



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 10:49 pm BST

PDB ID : 9F2D / pdb\_00009f2d  
Title : KIR2DL1 bound to RIFIN RBK21  
Authors : Chamberlain, S.G.; Higgins, M.K.  
Deposited on : 2024-04-22  
Resolution : 2.89 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

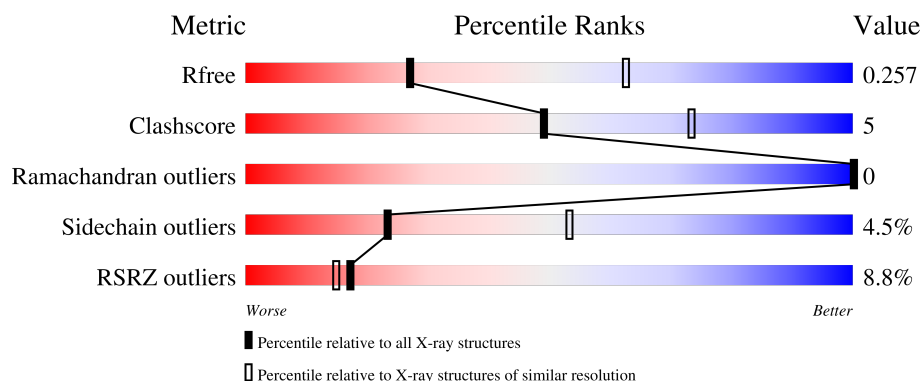
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	152	<div> <div>3%</div> <div>64%</div> <div>5%</div> <div>32%</div> </div>
1	C	152	<div> <div>15%</div> <div>52%</div> <div>14%</div> <div>33%</div> </div>
1	E	152	<div> <div>2%</div> <div>64%</div> <div>33%</div> </div>
1	G	152	<div> <div>10%</div> <div>54%</div> <div>11%</div> <div>34%</div> </div>
1	I	152	<div> <div>17%</div> <div>59%</div> <div>8%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	152	
1	M	152	
1	O	152	
2	B	195	
2	D	195	
2	F	195	
2	H	195	
2	J	195	
2	L	195	
2	N	195	
2	P	195	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18222 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 RIFIN RBK21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			760	476	129	151	4			
1	C	102	Total	C	N	O	S	0	0	0
			768	488	129	147	4			
1	E	102	Total	C	N	O	S	0	0	0
			749	469	127	149	4			
1	G	100	Total	C	N	O	S	0	0	0
			753	481	126	142	4			
1	I	102	Total	C	N	O	S	0	0	0
			765	487	128	146	4			
1	K	95	Total	C	N	O	S	0	0	0
			706	450	117	135	4			
1	M	87	Total	C	N	O	S	0	0	0
			650	414	105	127	4			
1	O	101	Total	C	N	O	S	0	0	0
			760	484	128	144	4			

- Molecule 2 is a protein called KIR2DL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	0
			1505	949	261	287	8			
2	D	194	Total	C	N	O	S	0	0	0
			1501	947	258	288	8			
2	F	195	Total	C	N	O	S	0	0	0
			1512	953	262	289	8			
2	H	192	Total	C	N	O	S	0	0	0
			1489	940	257	284	8			
2	J	195	Total	C	N	O	S	0	0	0
			1512	953	262	289	8			
2	L	189	Total	C	N	O	S	0	0	0
			1469	927	254	280	8			

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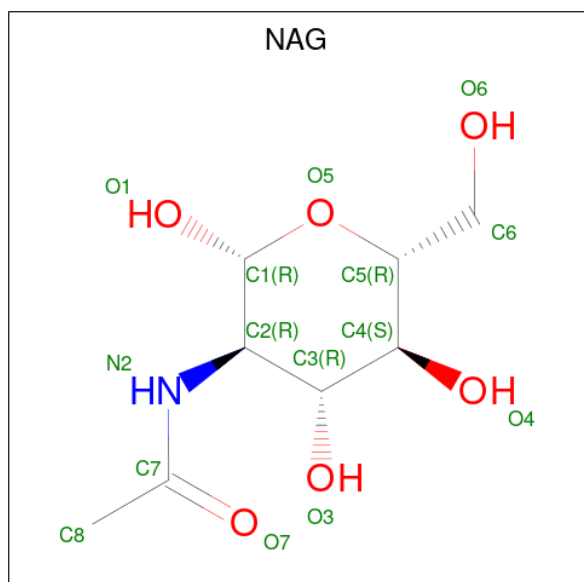
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	193	Total	C	N	O	S	0	0	0
			1492	941	256	287	8			
2	P	194	Total	C	N	O	S	0	0	0
			1501	947	258	288	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	R	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	S	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	T	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	U	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

