



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:27 AM BST

PDB ID : 4GMS
Title : Crystal structure of heterosubtypic Fab S139/1 in complex with influenza A H3 hemagglutinin
Authors : Lee, P.S.; Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-08-16
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

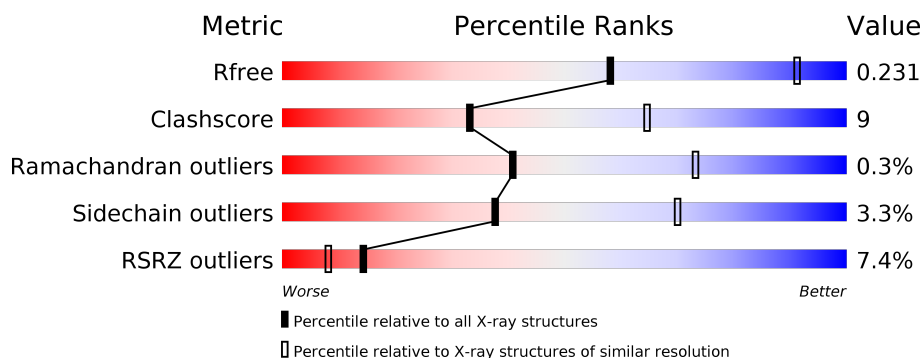
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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





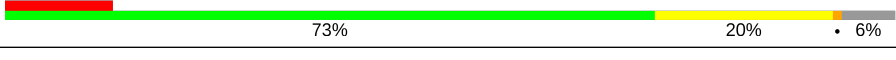


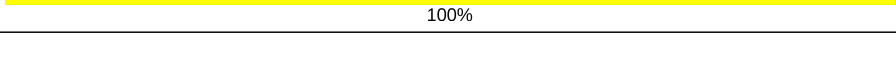
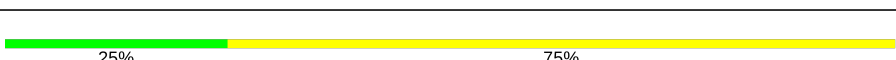
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	320	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	C	320	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	E	320	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
2	B	176	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
2	D	176	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
2	F	176	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	L	214	
3	M	214	
3	N	214	
4	H	225	
4	I	225	
4	J	225	
5	G	2	
5	O	2	
5	P	2	
5	U	2	
5	X	2	
6	K	5	
6	Q	5	
6	V	5	
7	R	3	
7	T	3	
8	S	4	
8	W	4	

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
10	SO4	A	514	-	-	-	X
10	SO4	A	515	-	-	-	X
10	SO4	B	203	-	-	X	-
7	BMA	R	3	-	-	-	X
8	MAN	W	4	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21460 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			
1	C	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			
1	E	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP P03435
C	10	GLY	-	expression tag	UNP P03435
E	10	GLY	-	expression tag	UNP P03435

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			
2	D	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			
2	F	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			

- Molecule 3 is a protein called Fab S139/1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1645	1022	275	341	7			
3	M	156	Total	C	N	O	S	0	0	0
			1209	758	195	250	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	213	Total	C	N	O	S	0	0	0
			1662	1031	278	346	7			

- Molecule 4 is a protein called Fab S139/1 heavy chain.

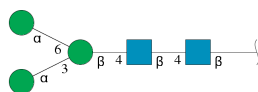
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1665	1062	267	329	7			
4	I	186	Total	C	N	O	S	0	0	0
			1429	918	226	280	5			
4	J	212	Total	C	N	O	S	0	0	0
			1629	1043	261	319	6			

- Molecule 5 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
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
6	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 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.



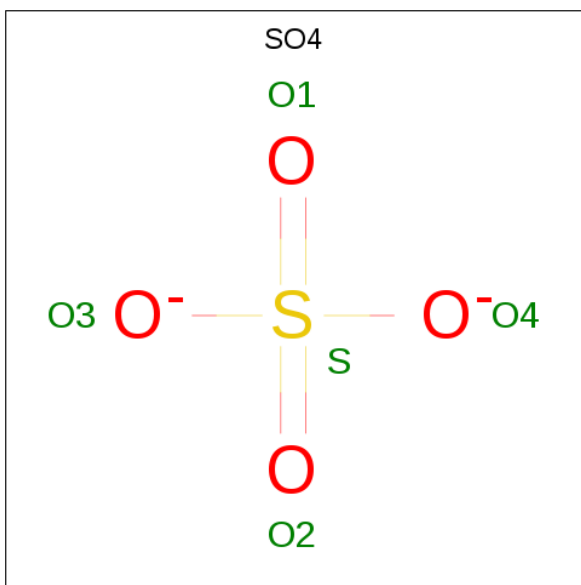
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	W	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



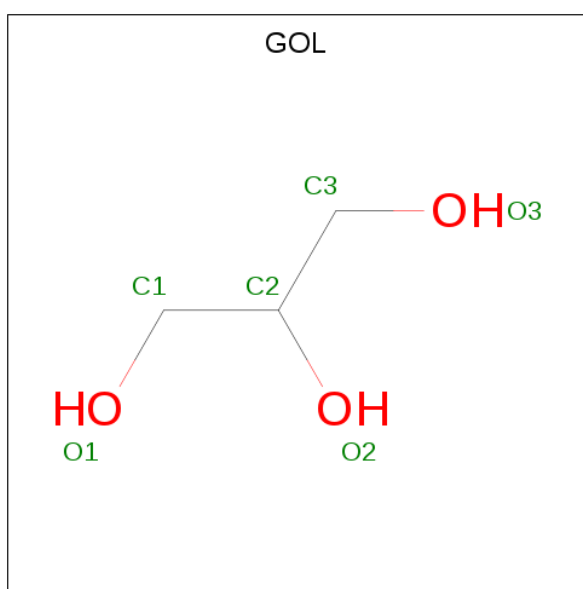
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10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

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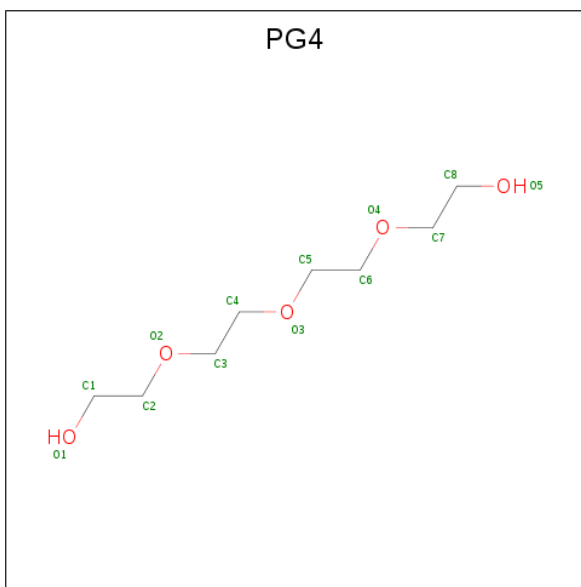
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total	O	S	0	0
			5	4	1		
10	H	1	Total	O	S	0	0
			5	4	1		
10	I	1	Total	O	S	0	0
			5	4	1		
10	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			13	8	5		

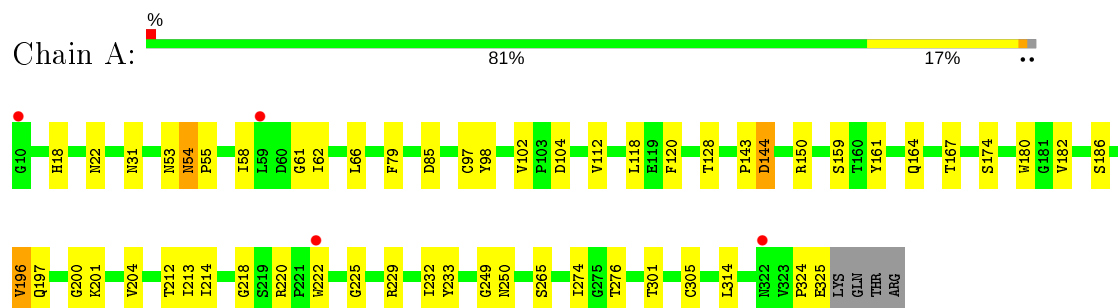
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	5	Total	O	0	0
			5	5		
13	C	6	Total	O	0	0
			6	6		
13	E	7	Total	O	0	0
			7	7		
13	L	1	Total	O	0	0
			1	1		
13	H	2	Total	O	0	0
			2	2		
13	M	3	Total	O	0	0
			3	3		
13	I	1	Total	O	0	0
			1	1		
13	N	4	Total	O	0	0
			4	4		
13	J	2	Total	O	0	0
			2	2		

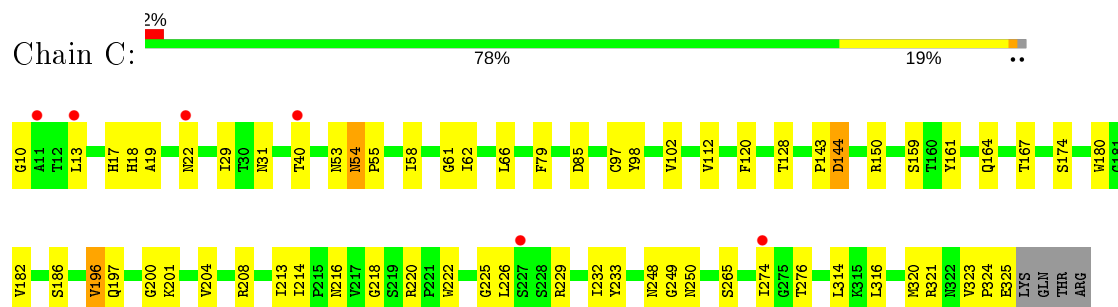
3 Residue-property plots [i](#)

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

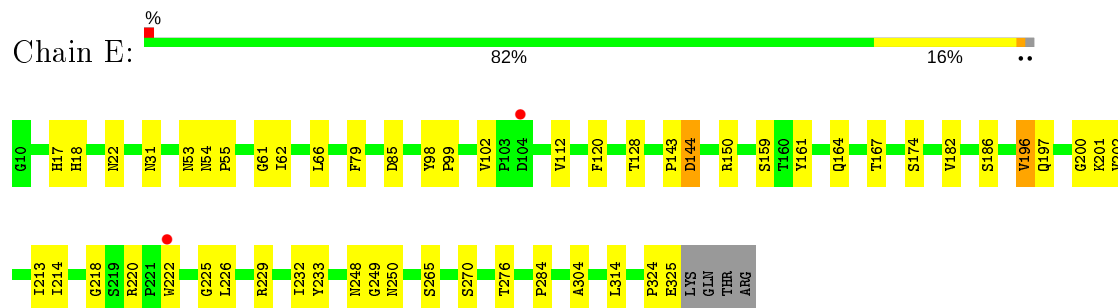
- Molecule 1: Hemagglutinin HA1 chain



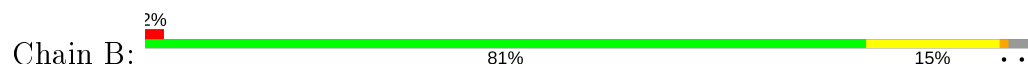
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

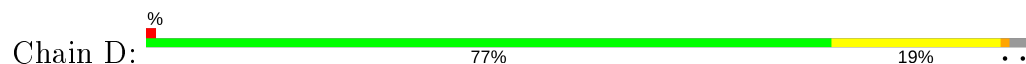


- Molecule 2: Hemagglutinin HA2 chain





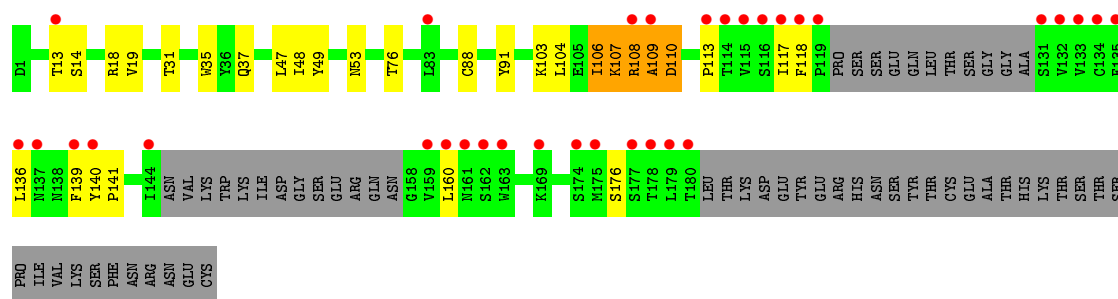
• Molecule 2: Hemagglutinin HA2 chain



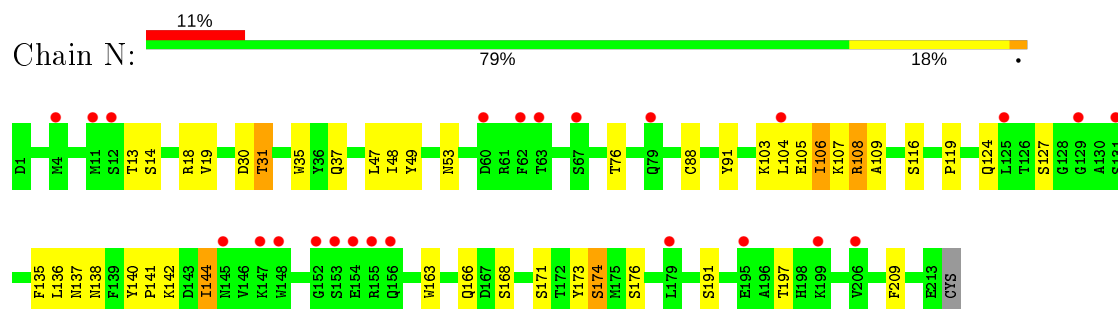
• Molecule 3: Fab S139/1 light chain



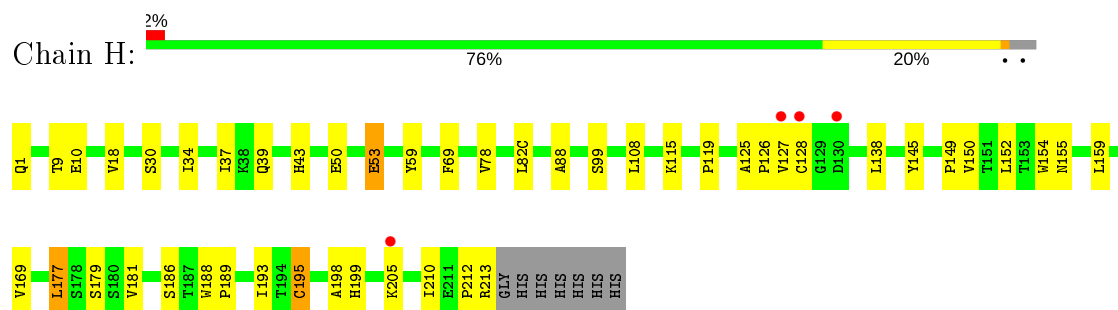
• Molecule 3: Fab S139/1 light chain



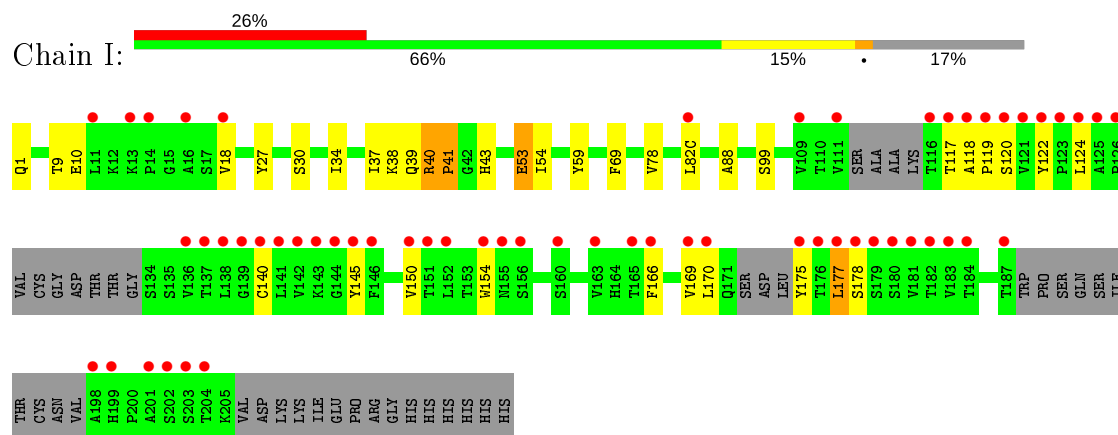
- Molecule 3: Fab S139/1 light chain



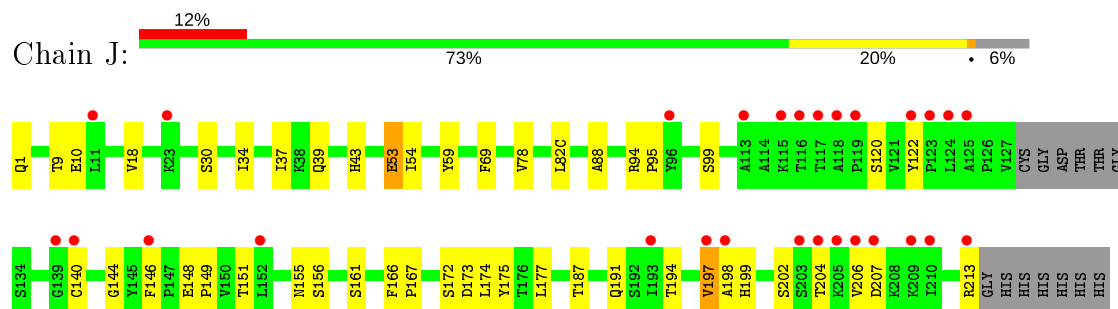
- Molecule 4: Fab S139/1 heavy chain



- Molecule 4: Fab S139/1 heavy chain



- Molecule 4: Fab S139/1 heavy chain

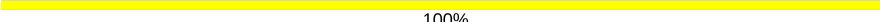


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%


MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%


MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

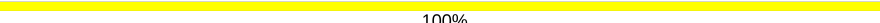

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%


MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%


MAG1
MAG2

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

Chain K:  20% 60% 20%


MAG1
MAG2
MAG3
MAG4
MAG5

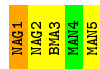
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  20% 60% 20%



