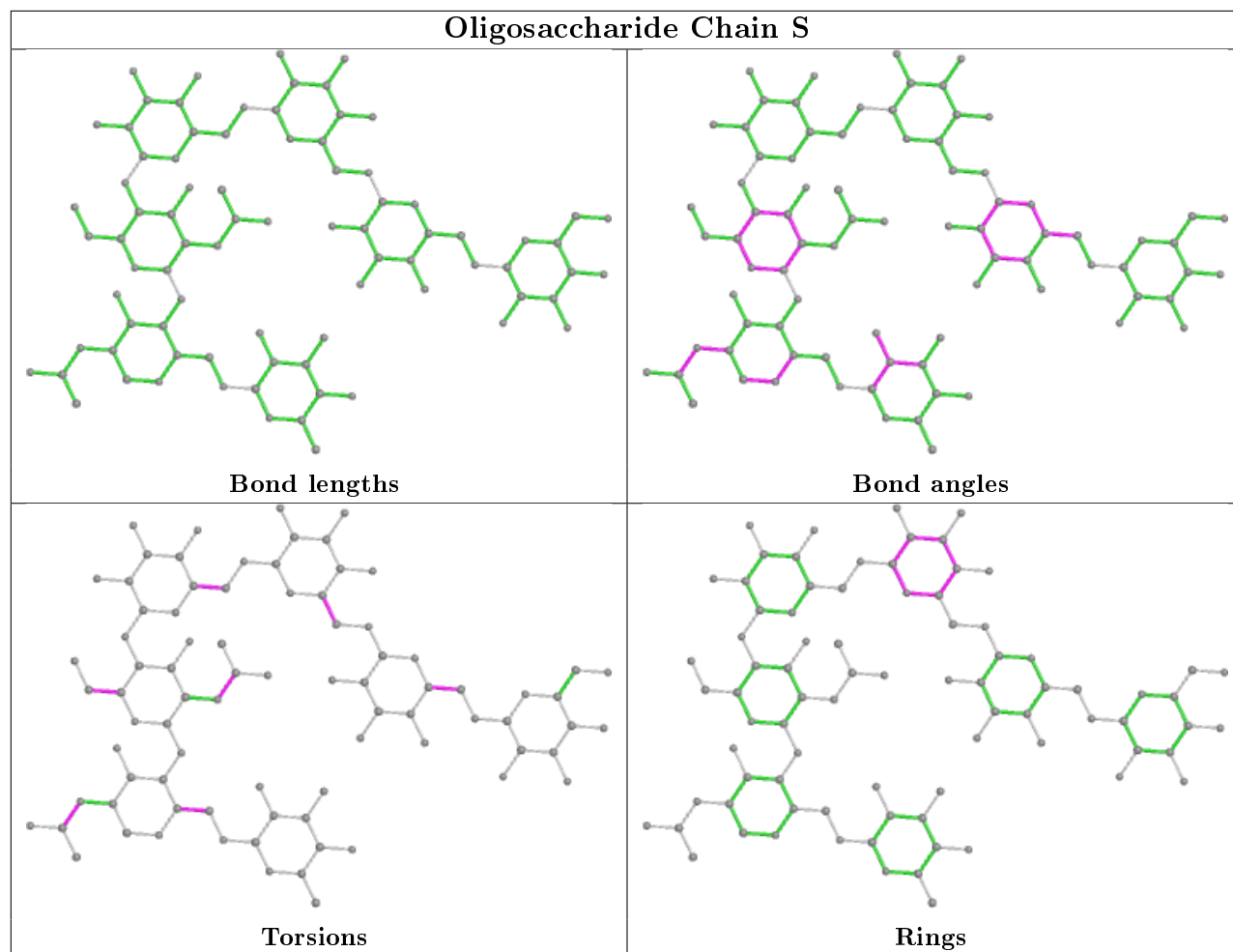
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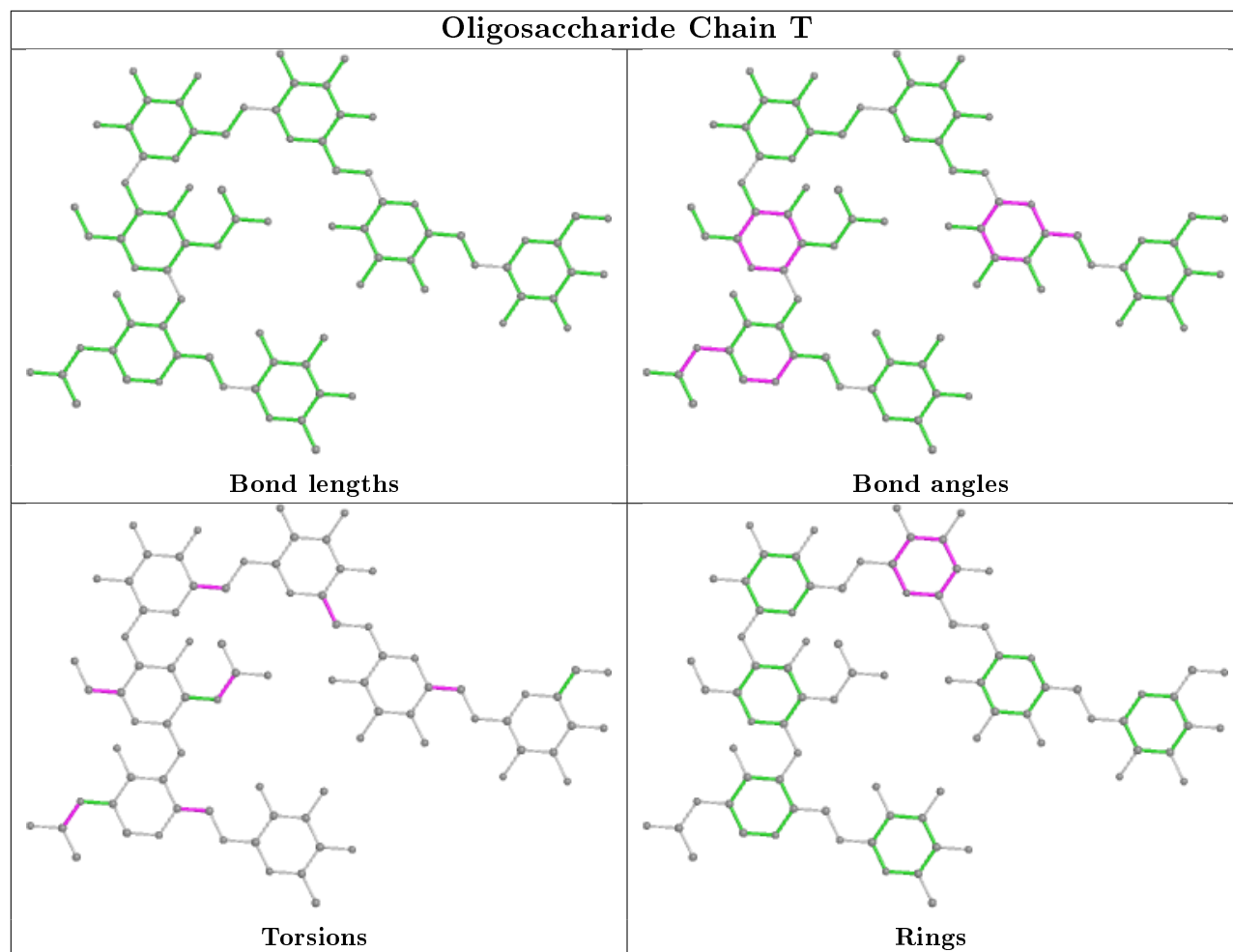
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	2	NAG	11	0
5	W	6	FUC	1	0
3	R	2	NAG	9	0
5	W	4	MAN	3	0
3	T	1	NAG	8	0
3	T	7	FUL	4	0
3	U	1	NAG	9	0
3	S	2	NAG	10	0
3	U	5	MAN	1	0