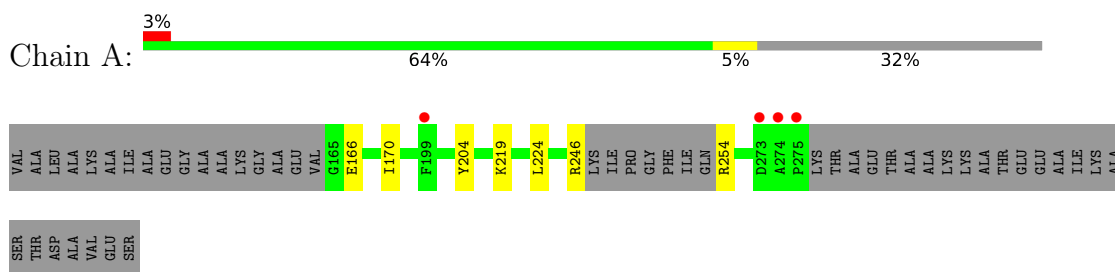


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	N	1	Total	C	N	O	0	0
			14	8	1	5		
4	N	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

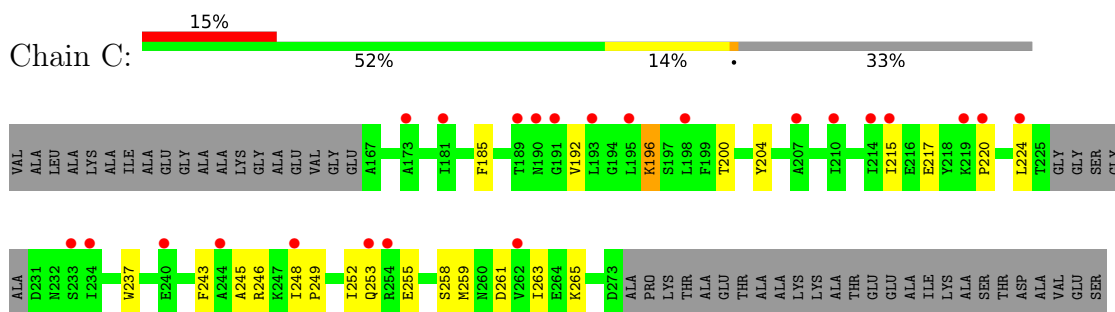
### 3 Residue-property plots

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

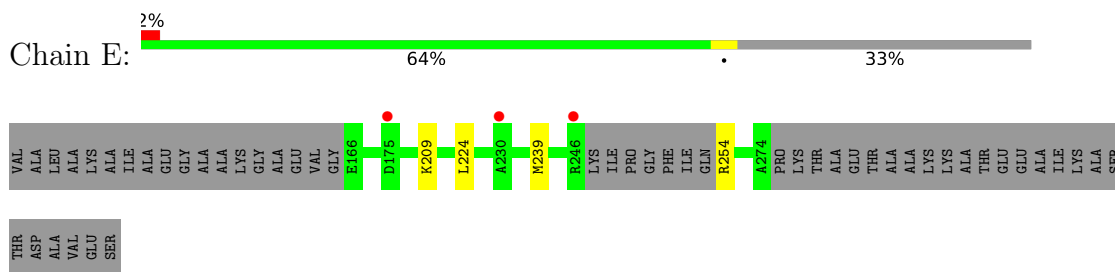
- Molecule 1: RIFIN RBK21



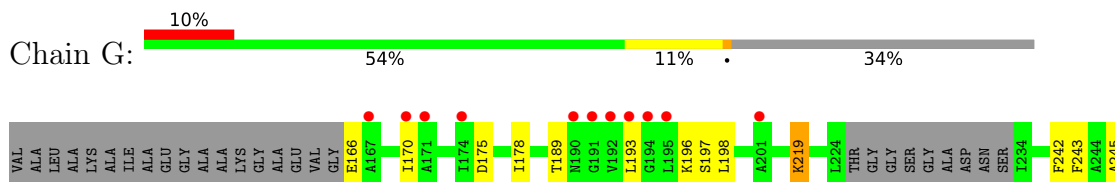
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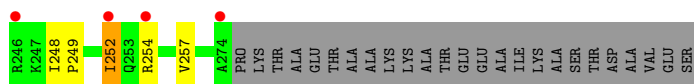