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

Chain V: 20% 60% 20%



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

Chain R: 100%



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

Chain T: 67% 33%



- Molecule 8: 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

Chain S: 25% 75%



- Molecule 8: 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

Chain W: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.51 Å 112.94 Å 196.97 Å 90.00° 118.76° 90.00°	Depositor
Resolution (Å)	48.41 – 2.95 48.41 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.41-2.95) 99.8 (48.41-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.207 , 0.233 0.205 , 0.231	Depositor DCC
R_{free} test set	4572 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21460	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: GOL, BMA, NAG, PG4, SO4, PCA, MAN

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	0.49	0/2488	0.63	0/3385
1	C	0.50	0/2488	0.61	0/3385
1	E	0.53	0/2488	0.64	0/3385
2	B	0.50	0/1408	0.61	0/1892
2	D	0.50	0/1408	0.59	0/1892
2	F	0.54	0/1408	0.59	0/1892
3	L	0.38	0/1681	0.54	0/2283
3	M	0.38	0/1234	0.53	0/1676
3	N	0.37	0/1698	0.55	0/2306
4	H	0.38	0/1705	0.56	0/2335
4	I	0.33	0/1461	0.53	0/1996
4	J	0.37	0/1668	0.53	0/2283
All	All	0.45	0/21135	0.58	0/28710

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
4	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	41	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	2375	35	0
1	C	2432	0	2375	47	0
1	E	2432	0	2375	38	0
2	B	1384	0	1305	21	0
2	D	1384	0	1305	28	0
2	F	1384	0	1305	24	0
3	L	1645	0	1563	41	0
3	M	1209	0	1148	34	0
3	N	1662	0	1575	40	0
4	H	1665	0	1612	38	0
4	I	1429	0	1375	27	0
4	J	1629	0	1582	31	0
5	G	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	U	28	0	25	0	0
5	X	28	0	25	0	0
6	K	61	0	52	1	0
6	Q	61	0	52	1	0
6	V	61	0	52	1	0
7	R	39	0	34	0	0
7	T	39	0	34	1	0
8	S	50	0	43	0	0
8	W	50	0	43	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
9	C	28	0	26	0	0
9	D	14	0	13	0	0
9	F	14	0	13	0	0
9	I	14	0	13	0	0
9	J	14	0	13	0	0
10	A	25	0	0	1	0
10	B	15	0	0	2	0
10	C	15	0	0	0	0
10	D	10	0	0	0	0
10	E	5	0	0	0	0
10	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	5	0	0	0	0
10	I	5	0	0	1	0
10	J	5	0	0	0	0
11	B	6	0	8	1	0
11	D	6	0	8	1	0
12	E	13	0	18	1	0
13	A	5	0	0	0	0
13	C	6	0	0	0	0
13	E	7	0	0	0	0
13	H	2	0	0	0	0
13	I	1	0	0	0	0
13	J	2	0	0	0	0
13	L	1	0	0	0	0
13	M	3	0	0	0	0
13	N	4	0	0	0	0
All	All	21460	0	20481	361	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 9.