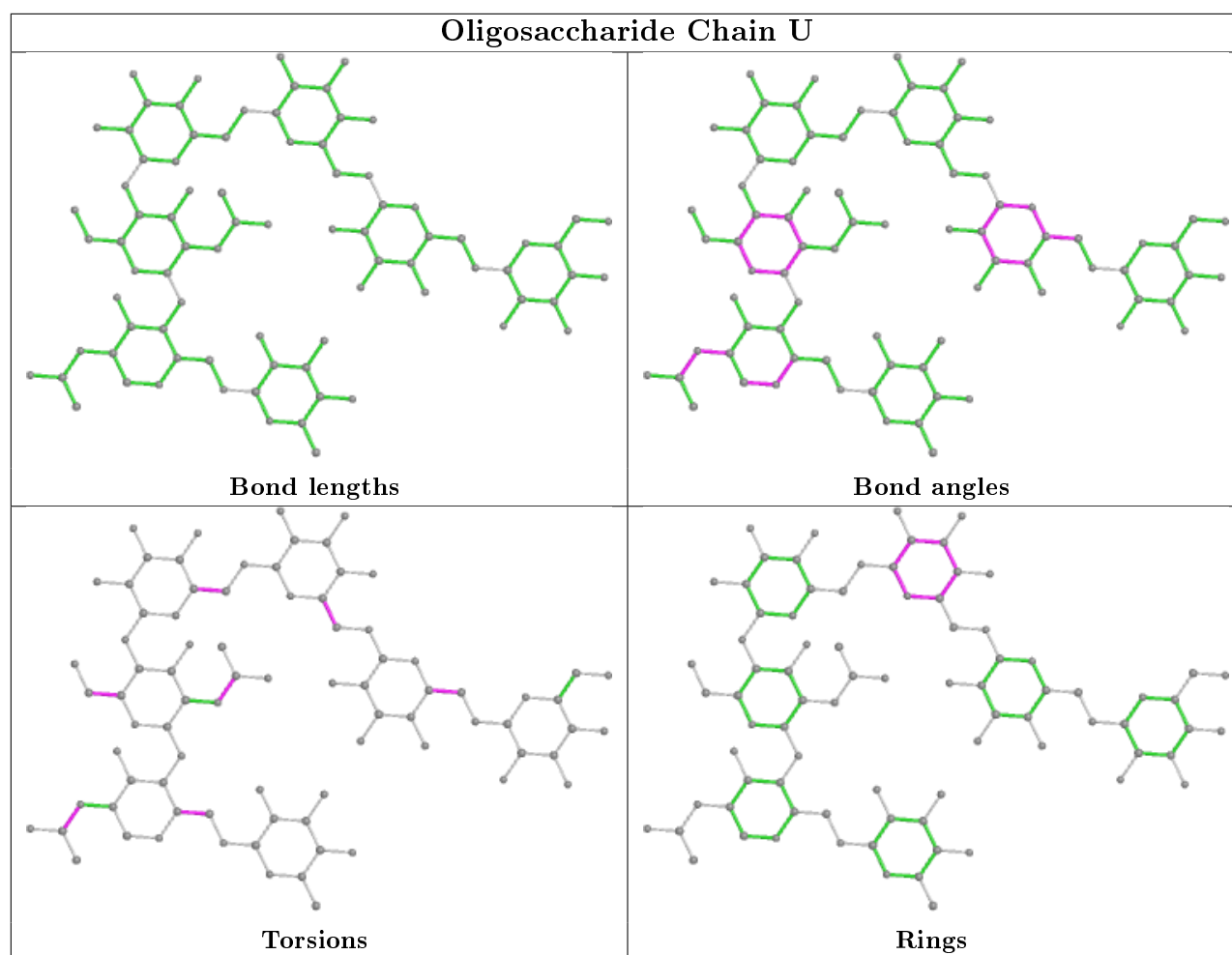
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