- Molecule 1: RIFIN RBK21

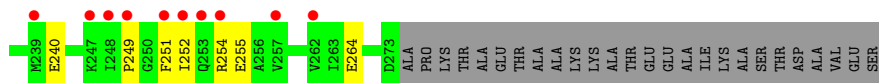
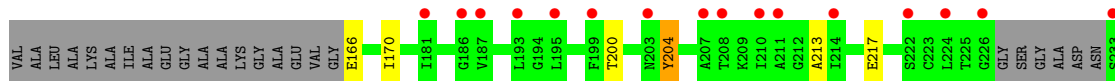


- Molecule 1: RIFIN RBK21

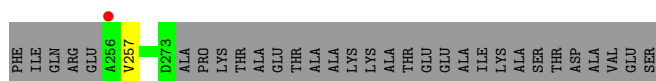
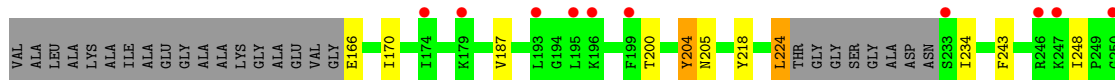




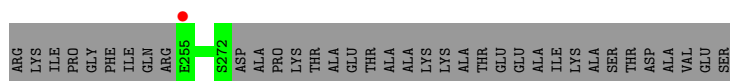
• Molecule 1: RIFIN RBK21



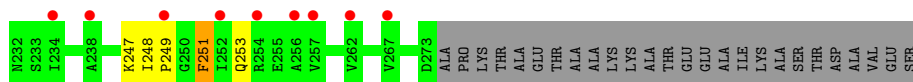
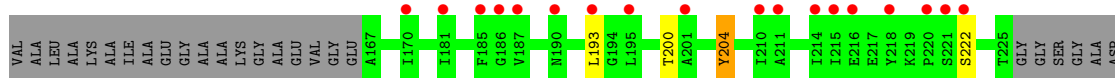
• Molecule 1: RIFIN RBK21



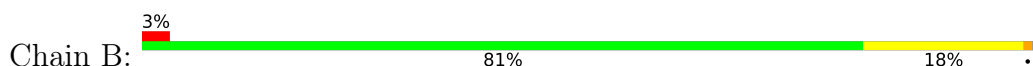
• Molecule 1: RIFIN RBK21



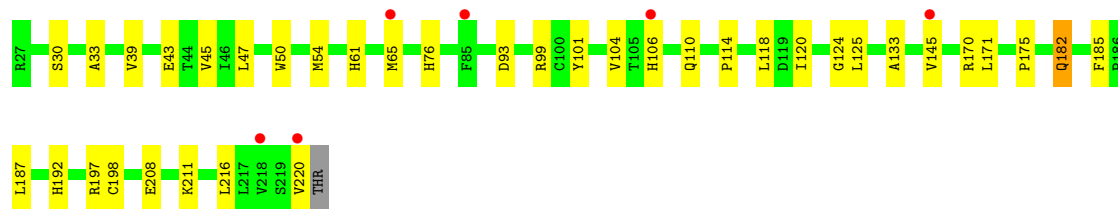
• Molecule 1: RIFIN RBK21



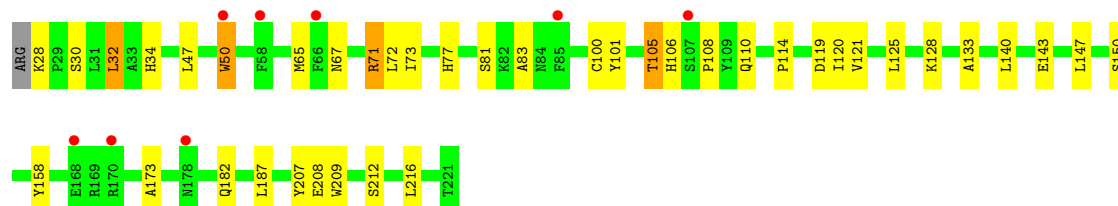
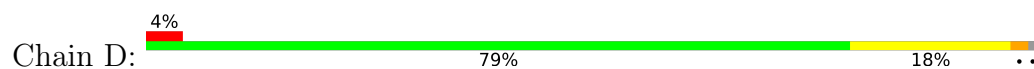
• Molecule 2: KIR2DL protein