All (361) 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)
3:M:107:LYS:HB2	3:M:140:TYR:OH	1.72	0.90
2:D:124:ARG:HD3	2:F:134:GLY:HA2	1.64	0.79
3:N:108:ARG:HG2	3:N:108:ARG:HH11	1.48	0.79
3:N:13:THR:O	3:N:106:ILE:HD13	1.87	0.75
3:L:13:THR:O	3:L:106:ILE:HD13	1.88	0.73
2:B:124:ARG:HD3	2:D:134:GLY:HA2	1.72	0.72
3:M:140:TYR:CD1	3:M:141:PRO:HA	2.24	0.72
2:B:17:MET:HE1	2:B:36:ALA:HA	1.70	0.72
2:B:134:GLY:HA2	2:F:124:ARG:HD3	1.70	0.72
2:F:17:MET:HE1	2:F:36:ALA:HA	1.72	0.70
3:M:13:THR:O	3:M:106:ILE:HD13	1.90	0.70
2:D:54:ARG:NH1	11:D:204:GOL:O3	2.27	0.68
2:B:17:MET:HE1	2:B:23:GLY:HA3	1.76	0.68
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.28	0.67
4:I:140:CYS:HB2	4:I:154:TRP:CH2	2.30	0.67
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.31	0.66
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.77	0.65
1:A:249:GLY:O	1:A:250:ASN:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.31	0.65
1:C:226:LEU:HD22	4:I:54:ILE:HG22	1.79	0.65
4:J:199:HIS:ND1	4:J:202:SER:HB2	2.11	0.65
3:N:140:TYR:CD1	3:N:141:PRO:HA	2.32	0.65
2:D:17:MET:HE1	2:D:36:ALA:HA	1.77	0.64
2:B:30:GLU:OE2	2:B:145:ASP:HB2	1.98	0.64
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.32	0.64
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.33	0.63
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.32	0.63
3:M:160:LEU:HG	4:I:169:VAL:HG11	1.81	0.63
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.80	0.63
1:C:66:LEU:HD21	1:C:112:VAL:HG12	1.80	0.63
4:H:126:PRO:HD3	4:H:138:LEU:CD2	2.29	0.63
4:H:154:TRP:CZ3	4:H:195:CYS:HB3	2.34	0.63
1:E:53:ASN:HD21	1:E:276:THR:HG22	1.63	0.63
3:M:107:LYS:C	3:M:107:LYS:CD	2.68	0.62
4:J:30:SER:HB2	4:J:53:GLU:HG2	1.80	0.62
1:A:66:LEU:HD21	1:A:112:VAL:HG12	1.81	0.62
1:C:249:GLY:O	1:C:250:ASN:HB2	1.99	0.62
1:A:53:ASN:HD21	1:A:276:THR:HG22	1.66	0.61
4:H:152:LEU:HD21	4:H:179:SER:CB	2.30	0.61
4:H:30:SER:HB2	4:H:53:GLU:HG2	1.81	0.61
2:F:30:GLU:OE2	2:F:145:ASP:HB2	2.01	0.61
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.01	0.60
4:I:30:SER:HB2	4:I:53:GLU:HG2	1.82	0.60
1:C:182:VAL:HG21	1:C:213:ILE:CG2	2.32	0.60
1:C:220:ARG:HD3	1:C:229:ARG:CG	2.31	0.60
4:H:177:LEU:HD12	4:H:177:LEU:C	2.22	0.60
1:E:66:LEU:HD21	1:E:112:VAL:HG12	1.83	0.60
1:C:53:ASN:HD21	1:C:276:THR:HG22	1.65	0.60
1:E:220:ARG:HD3	1:E:229:ARG:CG	2.32	0.59
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.85	0.59
4:I:177:LEU:C	4:I:177:LEU:HD12	2.23	0.59
1:C:220:ARG:HD3	1:C:229:ARG:HG3	1.84	0.59
1:E:249:GLY:O	1:E:250:ASN:HB2	2.02	0.59
3:N:105:GLU:HG3	3:N:173:TYR:OH	2.02	0.58
3:L:19:VAL:HG21	3:L:104:LEU:HD11	1.85	0.58
3:L:106:ILE:HG22	3:L:166:GLN:HE22	1.68	0.58
4:J:148:GLU:HB3	4:J:149:PRO:HA	1.85	0.58
1:C:314:LEU:HB3	2:D:100:VAL:HG21	1.84	0.58
3:N:142:LYS:HB2	3:N:173:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:PRO:HG2	1:C:144:ASP:OD1	2.04	0.57
1:A:220:ARG:HD3	1:A:229:ARG:CG	2.34	0.57
3:L:106:ILE:HG22	3:L:166:GLN:NE2	2.19	0.57
3:L:119:PRO:HG2	4:H:213:ARG:CZ	2.35	0.57
3:M:108:ARG:HD3	3:M:109:ALA:HB3	1.87	0.57
3:M:110:ASP:OD1	3:M:110:ASP:N	2.37	0.57
3:N:108:ARG:HG2	3:N:109:ALA:N	2.20	0.56
1:A:182:VAL:HG21	1:A:213:ILE:CG2	2.36	0.56
4:I:27:TYR:HB2	10:I:302:SO4:O1	2.05	0.56
7:T:2:NAG:O3	7:T:3:BMA:O5	2.18	0.56
2:B:17:MET:CE	2:B:36:ALA:HA	2.36	0.56
2:B:68:LYS:HE2	2:B:85:GLU:OE1	2.05	0.56
3:N:19:VAL:HG21	3:N:104:LEU:HD11	1.87	0.56
3:M:19:VAL:HG21	3:M:104:LEU:HD11	1.87	0.56
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.86	0.56
4:H:152:LEU:CD2	4:H:179:SER:HB2	2.35	0.56
1:A:104:ASP:N	10:A:514:SO4:O3	2.37	0.56
1:E:226:LEU:HD22	4:J:54:ILE:HG22	1.88	0.56
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.88	0.56
4:J:177:LEU:HD12	4:J:177:LEU:C	2.26	0.56
2:D:56:ILE:CG2	2:D:56:ILE:O	2.54	0.55
3:M:110:ASP:HA	3:M:140:TYR:HD2	1.72	0.55
2:B:56:ILE:CG2	2:B:56:ILE:O	2.54	0.55
3:M:14:SER:HA	3:M:106:ILE:HD12	1.88	0.55
1:E:324:PRO:O	1:E:325:GLU:CB	2.55	0.55
3:N:108:ARG:CG	3:N:108:ARG:HH11	2.18	0.55
3:N:136:LEU:HD12	3:N:136:LEU:N	2.21	0.55
3:M:108:ARG:HD3	3:M:109:ALA:CB	2.36	0.55
1:A:143:PRO:HG2	1:A:144:ASP:OD1	2.08	0.54
1:C:186:SER:HA	1:C:218:GLY:O	2.08	0.54
1:C:324:PRO:O	1:C:325:GLU:CB	2.56	0.54
3:L:140:TYR:CG	3:L:141:PRO:HA	2.41	0.54
2:D:17:MET:CE	2:D:36:ALA:HA	2.37	0.54
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.90	0.54
4:I:120:SER:HB3	4:I:122:TYR:CZ	2.43	0.54
4:I:140:CYS:HB2	4:I:154:TRP:CZ2	2.43	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.54
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.43	0.54
1:A:212:THR:HG21	1:C:216:ASN:CG	2.28	0.54
1:E:143:PRO:HG2	1:E:144:ASP:OD1	2.06	0.54
3:N:137:ASN:HA	3:N:174:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PRO:O	1:E:325:GLU:HB2	2.08	0.54
1:A:201:LYS:HG3	1:A:214:ILE:HD13	1.90	0.53
3:L:209:PHE:HB2	4:H:127:VAL:HG11	1.90	0.53
4:I:38:LYS:HE2	4:I:40:ARG:HD2	1.91	0.53
2:F:17:MET:CE	2:F:36:ALA:HA	2.39	0.53
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.44	0.53
1:C:182:VAL:HG21	1:C:213:ILE:HG21	1.91	0.53
1:E:220:ARG:HD3	1:E:229:ARG:HG3	1.89	0.53
2:F:26:HIS:CE1	2:F:33:GLY:HA3	2.43	0.53
3:L:155:ARG:HE	3:L:157:ASN:HB2	1.74	0.52
1:C:201:LYS:HG3	1:C:214:ILE:HD13	1.91	0.52
1:C:324:PRO:O	1:C:325:GLU:HB2	2.09	0.52
3:L:106:ILE:HG21	3:L:171:SER:HB3	1.91	0.52
1:A:324:PRO:O	1:A:325:GLU:CB	2.58	0.52
1:C:200:GLY:HA3	1:C:250:ASN:OD1	2.10	0.52
4:J:194:THR:HG21	4:J:207:ASP:HB3	1.91	0.52
4:J:37:ILE:HD12	4:J:37:ILE:N	2.24	0.52
3:N:138:ASN:H	3:N:174:SER:HB3	1.75	0.52
1:E:186:SER:HA	1:E:218:GLY:O	2.10	0.52
4:J:187:THR:HG22	4:J:191:GLN:NE2	2.25	0.52
3:M:106:ILE:O	3:M:106:ILE:HG22	2.10	0.52
3:M:107:LYS:O	3:M:108:ARG:HB2	2.08	0.52
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.45	0.51
4:H:152:LEU:HD21	4:H:179:SER:HB3	1.91	0.51
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.45	0.51
2:B:139:LYS:HD2	10:B:203:SO4:O3	2.09	0.51
3:L:167:ASP:OD2	3:L:168:SER:N	2.44	0.51
1:A:220:ARG:HD3	1:A:229:ARG:HG2	1.93	0.51
1:A:186:SER:HA	1:A:218:GLY:O	2.11	0.51
1:E:17:HIS:NE2	2:F:6:ILE:HG23	2.26	0.51
4:H:189:PRO:HB3	4:H:212:PRO:HG3	1.93	0.51
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.92	0.51
3:M:107:LYS:HB2	3:M:140:TYR:HH	1.75	0.51
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.11	0.51
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.45	0.51
1:E:213:ILE:HG12	1:E:233:TYR:CZ	2.46	0.50
2:F:56:ILE:CG2	2:F:56:ILE:O	2.59	0.50
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.92	0.50
4:I:37:ILE:N	4:I:37:ILE:HD12	2.26	0.50
4:J:151:THR:OG1	4:J:198:ALA:HB3	2.11	0.50
3:N:136:LEU:HD23	3:N:144:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:34:ILE:HG13	4:H:78:VAL:HG21	1.93	0.50
3:N:176:SER:HB2	4:J:166:PHE:CZ	2.47	0.50
2:D:26:HIS:CE1	2:D:33:GLY:HA3	2.47	0.50
1:A:220:ARG:HD3	1:A:229:ARG:HG3	1.93	0.50
4:H:37:ILE:N	4:H:37:ILE:HD12	2.27	0.50
3:L:18:ARG:HD3	3:L:76:THR:HG22	1.94	0.49
1:E:200:GLY:HA3	1:E:250:ASN:OD1	2.11	0.49
4:J:172:SER:O	4:J:173:ASP:HB2	2.13	0.49
10:B:203:SO4:O4	2:F:127:ARG:NH1	2.41	0.49
4:H:108:LEU:HD23	4:H:149:PRO:HD3	1.94	0.49
3:L:113:PRO:O	3:L:115:VAL:HG23	2.12	0.49
3:N:163:TRP:O	4:J:167:PRO:HD2	2.12	0.49
4:I:170:LEU:HD13	4:I:175:TYR:CD2	2.48	0.49
1:A:324:PRO:O	1:A:325:GLU:HB2	2.11	0.49
1:C:213:ILE:HG12	1:C:233:TYR:CZ	2.47	0.49
1:E:220:ARG:HD3	1:E:229:ARG:HG2	1.94	0.49
1:A:61:GLY:HA2	1:A:79:PHE:CZ	2.48	0.48
4:I:34:ILE:HG13	4:I:78:VAL:HG21	1.95	0.48
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.95	0.48
1:E:314:LEU:HB3	2:F:100:VAL:HG21	1.96	0.48
1:E:201:LYS:HG3	1:E:214:ILE:HD13	1.94	0.48
4:I:145:TYR:OH	4:I:177:LEU:HD23	2.13	0.48
3:N:107:LYS:HG3	3:N:140:TYR:OH	2.13	0.48
1:C:61:GLY:HA2	1:C:79:PHE:CZ	2.49	0.48
4:I:59:TYR:CE1	4:I:69:PHE:CE2	3.01	0.48
3:M:18:ARG:HD3	3:M:76:THR:HG22	1.96	0.48
3:N:91:TYR:HD1	4:J:99:SER:HB2	1.79	0.48
1:C:196:VAL:HG12	1:C:197:GLN:N	2.28	0.48
4:H:59:TYR:CE1	4:H:69:PHE:CE2	3.01	0.48
1:A:314:LEU:HB3	2:B:100:VAL:HG21	1.96	0.47
1:E:182:VAL:HG21	1:E:213:ILE:CG2	2.43	0.47
4:H:145:TYR:CE2	4:H:150:VAL:HG13	2.49	0.47
4:H:198:ALA:HB2	4:H:205:LYS:HD2	1.95	0.47
4:I:39:GLN:O	4:I:88:ALA:HB1	2.13	0.47
2:B:110:LEU:C	2:B:110:LEU:HD12	2.35	0.47
1:C:40:THR:HG21	2:D:52:LEU:HD11	1.95	0.47
4:H:126:PRO:HD3	4:H:138:LEU:HD22	1.95	0.47
4:H:152:LEU:HD21	4:H:179:SER:HB2	1.96	0.47
3:N:176:SER:HB2	4:J:166:PHE:CE2	2.49	0.47
4:H:159:LEU:HD23	4:H:181:VAL:HG21	1.95	0.47
3:L:184:ASP:O	3:L:188:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106:ILE:HG21	3:L:171:SER:CB	2.44	0.47
1:A:128:THR:H	1:A:164:GLN:NE2	2.12	0.47
1:E:61:GLY:HA2	1:E:79:PHE:CZ	2.50	0.47
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.97	0.47
4:J:197:VAL:O	4:J:197:VAL:HG12	2.15	0.47
4:I:18:VAL:HG12	4:I:82(C):LEU:HD11	1.96	0.46
3:N:108:ARG:HG2	3:N:109:ALA:H	1.78	0.46
3:N:136:LEU:N	3:N:136:LEU:CD1	2.78	0.46
1:E:167:THR:OG1	6:V:1:NAG:H62	2.15	0.46
3:M:107:LYS:HD2	3:M:107:LYS:O	2.15	0.46
3:N:18:ARG:HD3	3:N:76:THR:HG22	1.95	0.46
3:M:107:LYS:CD	3:M:107:LYS:O	2.63	0.46
3:N:106:ILE:HA	3:N:106:ILE:HD13	1.75	0.46
4:J:146:PHE:CD2	4:J:146:PHE:C	2.89	0.46
4:J:34:ILE:HG13	4:J:78:VAL:HG21	1.97	0.46
4:H:138:LEU:HD12	4:H:193:ILE:HG21	1.96	0.46
3:N:135:PHE:HB3	3:N:137:ASN:OD1	2.15	0.46
2:D:126:LEU:HD21	2:D:152:ILE:HD13	1.98	0.46
4:J:146:PHE:CD1	4:J:175:TYR:HE2	2.34	0.46
1:E:182:VAL:HG22	1:E:202:VAL:HG21	1.97	0.46
2:F:126:LEU:HD21	2:F:152:ILE:HD13	1.98	0.46
4:H:125:ALA:HB2	4:H:210:ILE:HG22	1.97	0.46
4:J:199:HIS:ND1	4:J:202:SER:CB	2.77	0.46
1:C:220:ARG:HD3	1:C:229:ARG:HG2	1.98	0.46
2:D:56:ILE:O	2:D:56:ILE:HG22	2.16	0.46
3:L:14:SER:HA	3:L:106:ILE:HD12	1.98	0.46
3:L:106:ILE:HA	3:L:106:ILE:HD13	1.77	0.46
3:N:135:PHE:C	3:N:136:LEU:HD12	2.37	0.46
1:A:97:CYS:SG	1:A:98:TYR:N	2.89	0.45
4:J:18:VAL:HG12	4:J:82(C):LEU:HD11	1.98	0.45
3:L:197:THR:HG23	3:L:204:PRO:HB3	1.98	0.45
3:N:14:SER:HA	3:N:106:ILE:HD12	1.97	0.45
4:H:39:GLN:O	4:H:88:ALA:HB1	2.16	0.45
4:I:150:VAL:CG2	4:I:177:LEU:HD21	2.47	0.45
3:M:91:TYR:HD1	4:I:99:SER:HB2	1.81	0.45
3:N:136:LEU:HD23	3:N:144:ILE:CD1	2.46	0.45
1:A:196:VAL:HG12	1:A:197:GLN:N	2.31	0.45
1:E:98:TYR:CZ	1:E:226:LEU:HD13	2.52	0.45
3:N:103:LYS:HE3	3:N:103:LYS:HB2	1.83	0.45
1:E:196:VAL:HG12	1:E:197:GLN:N	2.31	0.45
1:E:200:GLY:O	1:E:201:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ASN:C	1:E:248:ASN:OD1	2.55	0.45
3:M:103:LYS:HE3	3:M:103:LYS:HB2	1.86	0.45
3:M:176:SER:HB2	4:I:166:PHE:CE2	2.51	0.45
3:M:107:LYS:C	3:M:107:LYS:HD2	2.36	0.45
1:C:10:GLY:HA2	2:D:142:HIS:O	2.17	0.45
4:J:59:TYR:CE1	4:J:69:PHE:CE2	3.05	0.45
3:N:166:GLN:HE21	3:N:171:SER:HB3	1.82	0.44
1:A:182:VAL:HG21	1:A:213:ILE:HG21	1.98	0.44
2:F:57:GLU:HG2	2:F:58:LYS:N	2.32	0.44
3:L:14:SER:OG	3:L:107:LYS:HG3	2.17	0.44
3:N:140:TYR:CG	3:N:141:PRO:HA	2.52	0.44
1:A:167:THR:OG1	6:K:1:NAG:H62	2.17	0.44
1:E:128:THR:H	1:E:164:GLN:NE2	2.15	0.44
2:F:110:LEU:C	2:F:110:LEU:HD12	2.38	0.44
4:J:204:THR:CG2	4:J:206:VAL:HG13	2.47	0.44
1:C:323:VAL:O	2:D:12:ASN:HB2	2.18	0.44
1:A:212:THR:HG21	1:C:216:ASN:CB	2.48	0.44
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.53	0.44
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.99	0.44
3:M:136:LEU:HD12	3:M:136:LEU:N	2.33	0.44
3:M:35:TRP:HB2	3:M:48:ILE:HB	1.99	0.44
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.52	0.44
1:C:58:ILE:HG21	1:C:274:ILE:HD13	1.99	0.44
2:F:6:ILE:C	2:F:8:GLY:N	2.71	0.44
4:H:155:ASN:HD22	4:H:159:LEU:HD13	1.82	0.44
3:L:106:ILE:CG2	3:L:171:SER:HB3	2.48	0.44
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.52	0.44
2:F:57:GLU:CG	2:F:58:LYS:N	2.81	0.44
4:H:126:PRO:HD3	4:H:138:LEU:HD23	1.99	0.44
3:L:209:PHE:CB	4:H:127:VAL:HG11	2.47	0.43
4:I:117:THR:HG22	4:I:118:ALA:N	2.33	0.43
3:N:13:THR:O	3:N:106:ILE:CD1	2.63	0.43
1:A:120:PHE:CD2	1:A:150:ARG:NH1	2.86	0.43
1:E:304:ALA:HB2	2:F:61:GLU:HG3	1.99	0.43
4:I:119:PRO:HB3	4:I:145:TYR:HB3	1.99	0.43
4:J:39:GLN:O	4:J:88:ALA:HB1	2.18	0.43
4:H:188:TRP:CG	4:H:189:PRO:HA	2.53	0.43
3:M:106:ILE:HA	3:M:106:ILE:HD13	1.81	0.43
1:C:19:ALA:HB2	2:D:13:GLY:HA3	2.01	0.43
2:D:27:GLN:HG3	2:D:32:THR:HG22	2.00	0.43
1:C:17:HIS:NE2	2:D:6:ILE:HG23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:GLU:CG	2:F:58:LYS:H	2.32	0.43
1:A:54:ASN:ND2	1:A:55:PRO:HA	2.33	0.43
2:B:57:GLU:HG2	2:B:58:LYS:N	2.33	0.43
1:C:128:THR:H	1:C:164:GLN:NE2	2.17	0.43
1:E:304:ALA:HA	2:F:61:GLU:HA	2.00	0.43
4:I:170:LEU:HD13	4:I:175:TYR:CE2	2.53	0.43
3:N:107:LYS:HA	3:N:140:TYR:OH	2.19	0.43
3:N:35:TRP:HB2	3:N:48:ILE:HB	2.01	0.43
2:B:4:GLY:HA3	2:F:117:LYS:HD3	2.00	0.43
3:L:103:LYS:HE3	3:L:103:LYS:HB2	1.86	0.43
3:N:30:ASP:HB3	3:N:31:THR:H	1.68	0.43
1:C:54:ASN:ND2	1:C:55:PRO:HA	2.34	0.43
1:E:128:THR:H	1:E:164:GLN:HE22	1.67	0.43
3:L:136:LEU:N	3:L:136:LEU:HD12	2.34	0.43
1:A:58:ILE:HG21	1:A:274:ILE:HD13	2.00	0.43
4:I:9:THR:HG22	4:I:10:GLU:N	2.33	0.43
4:H:119:PRO:HD3	4:H:199:HIS:ND1	2.33	0.43
4:J:9:THR:HG22	4:J:10:GLU:N	2.34	0.43
3:M:108:ARG:NE	3:M:109:ALA:HB2	2.34	0.43
1:C:167:THR:OG1	6:Q:1:NAG:H62	2.18	0.42
1:C:320:MET:HB3	2:D:111:THR:HB	2.00	0.42
2:D:130:ALA:HA	2:D:139:LYS:O	2.20	0.42
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.54	0.42
4:I:177:LEU:HD12	4:I:178:SER:N	2.35	0.42
4:J:144:GLY:HA2	4:J:174:LEU:HB3	2.02	0.42
3:N:91:TYR:CD1	4:J:99:SER:HB2	2.55	0.42
1:C:248:ASN:OD1	1:C:248:ASN:C	2.58	0.42
2:B:6:ILE:C	2:B:8:GLY:N	2.73	0.42
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.54	0.42
3:M:49:TYR:O	3:M:53:ASN:HB2	2.20	0.42
2:B:54:ARG:NH1	11:B:205:GOL:O3	2.52	0.42
2:B:57:GLU:CG	2:B:58:LYS:N	2.82	0.42
3:L:160:LEU:HG	4:H:169:VAL:HG11	2.02	0.42
3:N:49:TYR:O	3:N:53:ASN:HB2	2.20	0.42
2:D:110:LEU:HD12	2:D:110:LEU:C	2.39	0.42
1:E:213:ILE:HG12	1:E:233:TYR:CE2	2.54	0.42
2:F:68:LYS:HE2	2:F:85:GLU:OE1	2.19	0.42
4:J:155:ASN:O	4:J:156:SER:HB2	2.20	0.42
3:L:34:ALA:HA	3:L:48:ILE:O	2.20	0.42
2:D:6:ILE:C	2:D:8:GLY:N	2.73	0.42
2:F:9:PHE:CD1	2:F:9:PHE:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:194:THR:CG2	4:J:207:ASP:HB3	2.50	0.42
3:L:209:PHE:HB2	4:H:127:VAL:CG1	2.50	0.42
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.91	0.41
1:A:128:THR:H	1:A:164:GLN:HE22	1.67	0.41
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.55	0.41
3:L:94:TYR:OH	4:H:50:GLU:OE2	2.24	0.41
1:C:208:ARG:HB3	12:E:520:PG4:H51	2.01	0.41
1:E:85:ASP:O	1:E:265:SER:HA	2.20	0.41
3:L:111:ALA:C	3:L:200:THR:HG21	2.40	0.41
1:C:85:ASP:O	1:C:265:SER:HA	2.20	0.41
3:N:119:PRO:HB3	3:N:209:PHE:CZ	2.55	0.41
2:B:57:GLU:CG	2:B:58:LYS:H	2.32	0.41
1:C:13:LEU:CD2	2:D:152:ILE:HG21	2.51	0.41
1:C:201:LYS:HG3	1:C:214:ILE:CD1	2.50	0.41
4:H:9:THR:HG22	4:H:10:GLU:N	2.35	0.41
4:H:152:LEU:HD23	4:H:179:SER:HB2	2.03	0.41
3:L:170:ASP:OD1	3:L:170:ASP:C	2.59	0.41
3:L:180:THR:O	3:L:181:LEU:HG	2.20	0.41
3:L:91:TYR:HD1	4:H:99:SER:HB2	1.85	0.41
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.01	0.41
3:M:117:ILE:C	3:M:118:PHE:CD2	2.94	0.41
3:M:113:PRO:HA	3:M:139:PHE:HB3	2.02	0.41
3:M:14:SER:HA	3:M:106:ILE:CD1	2.50	0.41
3:N:124:GLN:HB2	4:J:122:TYR:CD1	2.55	0.41
1:C:120:PHE:CD2	1:C:150:ARG:NH1	2.89	0.41
3:M:118:PHE:CD1	4:I:124:LEU:HB3	2.55	0.41
2:D:68:LYS:HE2	2:D:85:GLU:OE1	2.20	0.41
3:N:119:PRO:HG2	4:J:213:ARG:NH2	2.35	0.41
1:A:85:ASP:O	1:A:265:SER:HA	2.21	0.41
1:C:29:ILE:HD11	2:D:102:LEU:HD23	2.03	0.41
1:C:316:LEU:HD23	2:D:52:LEU:HD13	2.03	0.41
1:E:120:PHE:CD2	1:E:150:ARG:NH1	2.89	0.41
4:H:53:GLU:HA	4:H:53:GLU:OE2	2.20	0.41
4:I:40:ARG:HA	4:I:41:PRO:HD3	1.85	0.41
3:N:105:GLU:HG2	3:N:106:ILE:N	2.36	0.41
1:C:200:GLY:O	1:C:201:LYS:HB2	2.21	0.41
1:C:324:PRO:O	1:C:325:GLU:HG3	2.21	0.41
3:L:49:TYR:O	3:L:53:ASN:HB2	2.21	0.41
2:D:9:PHE:CD1	2:D:9:PHE:C	2.95	0.41
3:M:118:PHE:N	3:M:118:PHE:CD2	2.89	0.41
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:TYR:CE2	1:E:226:LEU:HD13	2.56	0.40
1:E:270:SER:HB2	1:E:284:PRO:HA	2.02	0.40
3:L:105:GLU:HG2	3:L:106:ILE:N	2.36	0.40
3:L:193:THR:HG22	3:L:194:CYS:N	2.36	0.40
4:H:127:VAL:HG12	4:H:128:CYS:N	2.36	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.91	0.40
1:E:324:PRO:O	1:E:325:GLU:HG3	2.21	0.40
3:L:83:LEU:HD11	3:L:166:GLN:HB3	2.02	0.40
3:M:91:TYR:CD1	4:I:99:SER:HB2	2.56	0.40
2:B:56:ILE:HG22	2:B:56:ILE:O	2.20	0.40
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.57	0.40
4:H:177:LEU:CD1	4:H:177:LEU:C	2.89	0.40
3:L:91:TYR:CD1	4:H:99:SER:HB2	2.56	0.40
4:J:94:ARG:HA	4:J:95:PRO:HD3	1.98	0.40
3:L:186:TYR:CE1	3:L:192:TYR:CE2	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	314/320 (98%)	305 (97%)	7 (2%)	2 (1%)	25	60
1	C	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	25	60
1	E	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	25	60
2	B	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
2	D	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
2	F	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
3	L	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
3	M	150/214 (70%)	140 (93%)	9 (6%)	1 (1%)	22	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
4	H	216/225 (96%)	211 (98%)	5 (2%)	0	100	100
4	I	176/225 (78%)	170 (97%)	6 (3%)	0	100	100
4	J	208/225 (92%)	197 (95%)	11 (5%)	0	100	100
All	All	2619/2805 (93%)	2532 (97%)	80 (3%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	C	196	VAL
1	E	196	VAL
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
3	M	109	ALA