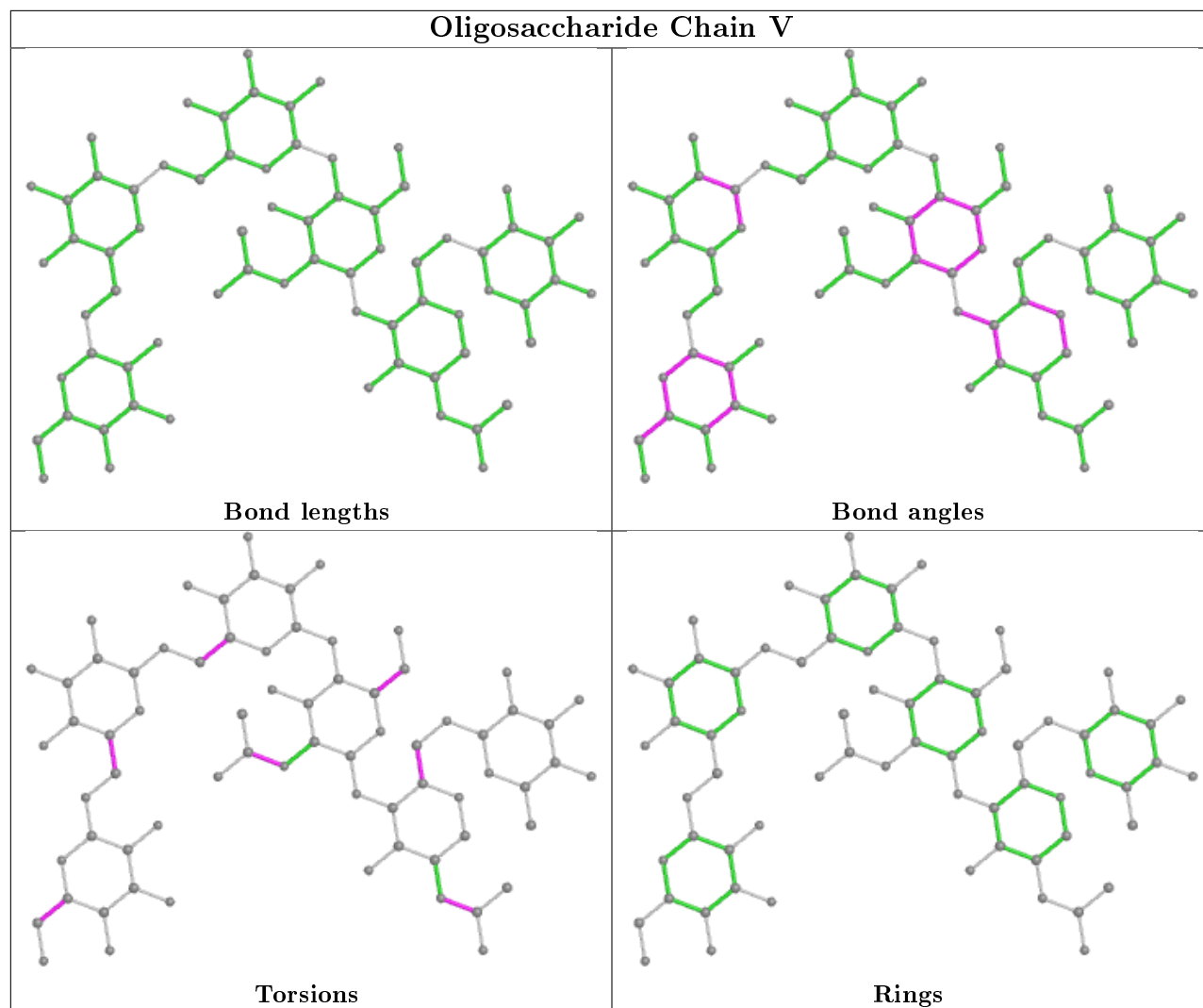


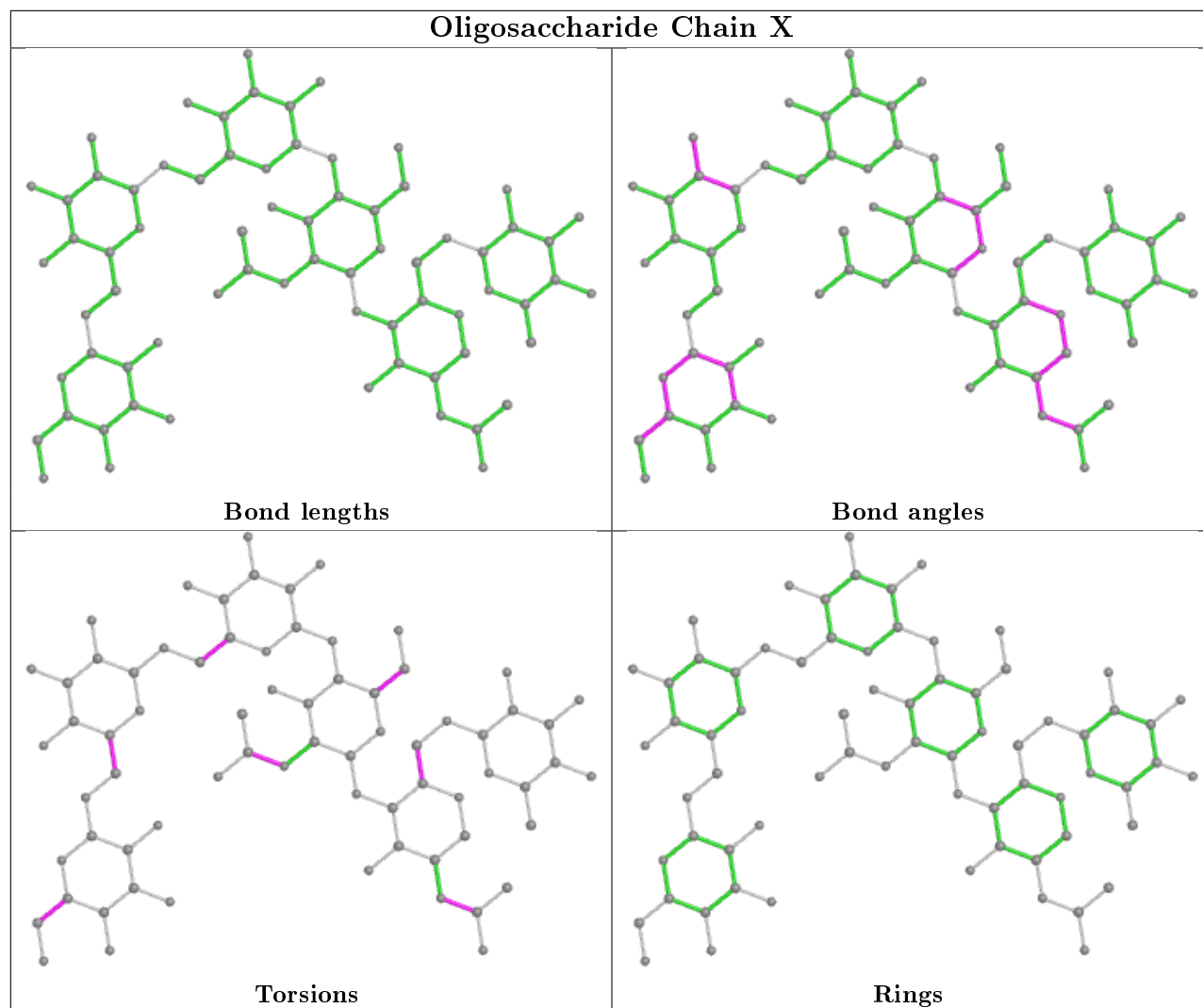


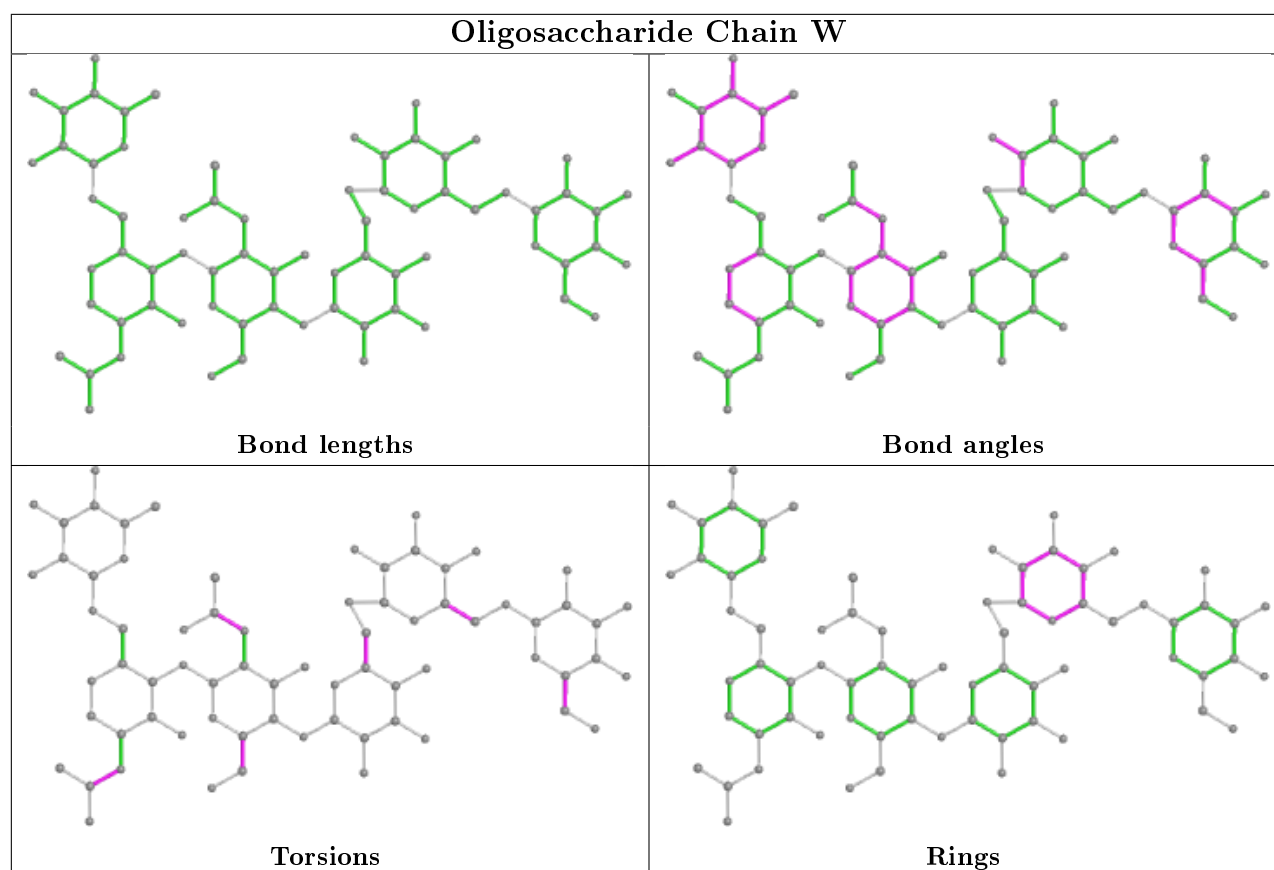












5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 4 are monoatomic - leaving 47 for Mogul analysis.