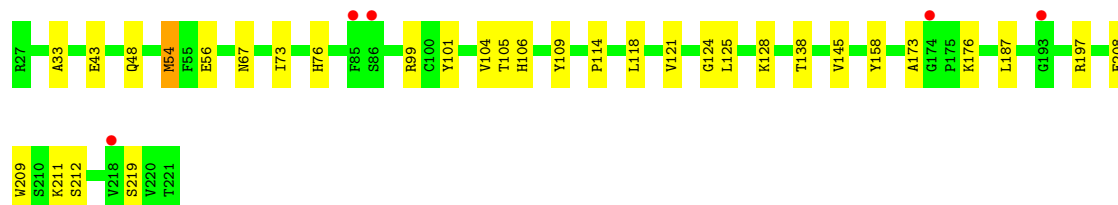
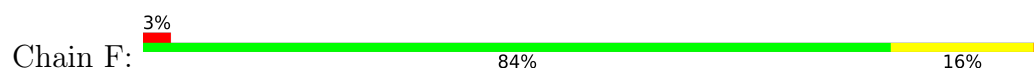




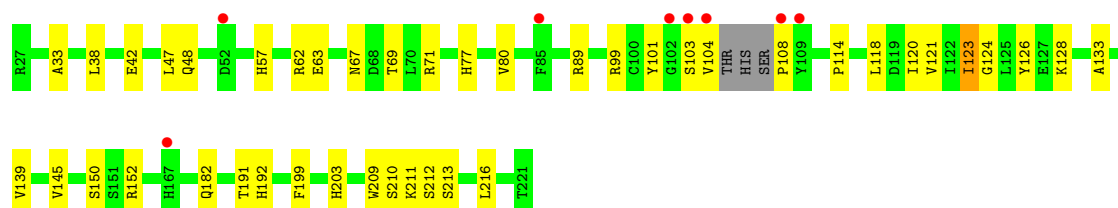
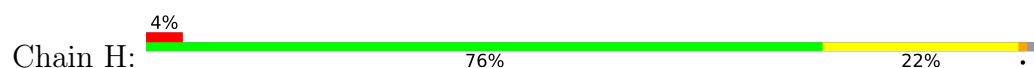
• Molecule 2: KIR2DL protein