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	276/280 (99%)	269 (98%)	7 (2%)	47	76
1	C	276/280 (99%)	268 (97%)	8 (3%)	42	73
1	E	276/280 (99%)	268 (97%)	8 (3%)	42	73
2	B	145/149 (97%)	139 (96%)	6 (4%)	30	64
2	D	145/149 (97%)	139 (96%)	6 (4%)	30	64
2	F	145/149 (97%)	140 (97%)	5 (3%)	37	69
3	L	189/192 (98%)	183 (97%)	6 (3%)	39	71
3	M	139/192 (72%)	134 (96%)	5 (4%)	35	67
3	N	191/192 (100%)	181 (95%)	10 (5%)	23	56
4	H	187/193 (97%)	181 (97%)	6 (3%)	39	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	159/193 (82%)	155 (98%)	4 (2%)	47	76
4	J	183/193 (95%)	177 (97%)	6 (3%)	38	70
All	All	2311/2442 (95%)	2234 (97%)	77 (3%)	38	70

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	22	ASN
1	A	31	ASN
1	A	54	ASN
1	A	144	ASP
1	A	159	SER
1	A	174	SER
2	B	12	ASN
2	B	56	ILE
2	B	110	LEU
2	B	120	GLU
2	B	121	LYS
2	B	144	CYS
1	C	18	HIS
1	C	22	ASN
1	C	31	ASN
1	C	54	ASN
1	C	144	ASP
1	C	159	SER
1	C	174	SER
1	C	321	ARG
2	D	12	ASN
2	D	51	LYS
2	D	56	ILE
2	D	120	GLU
2	D	121	LYS
2	D	144	CYS
1	E	18	HIS
1	E	22	ASN
1	E	31	ASN
1	E	54	ASN
1	E	55	PRO
1	E	144	ASP
1	E	159	SER

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Mol	Chain	Res	Type
1	E	174	SER
2	F	12	ASN
2	F	56	ILE
2	F	120	GLU
2	F	121	LYS
2	F	144	CYS
3	L	31	THR
3	L	106	ILE
3	L	116	SER
3	L	175	MET
3	L	176	SER
3	L	210	ASN
4	H	43	HIS
4	H	53	GLU
4	H	115	LYS
4	H	177	LEU
4	H	186	SER
4	H	195	CYS
3	M	31	THR
3	M	106	ILE
3	M	107	LYS
3	M	108	ARG
3	M	110	ASP
4	I	40	ARG
4	I	43	HIS
4	I	53	GLU
4	I	177	LEU
3	N	31	THR
3	N	106	ILE
3	N	108	ARG
3	N	116	SER
3	N	127	SER
3	N	144	ILE
3	N	168	SER
3	N	174	SER
3	N	191	SER
3	N	197	THR
4	J	43	HIS
4	J	53	GLU
4	J	120	SER
4	J	140	CYS
4	J	161	SER

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Mol	Chain	Res	Type
4	J	197	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	164	GLN
1	A	246	ASN
2	B	12	ASN
2	B	26	HIS
2	B	27	GLN
2	B	125	GLN
1	C	54	ASN
1	C	122	ASN
1	C	164	GLN
2	D	26	HIS
2	D	27	GLN
2	D	125	GLN
1	E	54	ASN
1	E	164	GLN
2	F	26	HIS
2	F	27	GLN
2	F	125	GLN
3	L	42	GLN
3	L	124	GLN
3	M	42	GLN
3	N	42	GLN
4	J	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PCA	H	1	4	7,8,9	2.17	2 (28%)	9,10,12	2.07	6 (66%)
4	PCA	I	1	4	7,8,9	2.24	2 (28%)	9,10,12	2.13	6 (66%)
4	PCA	J	1	4	7,8,9	2.34	2 (28%)	9,10,12	2.07	5 (55%)

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	PCA	H	1	4	-	0/0/11/13	0/1/1/1
4	PCA	I	1	4	-	0/0/11/13	0/1/1/1
4	PCA	J	1	4	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	PCA	CD-N	4.80	1.47	1.34
4	I	1	PCA	CD-N	4.56	1.46	1.34
4	H	1	PCA	CD-N	4.47	1.46	1.34
4	J	1	PCA	CA-N	3.75	1.50	1.46
4	I	1	PCA	CA-N	3.59	1.50	1.46
4	H	1	PCA	CA-N	3.40	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	PCA	CA-N-CD	-3.04	103.17	113.58
4	J	1	PCA	CA-N-CD	-3.00	103.32	113.58
4	H	1	PCA	CA-N-CD	-2.97	103.41	113.58
4	J	1	PCA	OE-CD-CG	-2.78	121.91	126.76
4	H	1	PCA	CB-CA-N	2.69	111.03	103.30
4	I	1	PCA	CB-CA-N	2.68	110.98	103.30
4	I	1	PCA	OE-CD-CG	-2.66	122.11	126.76
4	H	1	PCA	CB-CA-C	-2.62	109.09	112.70
4	J	1	PCA	CB-CA-N	2.62	110.83	103.30
4	I	1	PCA	CB-CA-C	-2.47	109.30	112.70
4	H	1	PCA	OE-CD-CG	-2.43	122.51	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	PCA	CG-CD-N	2.41	114.64	108.39
4	J	1	PCA	CG-CD-N	2.33	114.41	108.39
4	J	1	PCA	CB-CA-C	-2.22	109.64	112.70
4	H	1	PCA	CG-CD-N	2.20	114.08	108.39
4	I	1	PCA	O-C-CA	-2.13	119.21	124.78
4	H	1	PCA	O-C-CA	-2.02	119.48	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

39 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	$\# Z > 2$
5	NAG	G	1	1,5	14,14,15	0.66	0	17,19,21	1.03	1 (5%)
5	NAG	G	2	5	14,14,15	0.57	0	17,19,21	0.70	0
6	NAG	K	1	1,6	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
6	NAG	K	2	6	14,14,15	0.62	0	17,19,21	1.08	1 (5%)
6	BMA	K	3	6	11,11,12	0.70	0	15,15,17	0.90	1 (6%)
6	MAN	K	4	6	11,11,12	0.65	0	15,15,17	0.83	0
6	MAN	K	5	6	11,11,12	0.65	0	15,15,17	1.67	2 (13%)
5	NAG	O	1	1,5	14,14,15	0.51	0	17,19,21	1.38	2 (11%)
5	NAG	O	2	5	14,14,15	0.48	0	17,19,21	0.85	1 (5%)
5	NAG	P	1	1,5	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
5	NAG	P	2	5	14,14,15	0.59	0	17,19,21	0.72	0
6	NAG	Q	1	1,6	14,14,15	0.58	0	17,19,21	1.13	1 (5%)
6	NAG	Q	2	6	14,14,15	0.62	0	17,19,21	1.12	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	Q	3	6	11,11,12	0.78	0	15,15,17	1.14	1 (6%)
6	MAN	Q	4	6	11,11,12	0.63	0	15,15,17	0.92	0
6	MAN	Q	5	6	11,11,12	0.56	0	15,15,17	1.79	3 (20%)
7	NAG	R	1	1,7	14,14,15	0.55	0	17,19,21	1.54	1 (5%)
7	NAG	R	2	7	14,14,15	0.48	0	17,19,21	1.10	1 (5%)
7	BMA	R	3	7	11,11,12	0.64	0	15,15,17	1.30	2 (13%)
8	NAG	S	1	1,8	14,14,15	0.53	0	17,19,21	1.09	2 (11%)
8	NAG	S	2	8	14,14,15	0.57	0	17,19,21	0.94	1 (5%)
8	BMA	S	3	8	11,11,12	0.67	0	15,15,17	0.88	0
8	MAN	S	4	8	11,11,12	0.65	0	15,15,17	0.79	1 (6%)
7	NAG	T	1	1,7	14,14,15	0.72	0	17,19,21	1.02	2 (11%)
7	NAG	T	2	7	14,14,15	0.55	0	17,19,21	0.74	0
7	BMA	T	3	7	11,11,12	0.52	0	15,15,17	1.15	1 (6%)
5	NAG	U	1	1,5	14,14,15	0.53	0	17,19,21	1.02	1 (5%)
5	NAG	U	2	5	14,14,15	0.70	1 (7%)	17,19,21	1.05	1 (5%)
6	NAG	V	1	1,6	14,14,15	0.63	0	17,19,21	1.16	2 (11%)
6	NAG	V	2	6	14,14,15	0.64	0	17,19,21	1.09	2 (11%)
6	BMA	V	3	6	11,11,12	0.88	1 (9%)	15,15,17	1.11	1 (6%)
6	MAN	V	4	6	11,11,12	0.65	0	15,15,17	0.77	0
6	MAN	V	5	6	11,11,12	0.62	0	15,15,17	1.73	3 (20%)
8	NAG	W	1	1,8	14,14,15	0.45	0	17,19,21	1.54	1 (5%)
8	NAG	W	2	8	14,14,15	0.49	0	17,19,21	1.11	1 (5%)
8	BMA	W	3	8	11,11,12	0.55	0	15,15,17	1.13	2 (13%)
8	MAN	W	4	8	11,11,12	0.62	0	15,15,17	0.75	0
5	NAG	X	1	5,4	14,14,15	0.66	0	17,19,21	0.97	1 (5%)
5	NAG	X	2	5	14,14,15	0.54	0	17,19,21	1.18	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	3/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	0/2/19/22	0/1/1/1
7	NAG	R	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
8	NAG	S	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
7	NAG	T	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	2/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
8	NAG	W	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	0/2/19/22	0/1/1/1
8	MAN	W	4	8	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	2	NAG	C1-C2	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	3	BMA	O5-C1	-2.12	1.40	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	1	NAG	C1-O5-C5	5.46	119.59	112.19
8	W	1	NAG	C1-O5-C5	5.21	119.25	112.19
6	Q	5	MAN	C1-O5-C5	4.36	118.10	112.19
6	V	5	MAN	C1-O5-C5	4.29	118.01	112.19
5	O	1	NAG	C1-O5-C5	4.16	117.82	112.19
7	R	2	NAG	C1-O5-C5	3.75	117.27	112.19
8	W	2	NAG	C1-O5-C5	3.73	117.25	112.19
7	T	3	BMA	O5-C5-C6	3.61	112.86	107.20
6	K	5	MAN	C1-O5-C5	3.60	117.06	112.19
7	R	3	BMA	O5-C5-C6	3.42	112.56	107.20
6	V	1	NAG	C1-O5-C5	3.40	116.80	112.19
6	K	5	MAN	O5-C5-C6	-3.34	101.97	107.20
6	Q	1	NAG	C1-O5-C5	3.32	116.68	112.19
8	S	1	NAG	C2-N2-C7	-3.30	118.20	122.90
7	R	3	BMA	C1-C2-C3	3.23	113.63	109.67
8	W	3	BMA	O5-C5-C6	3.12	112.09	107.20
6	Q	5	MAN	O2-C2-C3	-3.00	104.13	110.14
6	K	1	NAG	C1-O5-C5	2.98	116.23	112.19
6	K	2	NAG	O5-C5-C6	2.89	111.73	107.20
6	Q	2	NAG	O5-C5-C6	2.87	111.70	107.20
6	Q	3	BMA	O5-C5-C6	2.86	111.69	107.20
6	V	5	MAN	O5-C5-C6	-2.85	102.74	107.20
5	U	1	NAG	C4-C3-C2	2.81	115.13	111.02
6	V	3	BMA	O5-C5-C6	2.73	111.49	107.20
5	U	2	NAG	O5-C5-C6	2.69	111.42	107.20
5	O	2	NAG	C1-O5-C5	2.68	115.83	112.19
5	X	2	NAG	C4-C3-C2	-2.64	107.15	111.02
8	S	2	NAG	O5-C5-C6	2.61	111.29	107.20
6	V	2	NAG	O5-C5-C6	2.55	111.21	107.20
6	V	5	MAN	C1-C2-C3	2.54	112.79	109.67
8	W	3	BMA	C1-C2-C3	2.51	112.75	109.67
5	X	1	NAG	O5-C1-C2	-2.51	107.33	111.29
6	K	3	BMA	O5-C5-C6	2.41	110.98	107.20
5	P	1	NAG	O5-C1-C2	-2.40	107.49	111.29
7	T	1	NAG	O5-C1-C2	-2.39	107.51	111.29
6	V	2	NAG	O5-C1-C2	-2.22	107.78	111.29
5	G	1	NAG	O5-C1-C2	-2.21	107.80	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C2-N2-C7	-2.21	119.76	122.90
6	Q	5	MAN	C1-C2-C3	2.19	112.36	109.67
6	Q	2	NAG	C2-N2-C7	-2.16	119.83	122.90
6	V	1	NAG	O5-C1-C2	-2.16	107.88	111.29
8	S	4	MAN	C1-C2-C3	2.13	112.28	109.67
5	X	2	NAG	C1-C2-N2	2.11	114.09	110.49
8	S	1	NAG	C1-O5-C5	2.11	115.05	112.19
6	Q	2	NAG	O5-C1-C2	-2.09	107.99	111.29
7	T	1	NAG	C2-N2-C7	-2.07	119.96	122.90

There are no chirality outliers.

All (28) torsion outliers are listed below:

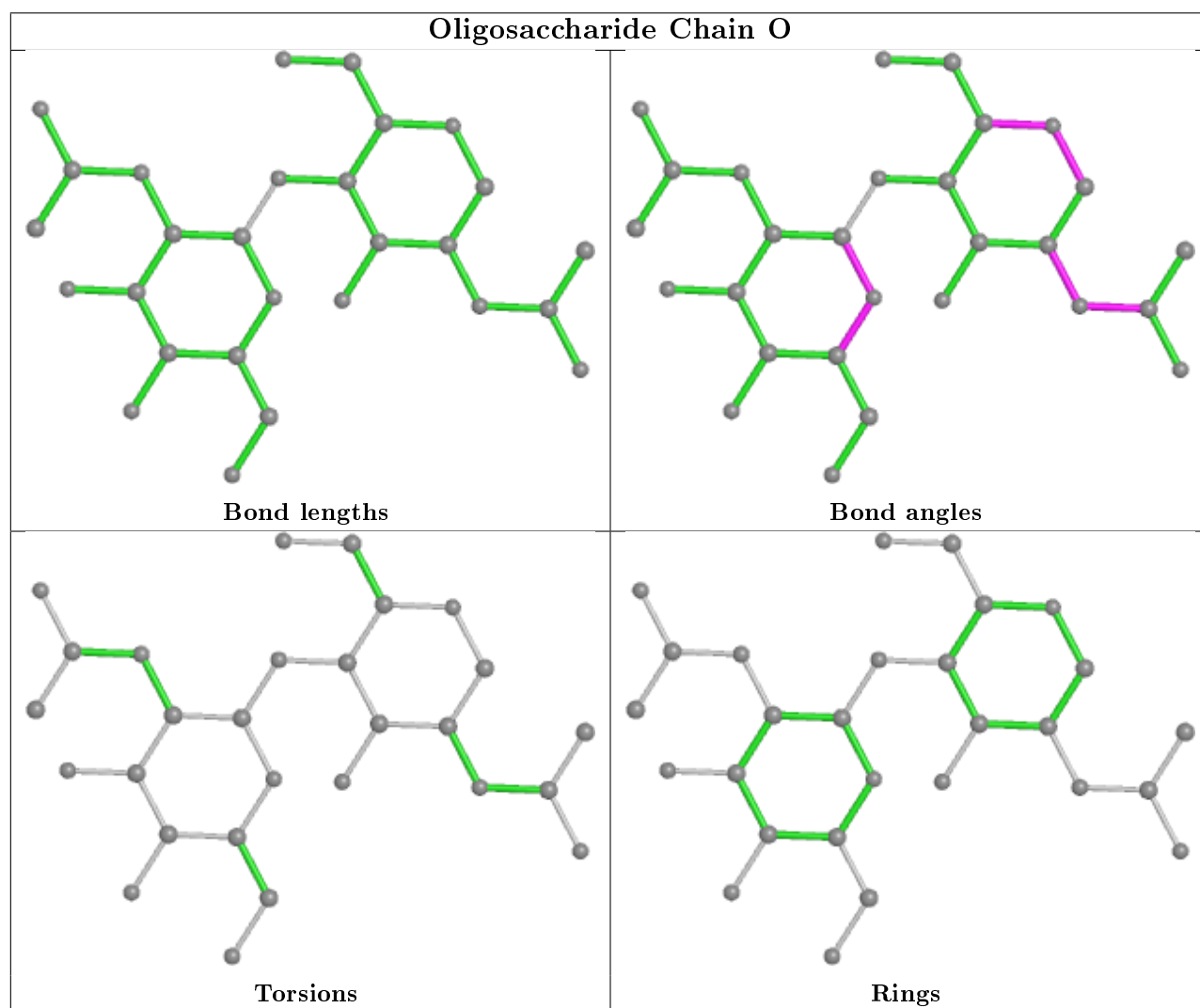
Mol	Chain	Res	Type	Atoms
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	K	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	3	BMA	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	V	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	Q	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O7-C7-N2-C2
6	V	3	BMA	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	V	2	NAG	O7-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
5	X	2	NAG	O5-C5-C6-O6
7	T	3	BMA	C4-C5-C6-O6
7	T	3	BMA	O5-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6