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	$\# Z > 2$
8	SO4	G	306	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	M	306	-	4,4,4	0.15	0	6,6,6	0.04	0
8	SO4	O	312	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	K	304	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	K	309	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	E	312	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	I	304	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	H	201	-	4,4,4	0.14	0	6,6,6	0.05	0
6	MAN	K	302	-	11,11,12	0.99	1 (9%)	15,15,17	2.11	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	L	201	-	4,4,4	0.15	0	6,6,6	0.05	0
8	SO4	E	313	-	4,4,4	0.14	0	6,6,6	0.04	0
6	MAN	I	301	-	11,11,12	0.80	0	15,15,17	2.05	4 (26%)
8	SO4	G	303	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	G	304	-	4,4,4	0.13	0	6,6,6	0.05	0
8	SO4	E	310	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	K	306	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	M	305	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	302	-	4,4,4	0.12	0	6,6,6	0.05	0
8	SO4	I	302	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	O	313	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	G	305	-	4,4,4	0.13	0	6,6,6	0.06	0
6	MAN	A	301	-	11,11,12	0.97	1 (9%)	15,15,17	2.19	4 (26%)
8	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	MAN	G	301	-	11,11,12	0.91	1 (9%)	15,15,17	2.18	4 (26%)
8	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.04	0
6	MAN	M	304	-	11,11,12	0.85	1 (9%)	15,15,17	1.84	5 (33%)
8	SO4	O	311	-	4,4,4	0.14	0	6,6,6	0.05	0
6	MAN	C	307	-	11,11,12	0.74	0	15,15,17	1.97	4 (26%)
8	SO4	C	306	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	M	307	-	4,4,4	0.15	0	6,6,6	0.05	0
6	MAN	O	307	-	11,11,12	0.82	0	15,15,17	2.00	4 (26%)
6	MAN	E	302	-	11,11,12	0.74	0	15,15,17	1.97	4 (26%)
8	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	I	303	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	O	310	-	4,4,4	0.20	0	6,6,6	0.33	0
8	SO4	K	303	-	4,4,4	0.20	0	6,6,6	0.17	0
8	SO4	A	306	-	4,4,4	0.13	0	6,6,6	0.05	0
8	SO4	I	305	-	4,4,4	0.14	0	6,6,6	0.04	0
8	SO4	K	305	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	M	309	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	O	309	-	4,4,4	0.24	0	6,6,6	0.20	0
8	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	H	202	-	4,4,4	0.21	0	6,6,6	0.32	0
8	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	E	311	-	4,4,4	0.14	0	6,6,6	0.05	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
6	MAN	C	307	-	-	2/2/19/22	0/1/1/1
6	MAN	O	307	-	-	2/2/19/22	0/1/1/1
6	MAN	E	302	-	-	2/2/19/22	0/1/1/1
6	MAN	K	302	-	-	2/2/19/22	0/1/1/1
6	MAN	A	301	-	-	2/2/19/22	0/1/1/1
6	MAN	G	301	-	-	2/2/19/22	0/1/1/1
6	MAN	I	301	-	-	2/2/19/22	0/1/1/1
6	MAN	M	304	-	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	302	MAN	O5-C1	-2.25	1.40	1.43
6	A	301	MAN	O5-C1	-2.25	1.40	1.43
6	M	304	MAN	O5-C1	-2.20	1.40	1.43
6	G	301	MAN	O5-C1	-2.09	1.40	1.43

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	301	MAN	O5-C1-C2	-4.92	103.17	110.77
6	G	301	MAN	C1-C2-C3	-4.72	103.86	109.67
6	A	301	MAN	O5-C1-C2	-4.65	103.59	110.77
6	K	302	MAN	O5-C1-C2	-4.63	103.62	110.77
6	E	302	MAN	O5-C1-C2	-4.43	103.93	110.77

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	301	MAN	O5-C5-C6-O6
6	I	301	MAN	O5-C5-C6-O6
6	A	301	MAN	O5-C5-C6-O6
6	G	301	MAN	C4-C5-C6-O6
6	M	304	MAN	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	301	MAN	4	0
8	K	306	SO4	1	0
6	A	301	MAN	7	0
6	G	301	MAN	1	0
6	O	307	MAN	1	0
8	C	305	SO4	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	208/219 (94%)	0.32	0 100 100	23, 45, 83, 109	0
1	C	209/219 (95%)	0.34	1 (0%) 91 88	23, 47, 86, 179	0
1	E	207/219 (94%)	0.54	11 (5%) 26 17	41, 69, 128, 160	0
1	G	209/219 (95%)	0.50	7 (3%) 46 36	17, 45, 92, 146	0
1	I	209/219 (95%)	0.56	12 (5%) 23 15	33, 66, 134, 171	0
1	K	209/219 (95%)	0.46	5 (2%) 59 49	25, 46, 88, 189	0
1	M	208/219 (94%)	0.60	10 (4%) 30 21	36, 67, 135, 153	0
1	O	208/219 (94%)	0.86	26 (12%) 3 2	34, 69, 142, 194	0
2	B	115/134 (85%)	0.60	9 (7%) 13 7	35, 68, 135, 151	0
2	D	117/134 (87%)	0.51	4 (3%) 45 35	31, 63, 135, 169	0
2	F	113/134 (84%)	0.89	16 (14%) 2 1	43, 80, 138, 189	0
2	H	116/134 (86%)	0.37	2 (1%) 70 63	28, 50, 102, 125	0
2	J	116/134 (86%)	0.44	5 (4%) 35 25	34, 60, 112, 140	0
2	L	110/134 (82%)	0.67	3 (2%) 54 44	36, 79, 121, 143	0
2	N	107/134 (79%)	0.77	9 (8%) 11 5	26, 98, 148, 194	0
2	P	110/134 (82%)	1.34	29 (26%) 0 0	52, 97, 152, 172	0
All	All	2571/2824 (91%)	0.58	149 (5%) 23 15	17, 63, 132, 194	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	160	ASP	7.4
2	P	120	HIS	6.7
2	L	62	ASN	6.5
1	O	160	ASP	6.4
2	P	62	ASN	6.3