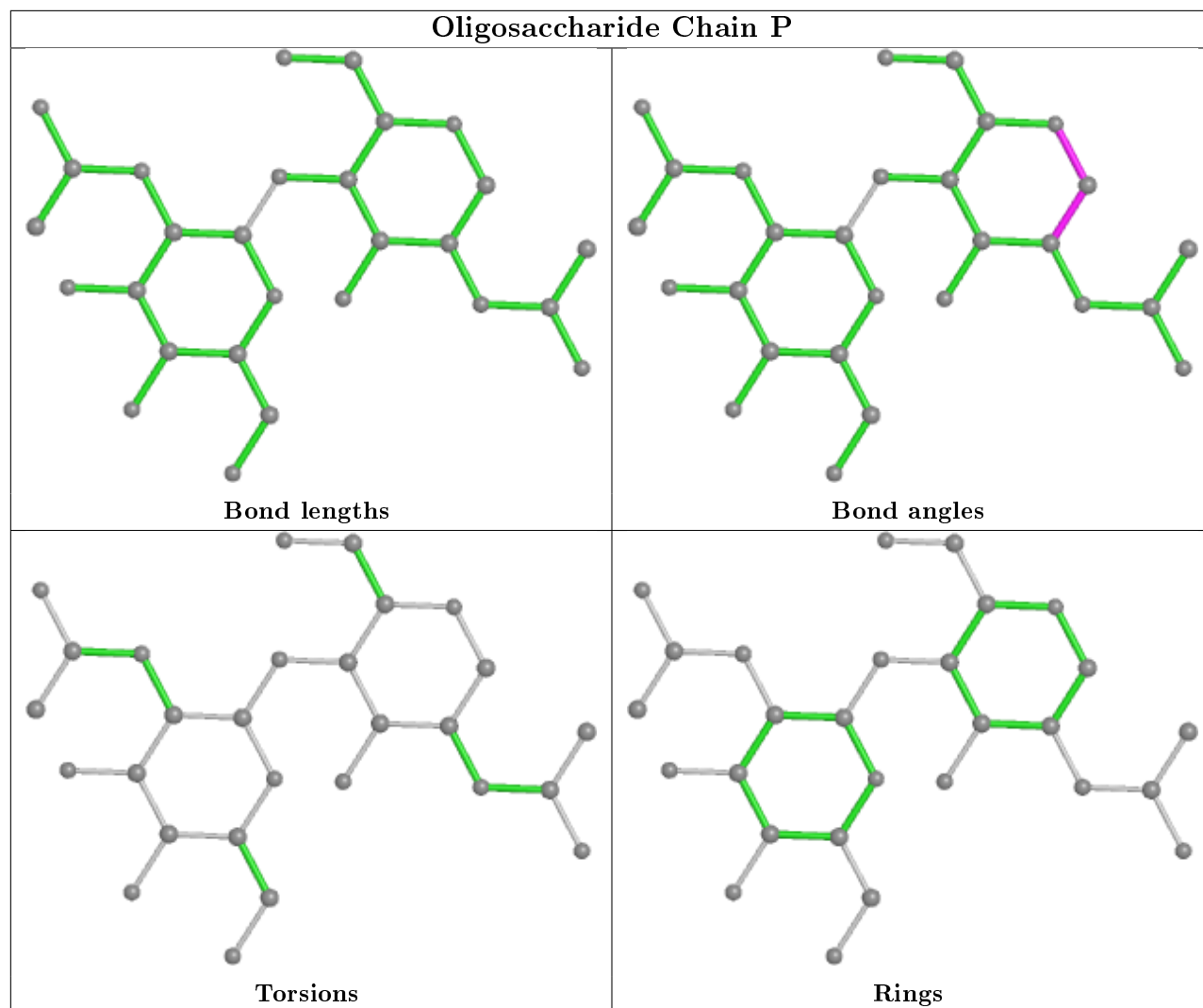
There are no ring outliers.

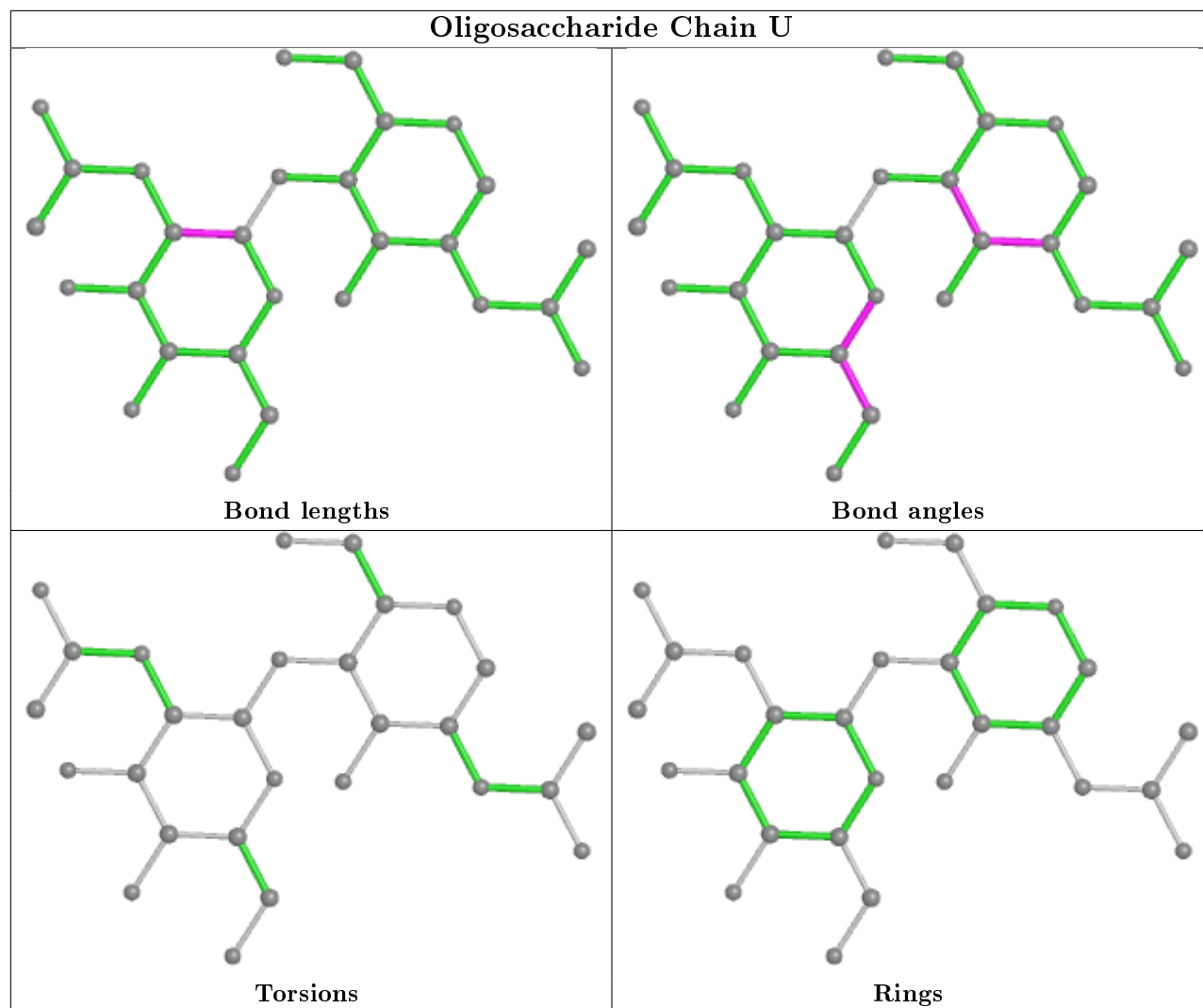
5 monomers are involved in 4 short contacts:

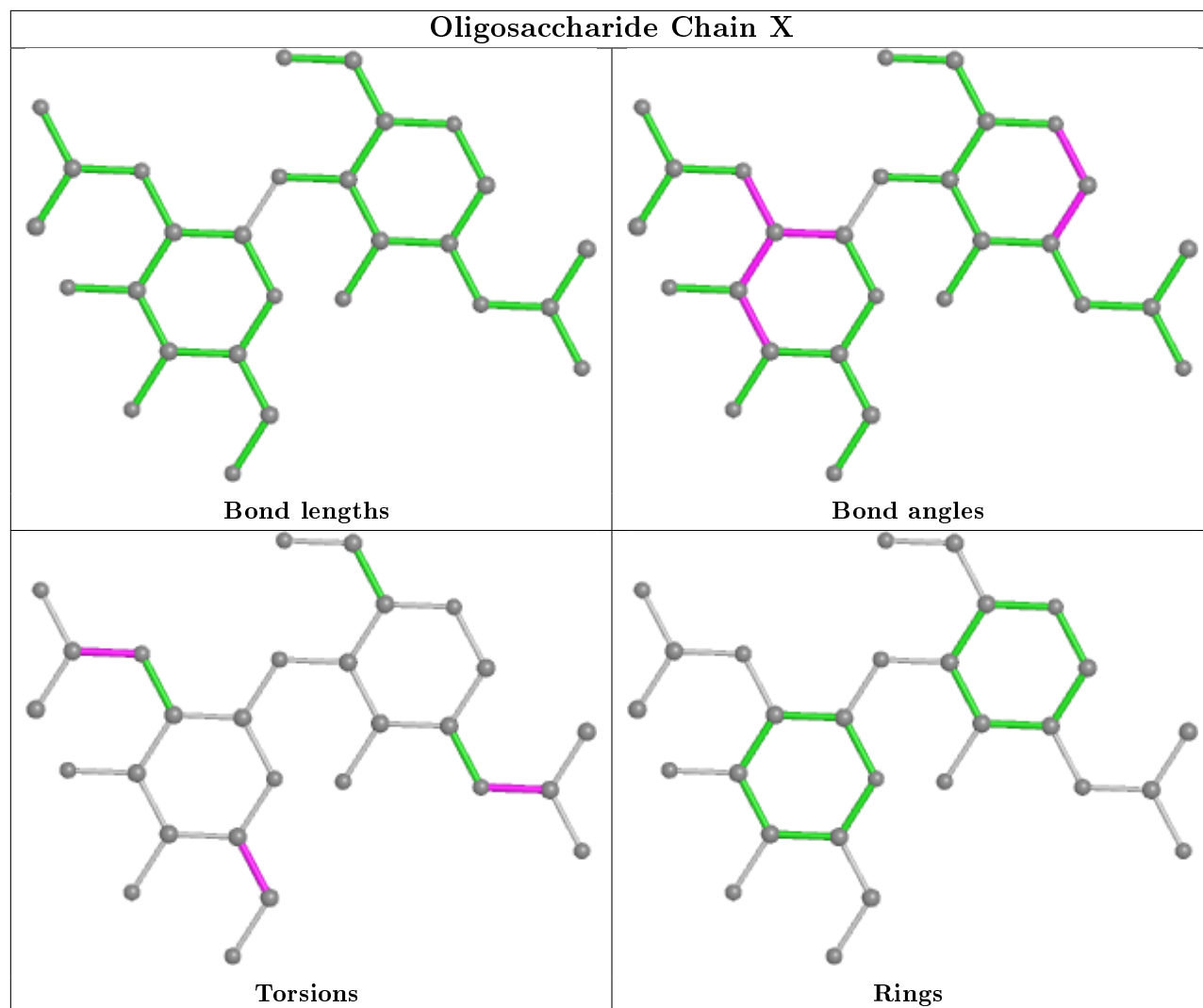
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	2	NAG	1	0
7	T	3	BMA	1	0
6	V	1	NAG	1	0
6	K	1	NAG	1	0
6	Q	1	NAG	1	0

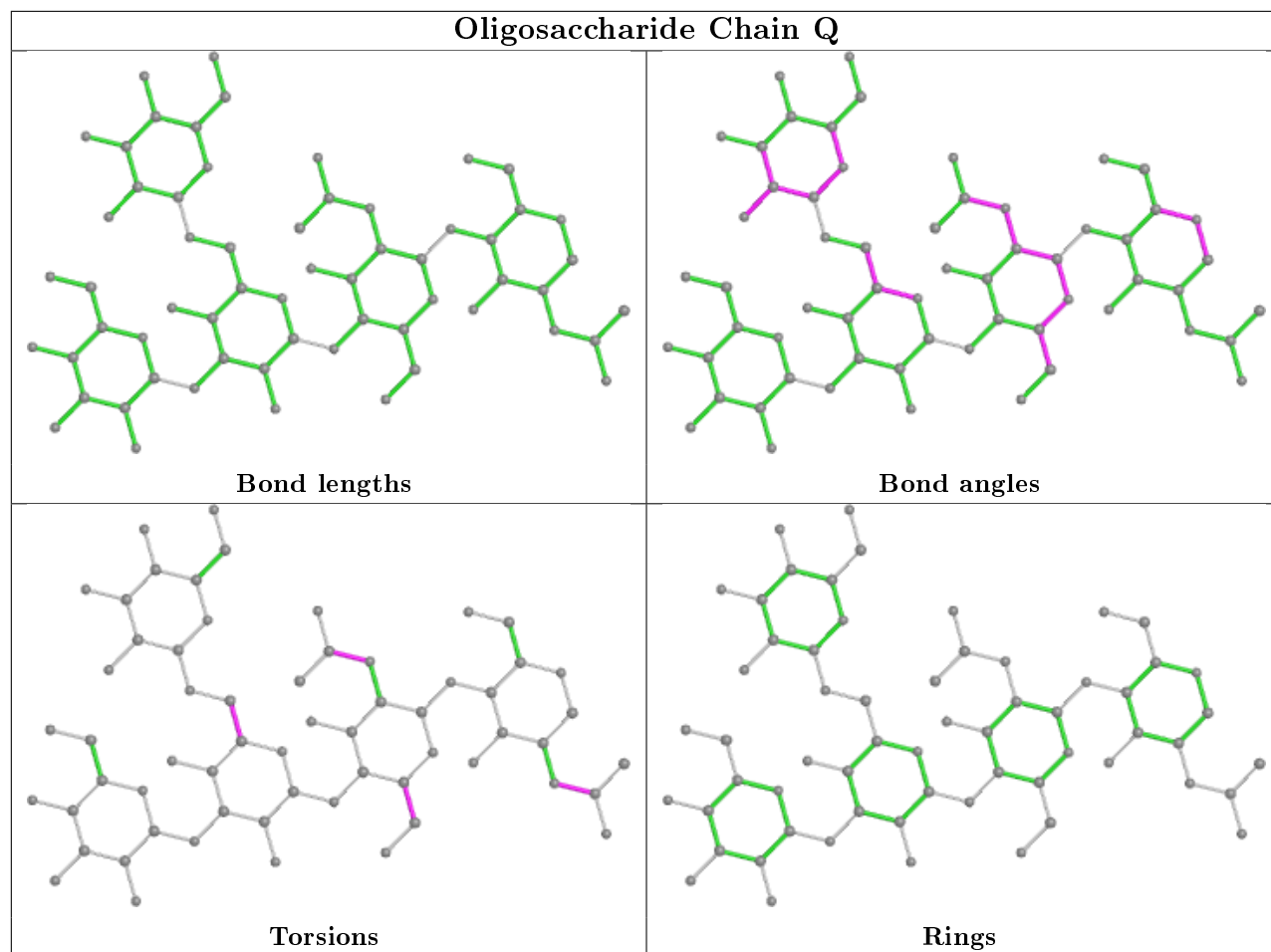
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

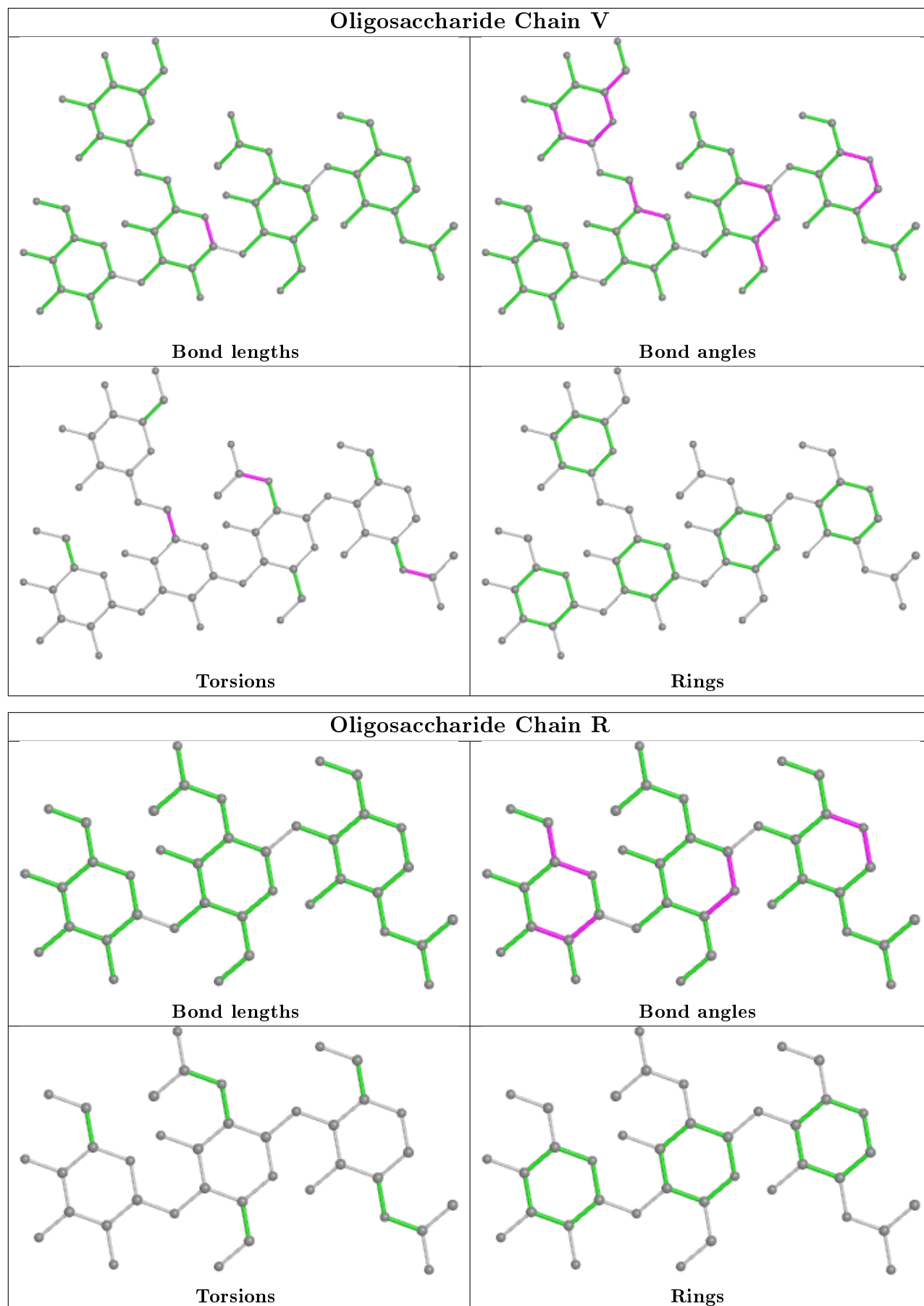


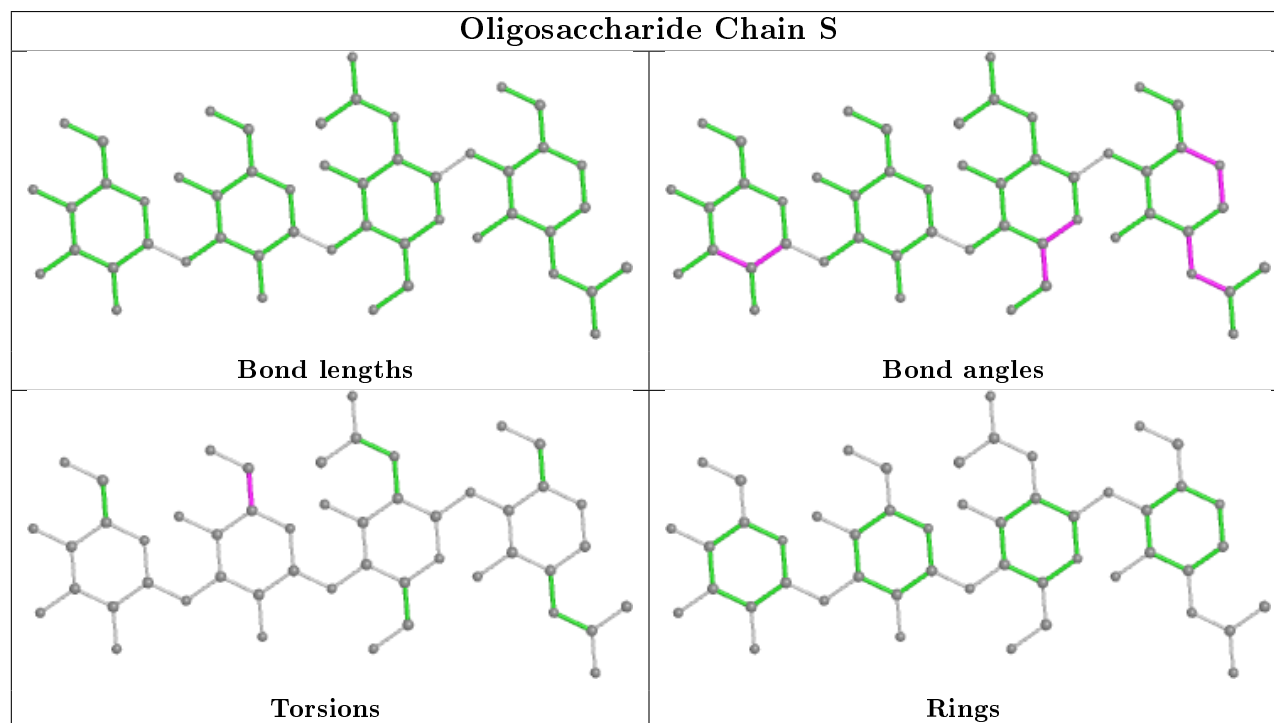
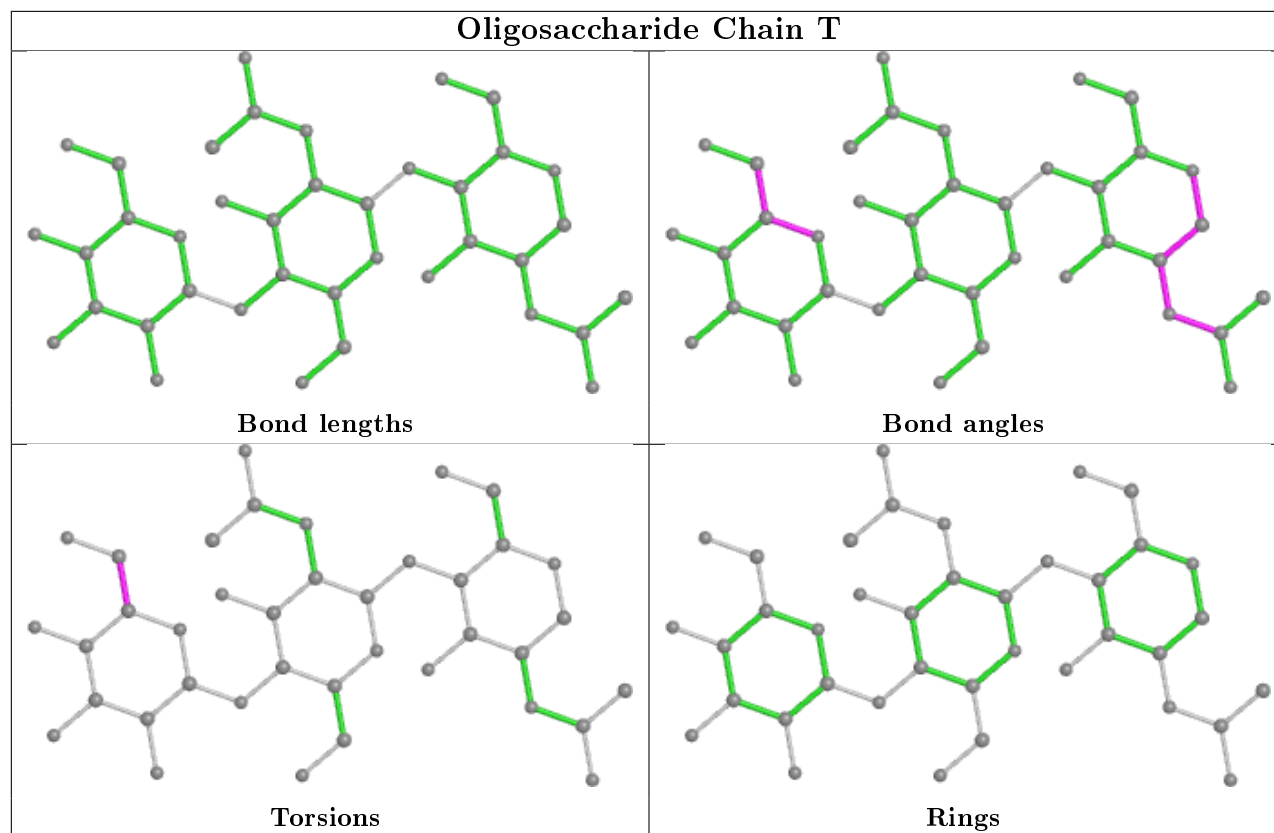