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	MAN	U	6	11/12	0.33	1.03	107,139,150,152	0
4	BMA	X	3	11/12	0.45	0.35	127,142,152,156	0
3	MAN	U	4	11/12	0.48	0.41	123,146,163,168	0
3	MAN	S	4	11/12	0.49	0.47	123,146,163,168	0
5	BMA	W	3	11/12	0.56	0.27	126,136,149,154	0
3	FUL	R	7	10/11	0.56	0.39	70,81,97,104	0
5	MAN	W	4	11/12	0.56	0.26	88,129,133,134	0
3	BMA	Q	3	11/12	0.57	0.22	128,140,152,153	0
3	MAN	T	6	11/12	0.58	0.46	107,139,150,152	0
3	FUL	U	7	10/11	0.59	0.39	70,81,97,104	0
3	FUL	Q	7	10/11	0.60	0.42	70,81,97,104	0
4	MAN	X	4	11/12	0.62	0.40	123,156,166,175	0
4	BMA	V	3	11/12	0.64	0.32	129,139,152,154	0
4	MAN	V	4	11/12	0.65	0.30	114,148,165,173	0
3	BMA	T	3	11/12	0.67	0.23	128,140,152,153	0
3	FUL	T	7	10/11	0.67	0.43	70,81,97,104	0
3	FUL	S	7	10/11	0.67	0.41	70,81,97,104	0
4	FUL	V	6	10/11	0.68	0.41	70,82,97,98	0
3	MAN	U	5	11/12	0.68	0.31	80,120,133,134	0
4	MAN	X	5	11/12	0.71	0.43	79,126,141,150	0
3	MAN	S	6	11/12	0.71	0.79	107,139,150,152	0
4	FUL	X	6	10/11	0.71	0.40	72,82,99,104	0
3	MAN	Q	4	11/12	0.71	0.21	123,146,163,168	0
3	MAN	R	4	11/12	0.72	0.20	123,146,163,168	0
3	MAN	Q	5	11/12	0.72	0.30	80,120,133,134	0
3	BMA	S	3	11/12	0.74	0.38	128,140,152,153	0
3	MAN	Q	6	11/12	0.75	0.41	107,139,150,152	0
3	BMA	U	3	11/12	0.77	0.26	128,140,152,153	0
3	MAN	T	5	11/12	0.79	0.33	80,120,133,134	0
3	BMA	R	3	11/12	0.79	0.16	128,140,152,153	0
3	MAN	S	5	11/12	0.80	0.28	80,120,133,134	0
3	MAN	R	5	11/12	0.81	0.35	80,120,133,134	0

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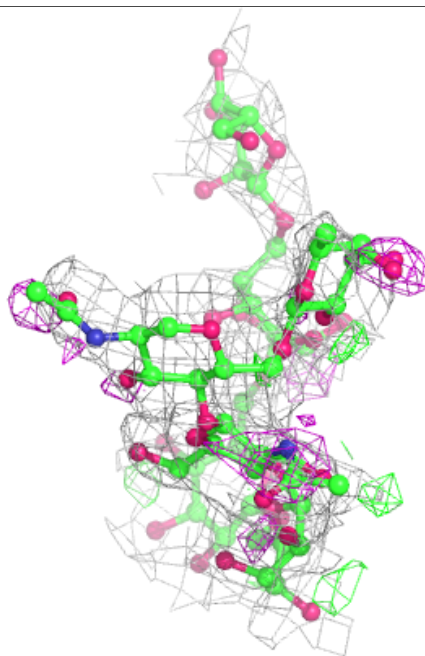
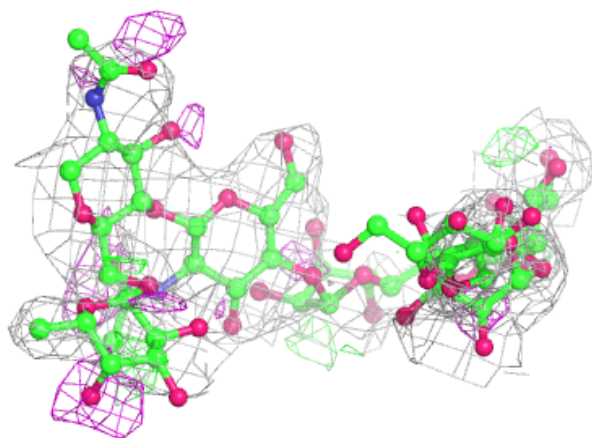
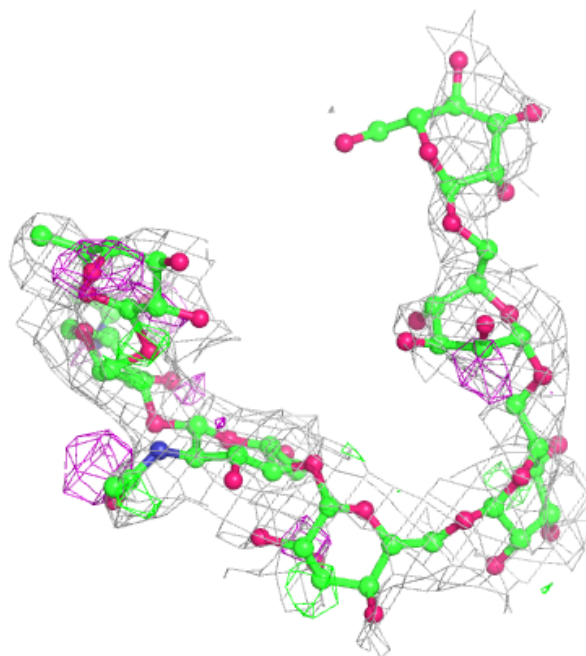
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	T	4	11/12	0.82	0.19	123,146,163,168	0
3	NAG	Q	2	14/15	0.83	0.25	52,84,107,117	0
3	MAN	R	6	11/12	0.83	0.57	107,139,150,152	0
5	MAN	W	5	11/12	0.83	0.34	76,111,132,133	0
4	NAG	V	1	14/15	0.86	0.18	37,48,56,73	0
4	NAG	V	2	14/15	0.86	0.21	55,87,106,122	0
3	NAG	U	2	14/15	0.87	0.19	52,84,107,117	0
4	MAN	V	5	11/12	0.87	0.36	49,96,120,121	0
5	FUC	W	6	10/11	0.88	0.38	73,85,99,102	0
3	NAG	R	2	14/15	0.88	0.17	52,84,107,117	0
3	NAG	U	1	14/15	0.88	0.16	46,54,61,76	0
3	NAG	S	2	14/15	0.88	0.18	52,84,107,117	0
3	NAG	T	2	14/15	0.88	0.22	52,84,107,117	0
3	NAG	T	1	14/15	0.89	0.22	46,54,61,76	0
4	NAG	X	2	14/15	0.89	0.18	54,90,111,120	0
3	NAG	Q	1	14/15	0.90	0.25	46,54,61,76	0
4	NAG	X	1	14/15	0.90	0.17	43,52,57,75	0
5	NAG	W	2	14/15	0.90	0.18	57,85,108,123	0
3	NAG	S	1	14/15	0.91	0.16	46,54,61,76	0
3	NAG	R	1	14/15	0.92	0.19	46,54,61,76	0
5	NAG	W	1	14/15	0.96	0.15	41,49,57,71	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.