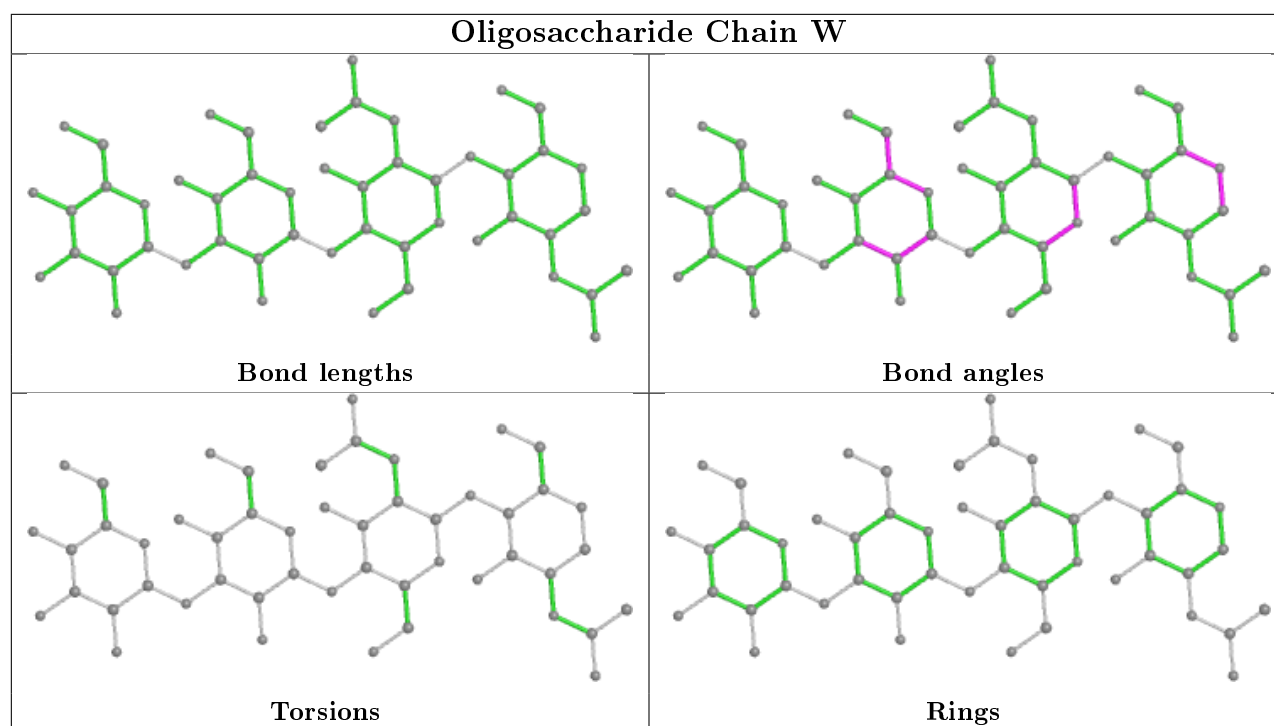












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
10	SO4	F	202	-	4,4,4	0.17	0	6,6,6	0.25	0
9	NAG	J	301	4	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
10	SO4	D	202	-	4,4,4	0.13	0	6,6,6	0.15	0
9	NAG	I	301	4	14,14,15	0.49	0	17,19,21	0.90	1 (5%)
9	NAG	F	201	2	14,14,15	0.54	0	17,19,21	0.92	1 (5%)
10	SO4	B	203	-	4,4,4	0.15	0	6,6,6	0.09	0
10	SO4	A	516	-	4,4,4	0.13	0	6,6,6	0.27	0
9	NAG	A	504	1	14,14,15	0.53	0	17,19,21	0.92	1 (5%)
9	NAG	A	501	1	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
11	GOL	D	204	-	5,5,5	0.56	0	5,5,5	0.70	0
9	NAG	B	201	2	14,14,15	0.56	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	C	514	-	4,4,4	0.14	0	6,6,6	0.18	0
10	SO4	C	513	-	4,4,4	0.14	0	6,6,6	0.13	0
10	SO4	I	302	-	4,4,4	0.14	0	6,6,6	0.18	0
9	NAG	D	201	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
10	SO4	H	303	-	4,4,4	0.16	0	6,6,6	0.22	0
10	SO4	B	202	-	4,4,4	0.13	0	6,6,6	0.15	0
10	SO4	C	515	-	4,4,4	0.15	0	6,6,6	0.33	0
12	PG4	E	520	-	12,12,12	0.54	0	11,11,11	0.27	0
10	SO4	A	514	-	4,4,4	0.15	0	6,6,6	0.23	0
10	SO4	A	513	-	4,4,4	0.15	0	6,6,6	0.49	0
10	SO4	B	204	-	4,4,4	0.18	0	6,6,6	0.33	0
10	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.16	0
10	SO4	A	512	-	4,4,4	0.13	0	6,6,6	0.07	0
9	NAG	C	504	1	14,14,15	0.54	0	17,19,21	0.94	3 (17%)
10	SO4	A	515	-	4,4,4	0.12	0	6,6,6	0.33	0
9	NAG	C	501	1	14,14,15	0.53	0	17,19,21	0.83	0
11	GOL	B	205	-	5,5,5	0.53	0	5,5,5	0.69	0
10	SO4	E	519	-	4,4,4	0.12	0	6,6,6	0.73	0
10	SO4	D	203	-	4,4,4	0.15	0	6,6,6	0.54	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
9	NAG	B	201	2	-	2/6/23/26	0/1/1/1
9	NAG	D	201	2	-	2/6/23/26	0/1/1/1
9	NAG	J	301	4	-	2/6/23/26	0/1/1/1
9	NAG	A	501	1	-	0/6/23/26	0/1/1/1
9	NAG	C	504	1	-	0/6/23/26	0/1/1/1
12	PG4	E	520	-	-	5/10/10/10	-
11	GOL	D	204	-	-	3/4/4/4	-
9	NAG	A	504	1	-	0/6/23/26	0/1/1/1
9	NAG	C	501	1	-	0/6/23/26	0/1/1/1
11	GOL	B	205	-	-	2/4/4/4	-
9	NAG	I	301	4	-	2/6/23/26	0/1/1/1
9	NAG	F	201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	201	NAG	C1-O5-C5	3.04	116.31	112.19
9	B	201	NAG	C1-O5-C5	2.99	116.25	112.19
9	F	201	NAG	C1-O5-C5	2.98	116.22	112.19
9	I	301	NAG	O5-C5-C6	2.30	110.80	107.20
9	A	501	NAG	C2-N2-C7	-2.21	119.75	122.90
9	C	504	NAG	C4-C3-C2	2.15	114.16	111.02
9	A	504	NAG	C4-C3-C2	2.12	114.12	111.02
9	J	301	NAG	O5-C5-C6	2.07	110.44	107.20
9	C	504	NAG	C1-O5-C5	2.04	114.96	112.19
9	C	504	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	301	NAG	C8-C7-N2-C2
9	J	301	NAG	O7-C7-N2-C2
9	I	301	NAG	C8-C7-N2-C2
9	I	301	NAG	O7-C7-N2-C2
11	D	204	GOL	O1-C1-C2-C3
12	E	520	PG4	O2-C3-C4-O3
11	B	205	GOL	O1-C1-C2-C3
12	E	520	PG4	O4-C7-C8-O5
11	D	204	GOL	O1-C1-C2-O2
9	B	201	NAG	C4-C5-C6-O6
9	D	201	NAG	C4-C5-C6-O6
12	E	520	PG4	O3-C5-C6-O4
11	B	205	GOL	O1-C1-C2-O2
9	F	201	NAG	C4-C5-C6-O6
9	B	201	NAG	O5-C5-C6-O6
9	D	201	NAG	O5-C5-C6-O6
12	E	520	PG4	O1-C1-C2-O2
9	F	201	NAG	O5-C5-C6-O6
11	D	204	GOL	O2-C2-C3-O3
12	E	520	PG4	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	203	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	204	GOL	1	0
10	I	302	SO4	1	0
12	E	520	PG4	1	0
10	A	514	SO4	1	0
11	B	205	GOL	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	316/320 (98%)	0.24	4 (1%) 77 61	62, 83, 113, 146	0
1	C	316/320 (98%)	0.27	6 (1%) 66 49	60, 83, 120, 188	0
1	E	316/320 (98%)	0.15	2 (0%) 89 78	49, 74, 105, 166	0
2	B	171/176 (97%)	0.13	3 (1%) 68 51	52, 86, 118, 189	0
2	D	171/176 (97%)	0.20	2 (1%) 79 63	56, 92, 128, 160	0
2	F	171/176 (97%)	0.18	3 (1%) 68 51	53, 82, 116, 166	0
3	L	211/214 (98%)	0.80	28 (13%) 3 2	84, 122, 154, 196	0
3	M	156/214 (72%)	1.27	33 (21%) 0 0	66, 132, 197, 239	0
3	N	213/214 (99%)	0.79	24 (11%) 5 3	85, 131, 174, 199	0
4	H	217/225 (96%)	0.18	4 (1%) 68 51	78, 101, 135, 200	0
4	I	185/225 (82%)	1.68	59 (31%) 0 0	85, 141, 218, 287	0
4	J	211/225 (93%)	0.70	28 (13%) 3 2	74, 129, 188, 226	0
All	All	2654/2805 (94%)	0.50	196 (7%) 14 8	49, 97, 174, 287	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	152	LEU	9.1
4	I	141	LEU	8.7
4	I	144	GLY	8.3
4	I	183	VAL	8.2
3	M	136	LEU	8.2
4	I	151	THR	7.1
4	I	121	VAL	6.8
3	M	135	PHE	6.8
4	I	202	SER	6.7
3	M	132	VAL	6.7
4	I	123	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
4	I	126	PRO	6.6
4	I	118	ALA	6.5
3	M	159	VAL	6.5
3	M	114	THR	6.2
3	M	134	CYS	6.2
4	I	124	LEU	6.2
3	M	160	LEU	5.9
4	I	119	PRO	5.5
4	I	150	VAL	5.5
4	I	203	SER	5.5
4	I	140	CYS	5.4
4	I	179	SER	5.4
2	B	58	LYS	5.3
4	I	136	VAL	5.3
3	M	118	PHE	5.2
4	J	213	ARG	5.2
3	M	180	THR	5.1
3	M	133	VAL	5.1
3	M	161	ASN	5.0
4	I	111	VAL	4.9
3	M	113	PRO	4.8
4	I	175	TYR	4.7
4	J	197	VAL	4.6
3	L	155	ARG	4.6
4	I	125	ALA	4.5
3	M	116	SER	4.5
4	I	122	TYR	4.5
3	N	104	LEU	4.5
3	L	186	TYR	4.4
4	I	165	THR	4.4
3	L	19	VAL	4.3
4	J	203	SER	4.3
3	M	144	ILE	4.3
4	J	152	LEU	4.2
4	I	82(C)	LEU	4.2
4	I	145	TYR	4.2
4	I	170	LEU	4.1
4	J	205	LYS	4.1
4	I	137	THR	4.0
4	I	138	LEU	3.9
4	I	142	VAL	3.9
3	M	179	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
4	J	123	PRO	3.9
3	M	119	PRO	3.8
4	I	156	SER	3.8
4	I	166	PHE	3.8
4	I	181	VAL	3.7
4	H	205	LYS	3.7
3	M	109	ALA	3.7
4	J	117	THR	3.6
3	M	178	THR	3.6
4	I	184	THR	3.6
4	I	169	VAL	3.6
4	I	198	ALA	3.5
2	D	171	PHE	3.5
4	J	118	ALA	3.5
3	N	179	LEU	3.4
4	I	155	ASN	3.4
4	I	176	THR	3.4
3	N	147	LYS	3.3
3	L	76	THR	3.3
4	J	124	LEU	3.3
3	M	131	SER	3.3
4	J	206	VAL	3.3
3	M	115	VAL	3.3
3	L	148	TRP	3.3
3	N	12	SER	3.3
3	N	11	MET	3.3
4	J	210	ILE	3.2
3	M	117	ILE	3.2
4	I	16	ALA	3.2
3	L	13	THR	3.2
4	J	139	GLY	3.1
4	I	117	THR	3.1
4	J	207	ASP	3.1
3	L	73	LEU	3.1
3	N	153	SER	3.1
4	J	193	ILE	3.1
4	I	139	GLY	3.0
4	I	163	VAL	3.0
4	I	11	LEU	3.0
1	E	222	TRP	3.0
4	I	154	TRP	3.0
4	I	180	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	I	201	ALA	2.9
3	L	81	GLU	2.9
4	I	13	LYS	2.9
3	N	62	PHE	2.9
4	J	140	CYS	2.9
3	N	152	GLY	2.9
3	M	139	PHE	2.9
4	H	128	CYS	2.8
4	J	122	TYR	2.8
4	J	146	PHE	2.8
3	L	1	ASP	2.8
3	M	137	ASN	2.8
4	J	116	THR	2.8
3	N	145	ASN	2.7
2	F	58	LYS	2.7
3	L	104	LEU	2.7
2	B	171	PHE	2.7
4	J	204	THR	2.7
3	N	155	ARG	2.7
3	L	20	SER	2.7
3	M	175	MET	2.7
3	L	9	LYS	2.7
4	J	96	TYR	2.6
1	A	322	ASN	2.6
1	C	40	THR	2.6
1	A	10	GLY	2.6
1	C	227	SER	2.6
4	J	113	ALA	2.6
4	I	182	THR	2.6
4	J	125	ALA	2.6
3	L	21	VAL	2.6
3	L	91	TYR	2.5
1	A	222	TRP	2.5
4	J	11	LEU	2.5
4	I	160	SER	2.5
4	I	204	THR	2.5
4	I	120	SER	2.4
3	M	177	SER	2.4
4	I	146	PHE	2.4
3	L	86	TYR	2.4
2	F	171	PHE	2.4
2	D	58	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	N	4	MET	2.4
1	C	22	ASN	2.4
3	L	63	THR	2.4
3	M	163	TRP	2.4
4	J	198	ALA	2.4
3	L	74	THR	2.3
4	I	187	THR	2.3
1	C	11	ALA	2.3
4	J	209	LYS	2.3
4	H	130	ASP	2.3
3	M	83	LEU	2.3
4	J	119	PRO	2.3
4	J	115	LYS	2.3
4	I	18	VAL	2.3
3	L	185	GLU	2.3
4	I	14	PRO	2.3
4	I	143	LYS	2.3
3	M	13	THR	2.3
4	I	116	THR	2.3
3	M	169	LYS	2.3
3	N	79	GLN	2.3
3	N	129	GLY	2.3
3	N	67	SER	2.2
1	E	104	ASP	2.2
3	N	131	SER	2.2
3	L	10	PHE	2.2
3	N	199	LYS	2.2
3	M	162	SER	2.2
3	N	63	THR	2.2
3	L	183	LYS	2.2
3	N	206	VAL	2.2
4	I	177	LEU	2.2
3	N	156	GLN	2.2
2	F	1	GLY	2.2
4	I	199	HIS	2.2
3	M	140	TYR	2.2
3	L	83	LEU	2.1
3	N	154	GLU	2.1
3	N	148	TRP	2.1
3	M	108	ARG	2.1
4	J	23	LYS	2.1
3	L	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	LEU	2.1
3	L	75	ILE	2.1
3	L	205	ILE	2.1
3	N	60	ASP	2.1
4	I	178	SER	2.1
1	C	274	ILE	2.1
3	L	100	GLY	2.1
2	B	60	ASN	2.1
4	H	127	VAL	2.1
1	C	13	LEU	2.1
3	L	181	LEU	2.1
3	N	195	GLU	2.1
4	I	109	VAL	2.0
3	N	125	LEU	2.0
3	L	48	ILE	2.0
3	M	174	SER	2.0
3	L	192	TYR	2.0

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

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	PCA	J	1	8/9	0.91	0.30	160,164,167,168	0
4	PCA	I	1	8/9	0.92	0.18	152,156,161,164	0
4	PCA	H	1	8/9	0.95	0.16	123,125,127,127	0

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
8	MAN	W	4	11/12	0.59	0.52	214,234,255,259	0
7	BMA	T	3	11/12	0.66	0.29	195,200,206,208	0
6	MAN	Q	5	11/12	0.69	0.40	209,225,234,235	0

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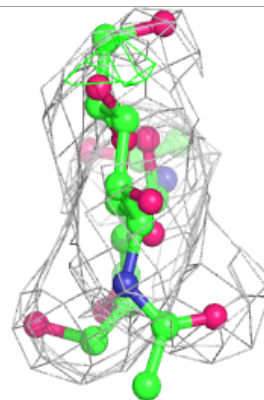
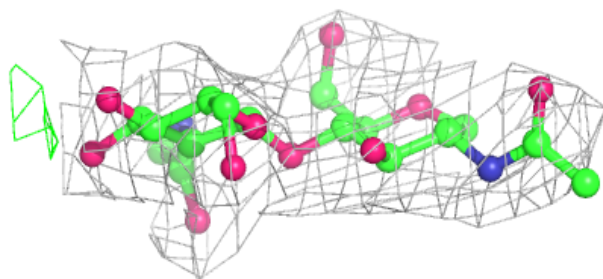
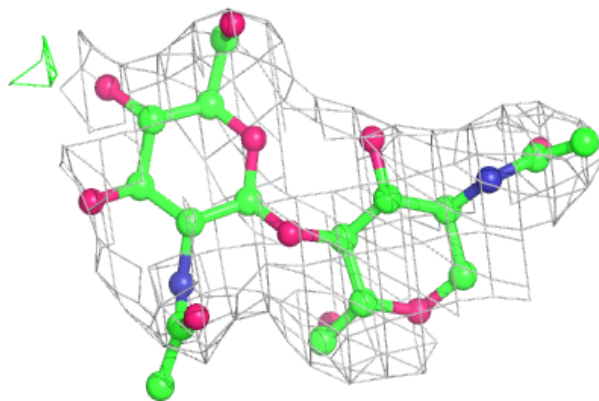
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	BMA	R	3	11/12	0.70	0.41	209,215,227,230	0
6	MAN	K	5	11/12	0.71	0.36	182,197,207,208	0
8	BMA	S	3	11/12	0.72	0.36	179,190,194,196	0
6	MAN	K	4	11/12	0.73	0.35	134,157,185,188	0
8	MAN	S	4	11/12	0.73	0.31	142,168,179,197	0
6	MAN	V	4	11/12	0.75	0.29	132,157,187,187	0
8	NAG	W	2	14/15	0.75	0.27	121,142,150,156	0
5	NAG	U	2	14/15	0.76	0.30	154,181,201,201	0
5	NAG	G	2	14/15	0.76	0.39	164,187,198,205	0
7	NAG	T	2	14/15	0.79	0.34	158,178,183,190	0
6	MAN	Q	4	11/12	0.80	0.33	125,145,170,174	0
5	NAG	P	2	14/15	0.81	0.21	150,173,177,185	0
5	NAG	G	1	14/15	0.84	0.28	99,117,131,137	0
6	MAN	V	5	11/12	0.86	0.23	155,166,182,191	0
8	BMA	W	3	11/12	0.87	0.38	186,193,200,204	0
5	NAG	O	2	14/15	0.87	0.19	125,148,161,162	0
7	NAG	R	2	14/15	0.88	0.21	128,155,169,173	0
8	NAG	S	2	14/15	0.88	0.20	111,132,137,138	0
5	NAG	X	2	14/15	0.89	0.22	165,171,175,177	0
5	NAG	U	1	14/15	0.89	0.40	153,173,185,186	0
6	BMA	K	3	11/12	0.89	0.22	123,134,148,158	0
8	NAG	S	1	14/15	0.90	0.21	102,124,133,136	0
6	BMA	Q	3	11/12	0.90	0.20	116,126,136,143	0
5	NAG	P	1	14/15	0.91	0.19	91,113,128,134	0
6	BMA	V	3	11/12	0.91	0.16	97,110,121,128	0
6	NAG	K	2	14/15	0.92	0.23	103,137,158,163	0
5	NAG	X	1	14/15	0.92	0.12	131,141,153,160	0
7	NAG	R	1	14/15	0.93	0.18	88,109,112,114	0
7	NAG	T	1	14/15	0.93	0.18	76,97,110,115	0
6	NAG	Q	2	14/15	0.94	0.22	102,128,147,149	0
6	NAG	Q	1	14/15	0.95	0.19	88,106,117,118	0
6	NAG	K	1	14/15	0.95	0.21	94,113,128,129	0
6	NAG	V	2	14/15	0.95	0.20	92,122,139,145	0
8	NAG	W	1	14/15	0.96	0.20	72,87,94,96	0
6	NAG	V	1	14/15	0.96	0.18	80,98,111,113	0
5	NAG	O	1	14/15	0.98	0.19	81,98,105,105	0

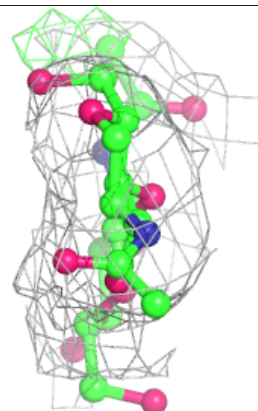
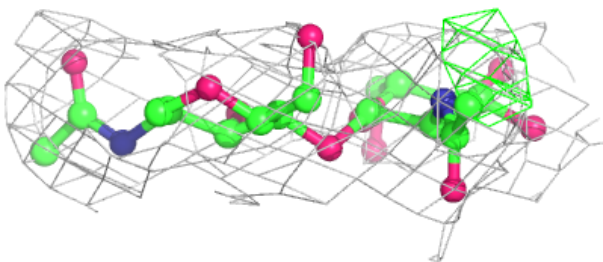
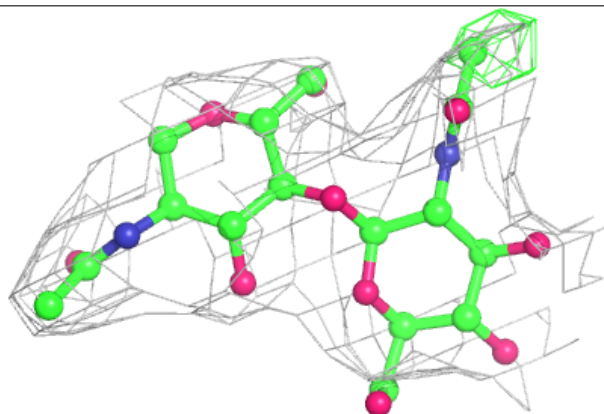
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain O:

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

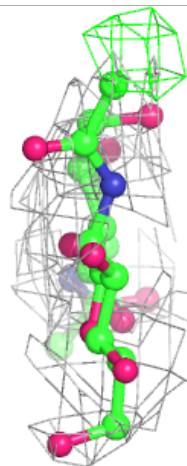
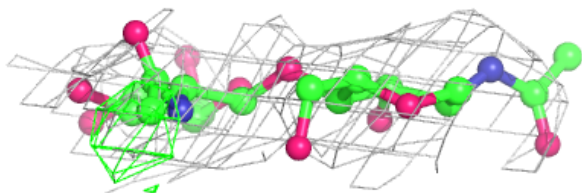
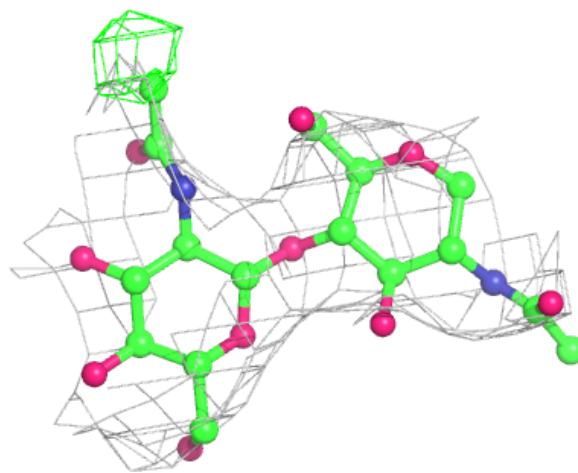
**Electron density around Chain P:**

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



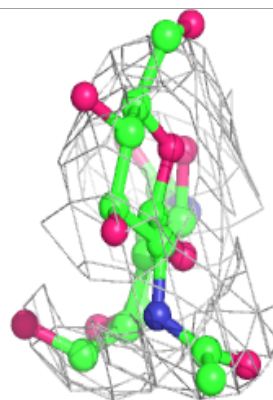
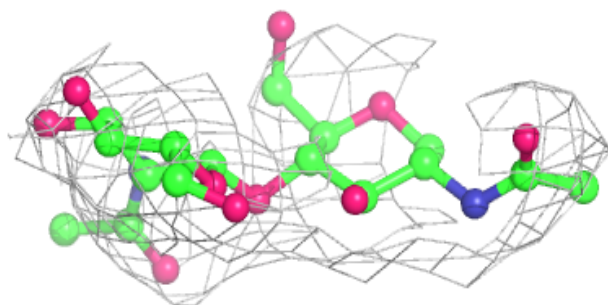
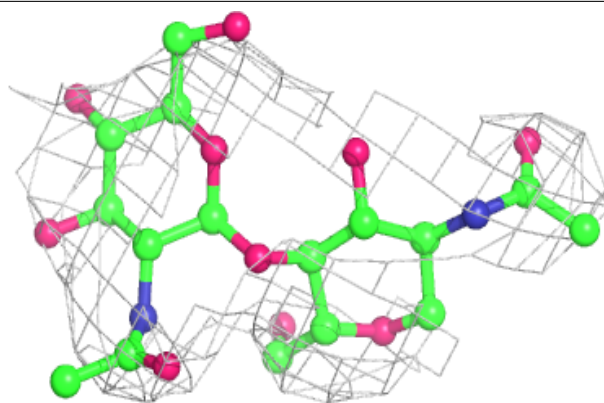
Electron density around Chain U:

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

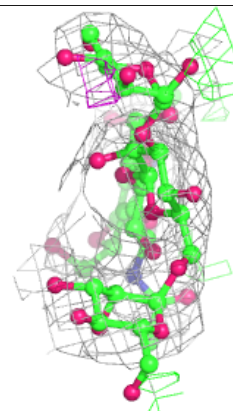
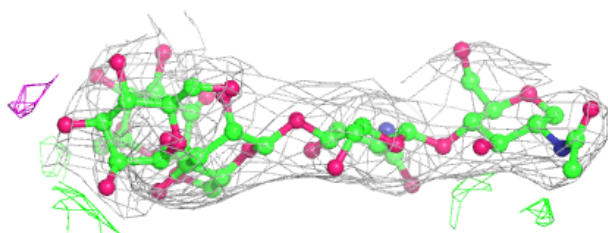
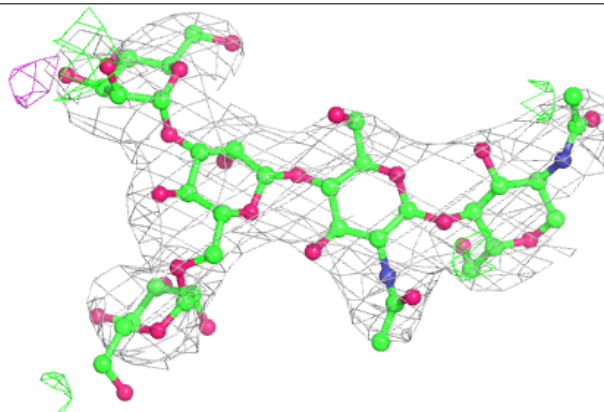


Electron density around Chain X:

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

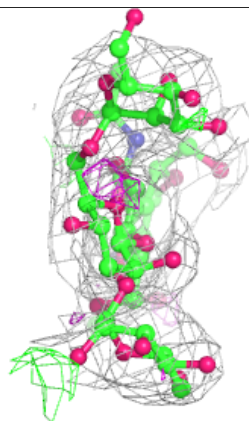
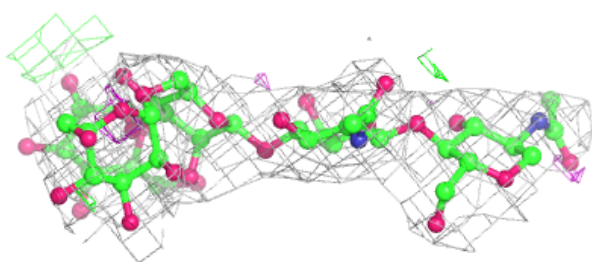
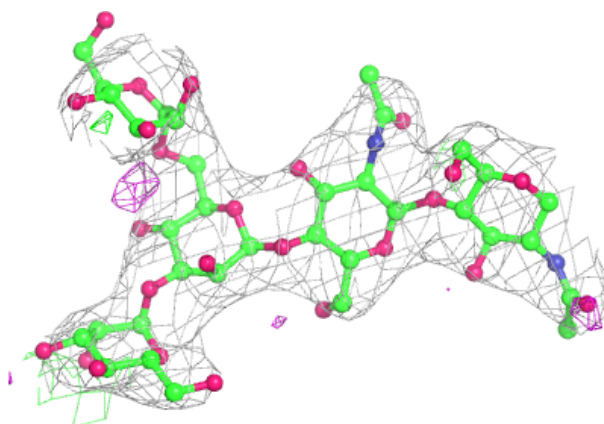
**Electron density around Chain Q:**

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

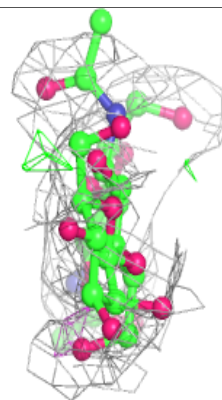
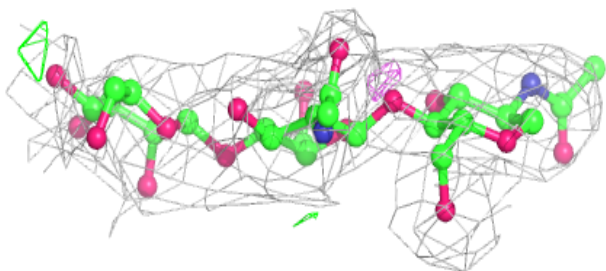
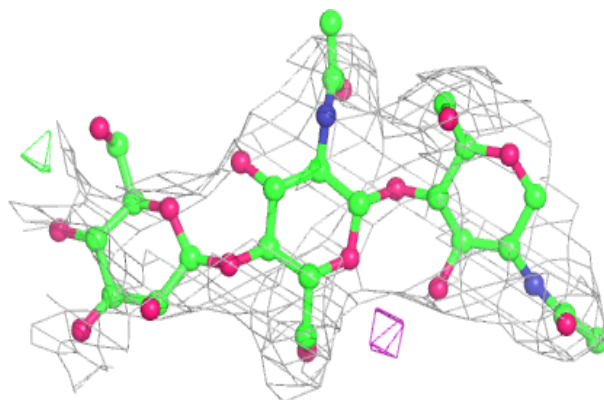


Electron density around Chain V:

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

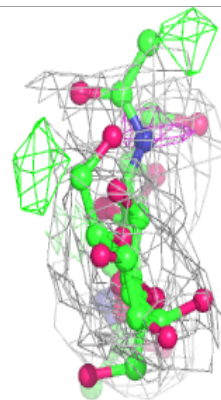
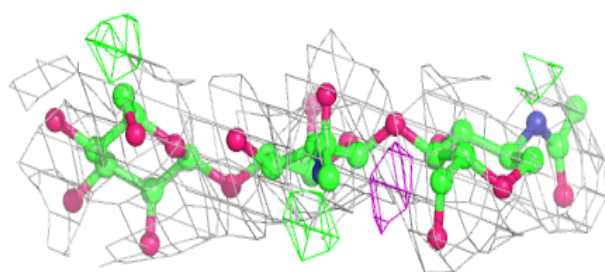
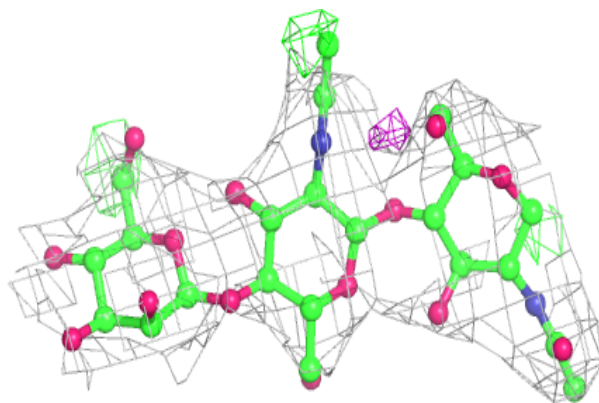
**Electron density around Chain R:**

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

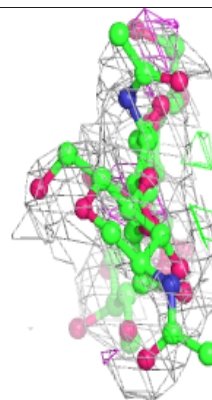
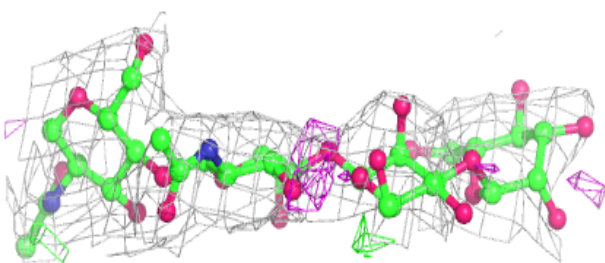
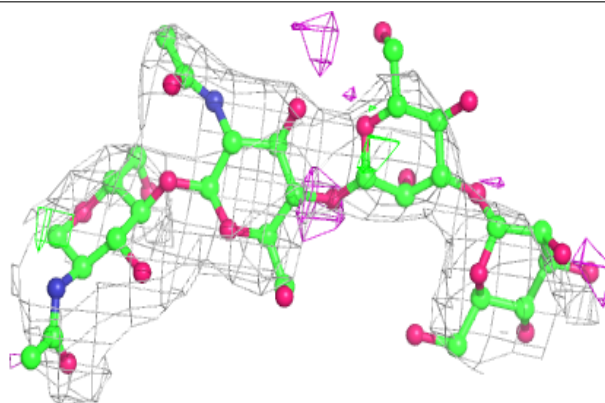


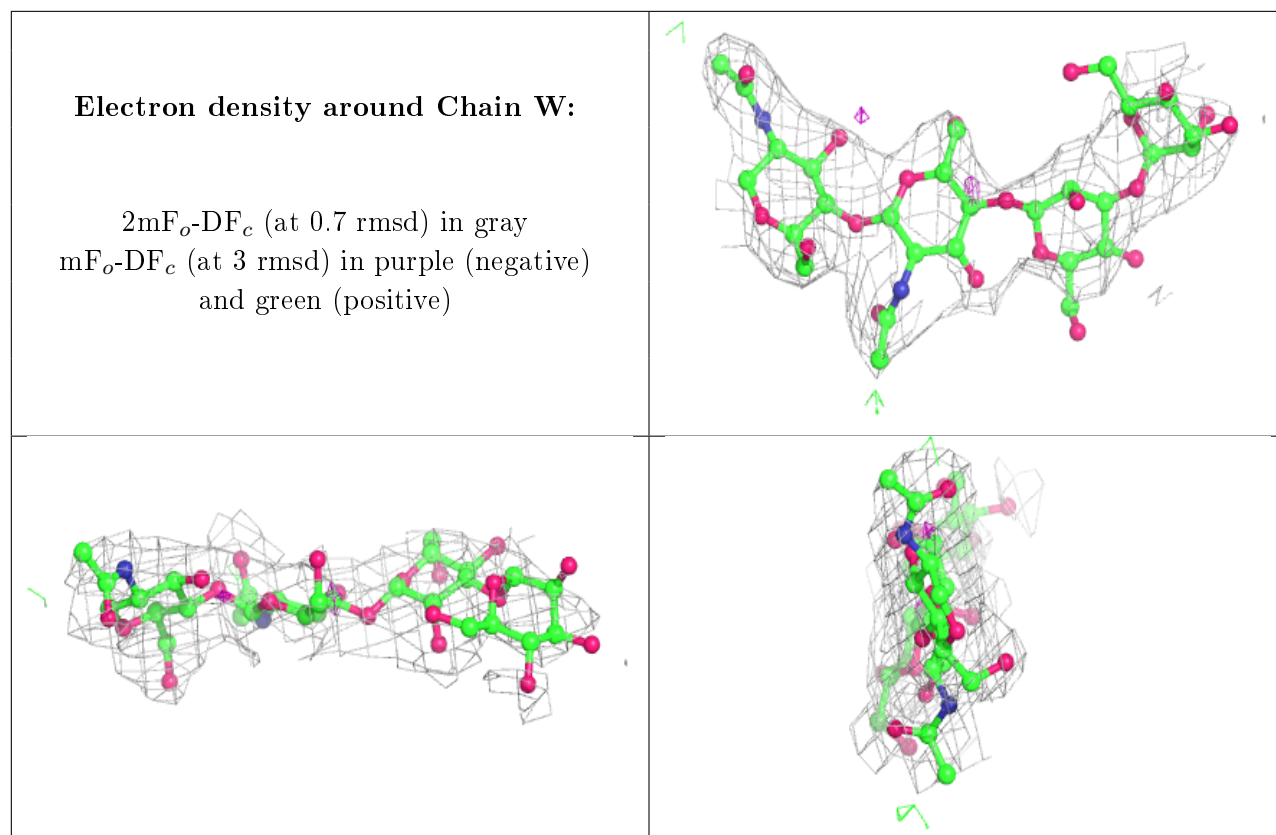
Electron density around Chain T:

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

**Electron density around Chain S:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
10	SO4	A	515	5/5	0.58	0.47	197,197,197,197	0
11	GOL	B	205	6/6	0.64	0.34	100,100,100,100	0
9	NAG	B	201	14/15	0.67	0.29	152,166,178,185	0
11	GOL	D	204	6/6	0.68	0.33	103,103,103,103	0
9	NAG	C	501	14/15	0.75	0.30	145,168,180,184	0
10	SO4	C	515	5/5	0.76	0.35	181,181,181,181	0
10	SO4	I	302	5/5	0.77	0.19	161,161,161,161	0
10	SO4	A	514	5/5	0.78	0.76	181,181,181,181	0
9	NAG	A	501	14/15	0.82	0.28	132,153,159,160	0
9	NAG	A	504	14/15	0.82	0.48	160,181,195,195	0
10	SO4	C	513	5/5	0.82	0.21	183,183,183,183	0
12	PG4	E	520	13/13	0.83	0.31	110,110,110,110	0
9	NAG	I	301	14/15	0.83	0.17	166,184,208,216	0
9	NAG	C	504	14/15	0.83	0.39	145,168,179,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	NAG	D	201	14/15	0.84	0.30	146,155,171,178	0
10	SO4	J	302	5/5	0.86	0.19	168,168,168,168	0
10	SO4	A	516	5/5	0.87	0.20	166,166,166,166	0
10	SO4	D	202	5/5	0.88	0.17	159,159,159,159	0
9	NAG	F	201	14/15	0.89	0.26	125,136,146,152	0
9	NAG	J	301	14/15	0.92	0.19	126,139,155,161	0
10	SO4	D	203	5/5	0.92	0.14	109,109,109,109	0
10	SO4	C	514	5/5	0.93	0.20	133,133,133,133	0
10	SO4	H	303	5/5	0.93	0.10	155,155,155,155	0
10	SO4	B	202	5/5	0.93	0.13	149,149,149,149	0
10	SO4	E	519	5/5	0.94	0.17	101,101,101,101	0
10	SO4	A	512	5/5	0.94	0.15	178,178,178,178	0
10	SO4	F	202	5/5	0.95	0.16	106,106,106,106	0
10	SO4	A	513	5/5	0.97	0.14	98,98,98,98	0
10	SO4	B	204	5/5	0.97	0.15	104,104,104,104	0
10	SO4	B	203	5/5	0.98	0.09	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.