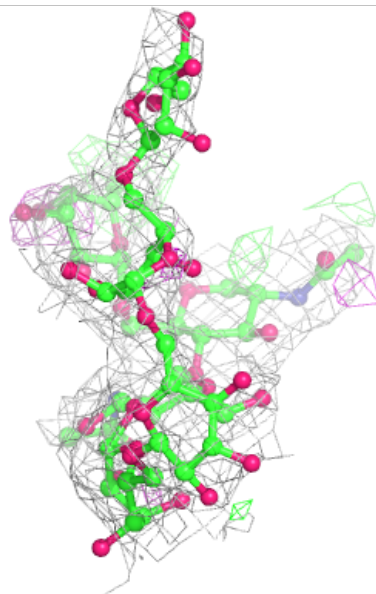
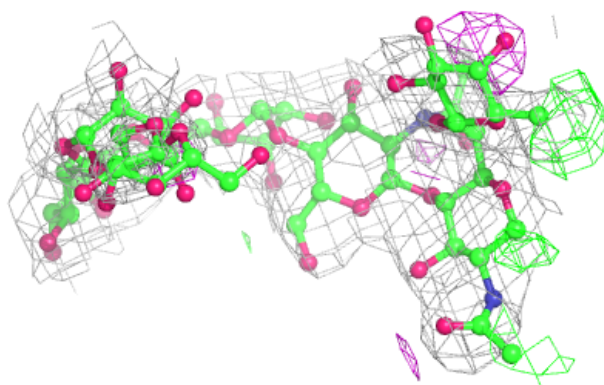
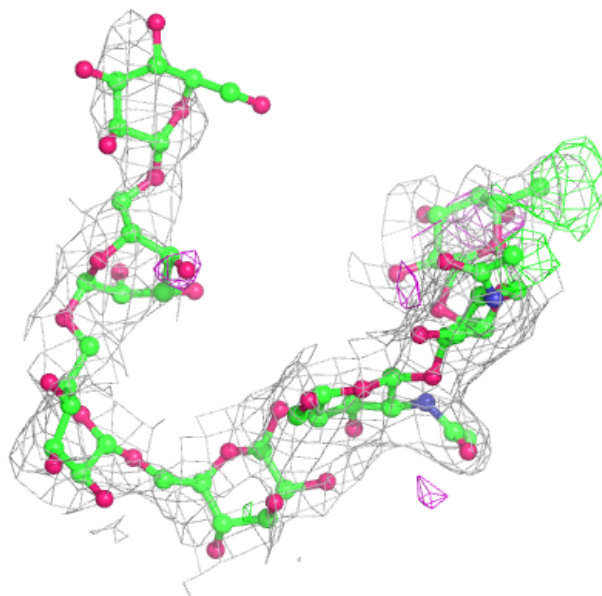
Electron density around Chain Q:

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



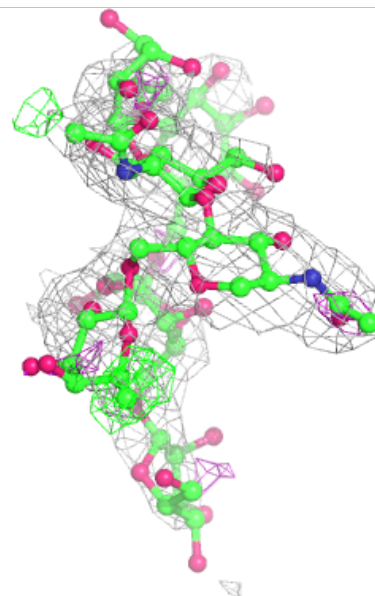
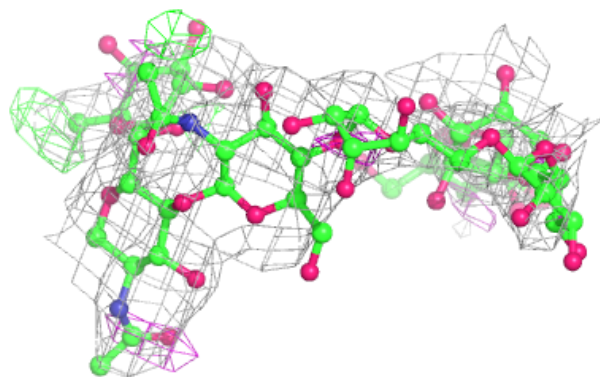
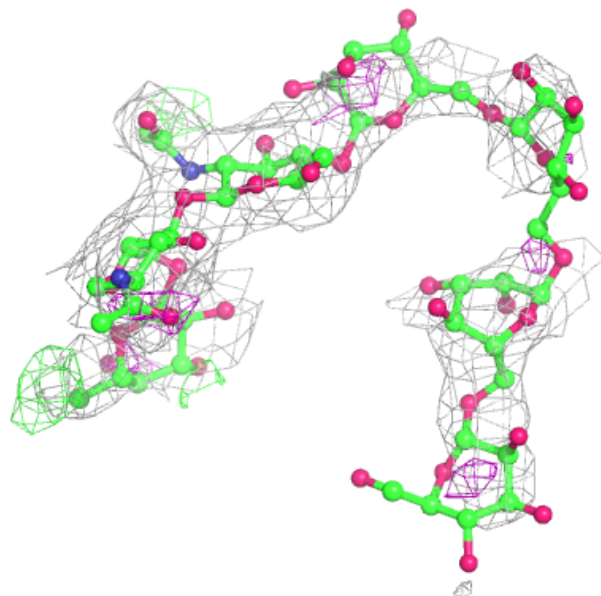
Electron density around Chain R:

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



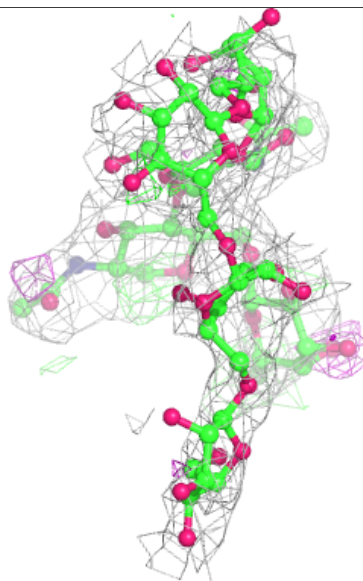
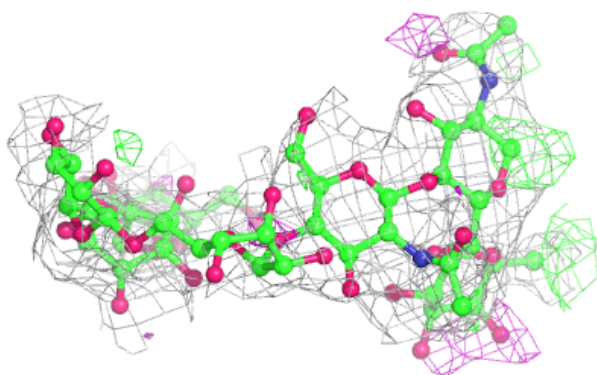
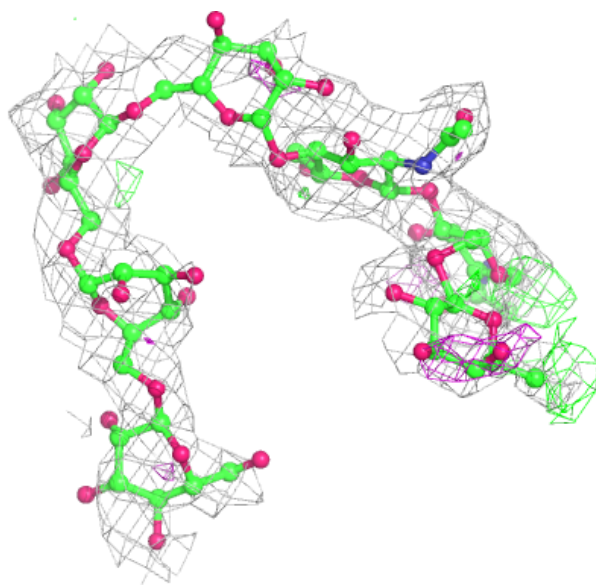
Electron density around Chain S:

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



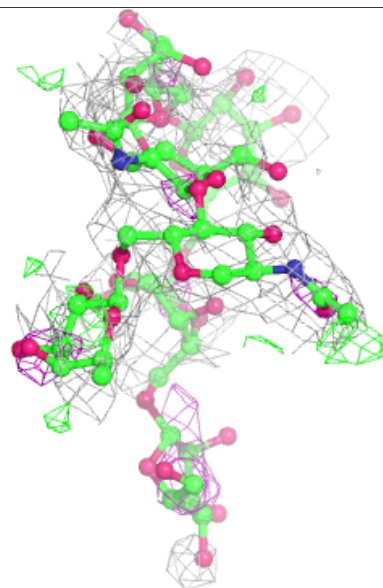
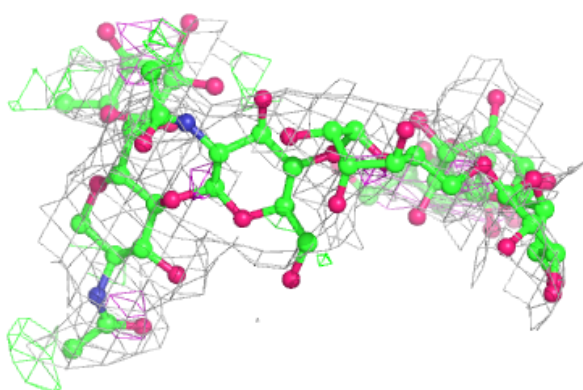
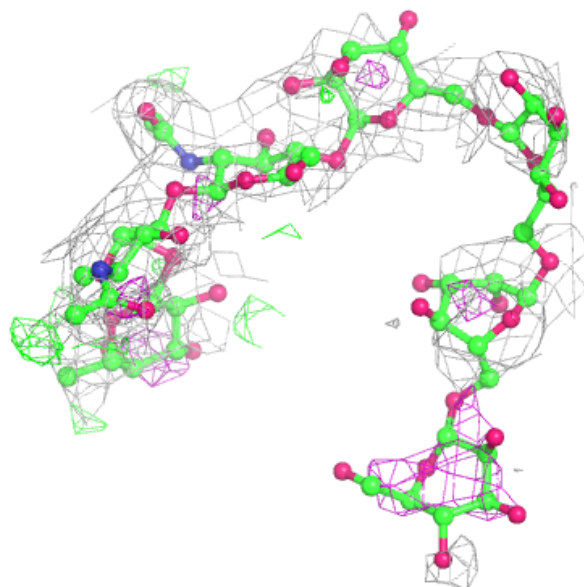
Electron density around Chain T:

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



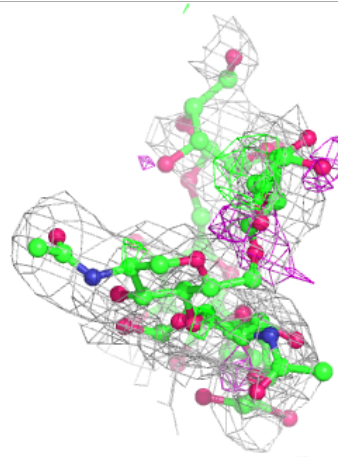
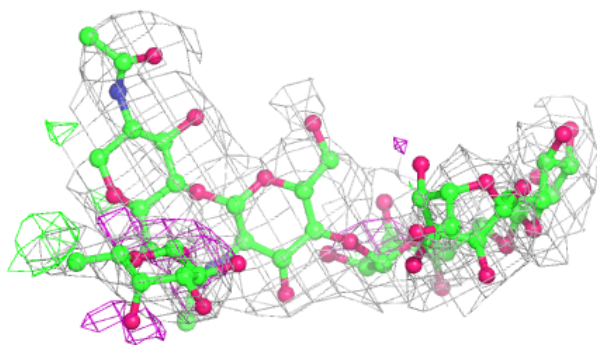
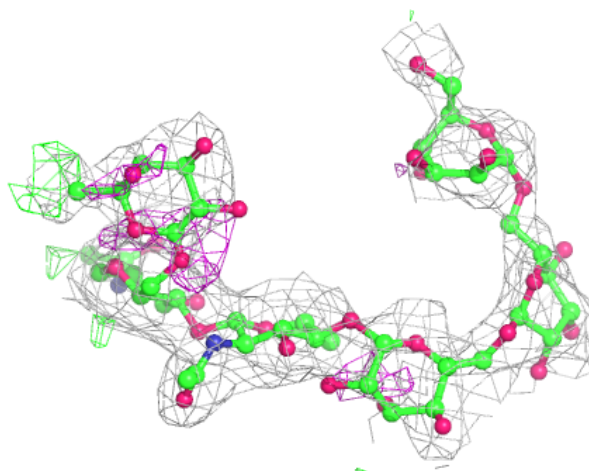
Electron density around Chain U:

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



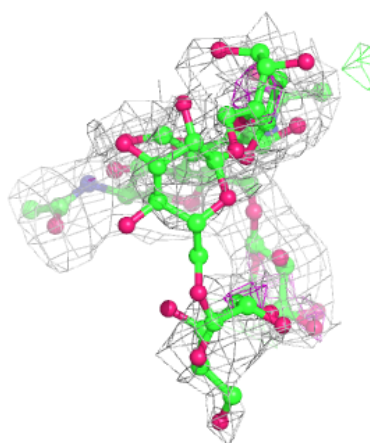
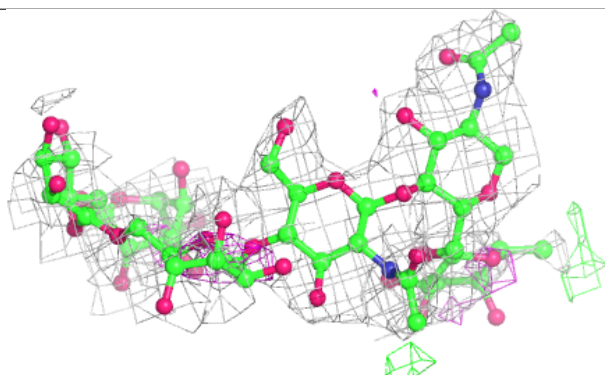
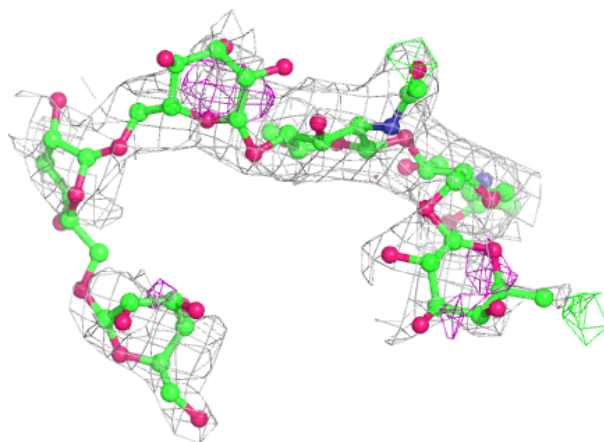
Electron density around Chain V:

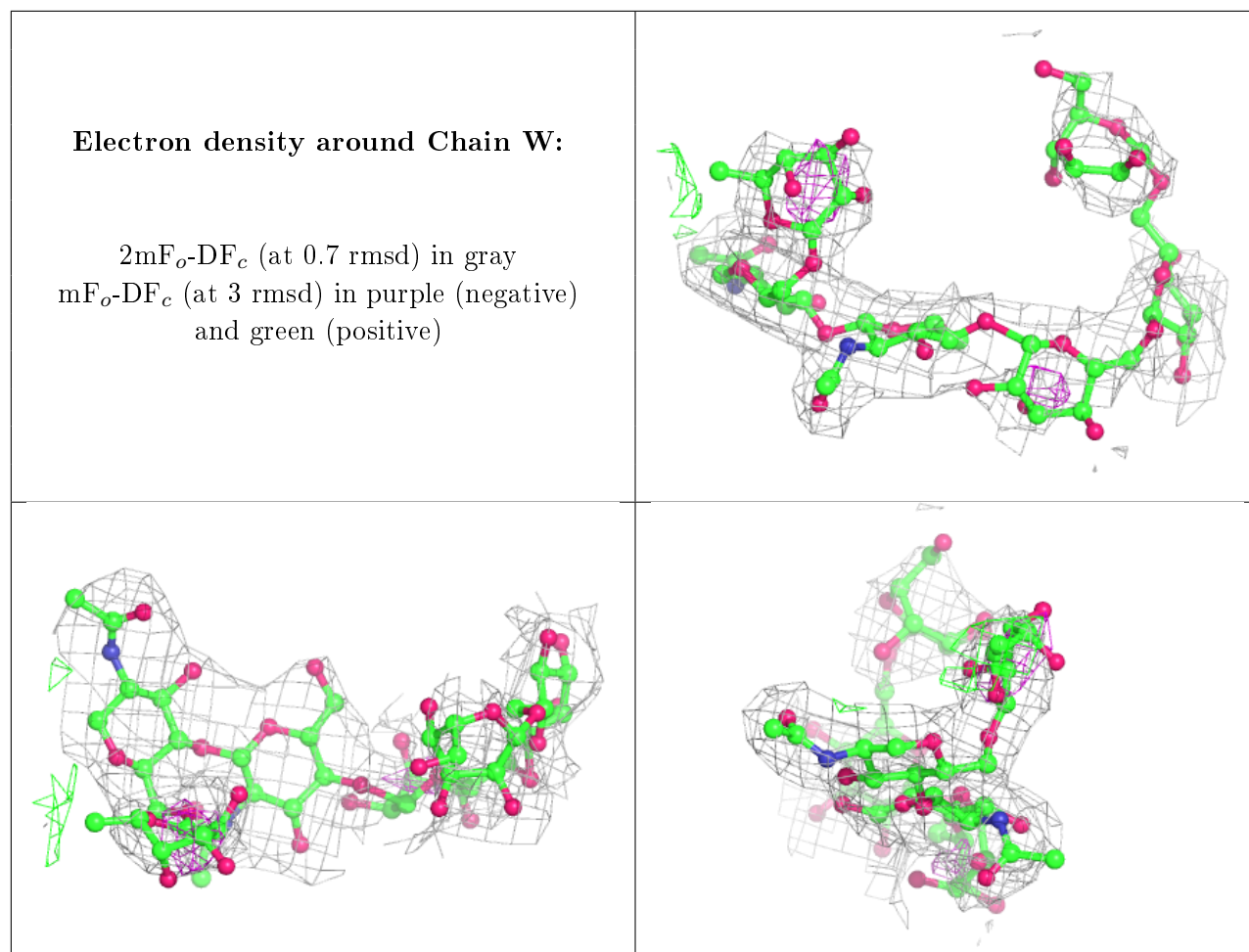
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain X:

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





6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
7	NI	O	308	1/1	0.41	0.30	76,76,76,76	0
8	SO4	M	307	5/5	0.57	0.38	139,149,151,153	0
8	SO4	G	305	5/5	0.58	0.29	110,122,137,140	0
8	SO4	A	305	5/5	0.61	0.44	145,145,151,153	0
8	SO4	O	312	5/5	0.66	0.45	154,155,160,166	0
8	SO4	O	313	5/5	0.66	0.65	163,164,166,169	0
8	SO4	A	306	5/5	0.68	0.37	135,142,143,144	0
8	SO4	I	305	5/5	0.68	0.46	140,141,152,159	0
8	SO4	O	311	5/5	0.68	0.31	166,166,169,173	0
8	SO4	C	305	5/5	0.73	0.29	144,148,150,153	0
8	SO4	E	312	5/5	0.73	0.36	142,150,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	A	301	11/12	0.74	0.30	54,76,89,97	0
8	SO4	K	304	5/5	0.75	0.33	112,121,124,133	0
8	SO4	K	306	5/5	0.79	0.21	112,116,118,118	0
8	SO4	E	313	5/5	0.80	0.29	123,129,137,150	0
8	SO4	L	201	5/5	0.81	0.18	138,143,149,152	0
8	SO4	M	309	5/5	0.81	0.57	128,135,142,143	0
8	SO4	E	310	5/5	0.82	0.28	124,131,134,137	0
8	SO4	I	304	5/5	0.83	0.16	133,140,142,147	0
6	MAN	E	302	11/12	0.85	0.21	63,77,91,94	0
6	MAN	I	301	11/12	0.85	0.24	62,78,89,98	0
8	SO4	K	303	5/5	0.85	0.29	64,65,103,105	0
6	MAN	C	307	11/12	0.86	0.26	63,77,91,94	0
8	SO4	C	306	5/5	0.86	0.21	130,132,137,141	0
8	SO4	G	306	5/5	0.86	0.32	114,118,118,122	0
6	MAN	O	307	11/12	0.87	0.29	62,80,90,99	0
8	SO4	C	304	5/5	0.87	0.36	136,139,141,146	0
8	SO4	H	202	5/5	0.87	0.41	30,30,30,30	0
6	MAN	G	301	11/12	0.88	0.25	52,70,88,101	0
8	SO4	K	309	5/5	0.89	0.41	128,129,133,139	0
8	SO4	C	303	5/5	0.89	0.22	145,147,148,152	0
7	NI	G	302	1/1	0.90	0.51	103,103,103,103	0
8	SO4	K	305	5/5	0.90	0.20	148,149,155,157	0
6	MAN	K	302	11/12	0.91	0.23	51,73,81,91	0
6	MAN	M	304	11/12	0.91	0.20	58,74,90,95	0
8	SO4	E	311	5/5	0.92	0.18	108,108,115,119	0
8	SO4	I	302	5/5	0.93	0.18	107,115,118,122	0
8	SO4	A	303	5/5	0.93	0.28	85,97,104,106	0
8	SO4	M	305	5/5	0.94	0.22	89,105,109,114	0
8	SO4	O	309	5/5	0.94	0.12	59,67,94,100	0
8	SO4	C	301	5/5	0.94	0.25	81,94,110,123	0
8	SO4	H	201	5/5	0.95	0.25	91,97,101,111	0
8	SO4	I	303	5/5	0.95	0.23	92,105,105,114	0
8	SO4	G	303	5/5	0.95	0.26	64,79,96,106	0
7	NI	E	305	1/1	0.96	0.30	64,64,64,64	0
8	SO4	G	304	5/5	0.96	0.21	57,65,73,77	0
7	NI	A	302	1/1	0.97	0.36	65,65,65,65	0
8	SO4	C	302	5/5	0.97	0.22	54,63,89,93	0
8	SO4	A	304	5/5	0.97	0.21	68,77,82,88	0
8	SO4	M	306	5/5	0.98	0.17	76,77,80,90	0
8	SO4	O	310	5/5	0.99	0.16	51,53,63,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.