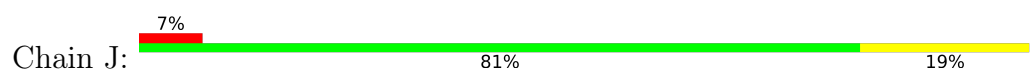
• Molecule 2: KIR2DL protein



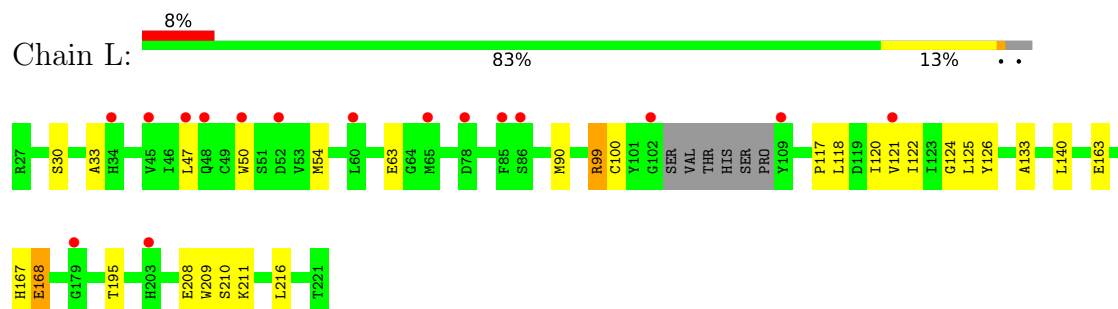
• Molecule 2: KIR2DL protein



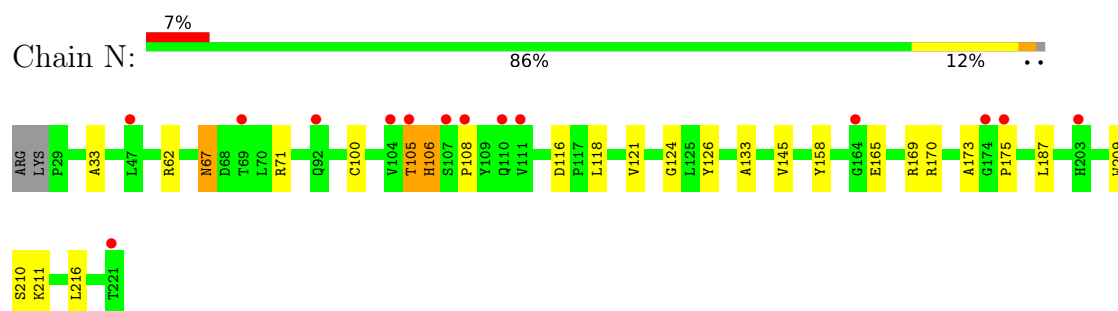
• Molecule 2: KIR2DL protein



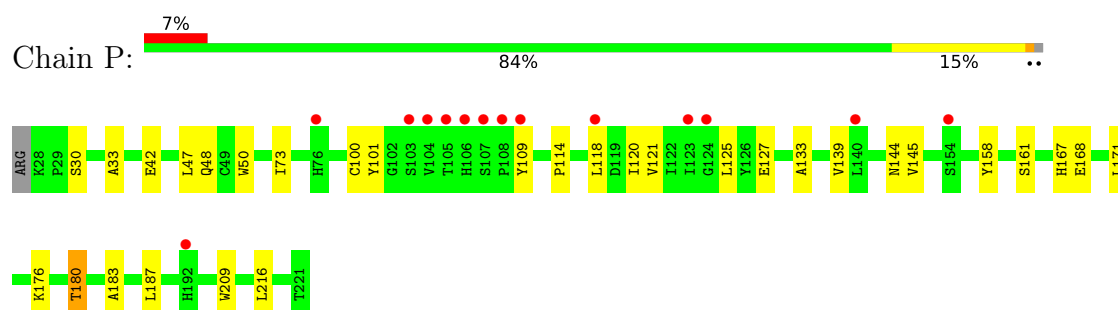
- Molecule 2: KIR2DL protein



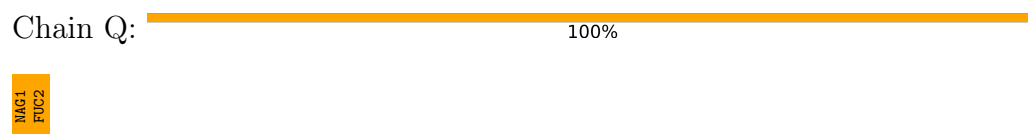
- Molecule 2: KIR2DL protein



- Molecule 2: KIR2DL protein



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



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



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





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

Chain T:  50%  50%



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

Chain U:  50%  50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40Å 99.05Å 321.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.37 – 2.89 57.37 – 2.89	Depositor EDS
% Data completeness (in resolution range)	78.8 (57.37-2.89) 78.8 (57.37-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.91Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, $R_{free}$	0.256 , 0.286 0.260 , 0.257	Depositor DCC
$R_{free}$ test set	17091 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1935e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/769	0.45	0/1039
1	C	0.28	0/778	0.46	0/1051
1	E	0.30	0/757	0.46	0/1022
1	G	0.28	0/763	0.45	0/1030
1	I	0.26	0/775	0.41	0/1046
1	K	0.26	0/714	0.43	0/963
1	M	0.23	0/657	0.38	0/886
1	O	0.26	0/770	0.44	0/1040
2	B	0.35	0/1549	0.54	0/2106
2	D	0.33	0/1545	0.52	0/2102
2	F	0.33	0/1556	0.52	0/2116
2	H	0.34	0/1531	0.55	0/2079
2	J	0.30	0/1556	0.48	0/2116
2	L	0.27	0/1510	0.48	0/2050
2	N	0.28	0/1536	0.53	0/2090
2	P	0.31	0/1545	0.52	0/2102
All	All	0.30	0/18311	0.49	0/24838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	760	0	757	3	0
1	C	768	0	780	15	0
1	E	749	0	747	3	0
1	G	753	0	769	12	0
1	I	765	0	778	8	0
1	K	706	0	721	6	0
1	M	650	0	655	3	0
1	O	760	0	775	8	0
2	B	1505	0	1436	18	0
2	D	1501	0	1431	22	0
2	F	1512	0	1444	15	0
2	H	1489	0	1425	25	0
2	J	1512	0	1444	17	0
2	L	1469	0	1403	16	0
2	N	1492	0	1419	13	0
2	P	1501	0	1431	16	0
3	Q	24	0	22	7	0
3	R	24	0	22	1	0
3	S	24	0	22	1	0
3	T	24	0	22	0	0
3	U	24	0	22	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	D	14	0	13	2	0
4	E	14	0	13	1	0
4	F	14	0	13	4	0
4	H	28	0	26	2	0
4	I	14	0	13	0	0
4	J	14	0	13	0	0
4	L	28	0	26	1	0
4	N	28	0	26	0	0
4	O	14	0	13	0	0
4	P	14	0	13	1	0
All	All	18222	0	17720	192	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 5.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:TYR:HB3	1:K:234:ILE:HG12	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:301:NAG:H83	4:F:301:NAG:H3	1.54	0.88
1:G:178:ILE:HD13	1:G:196:LYS:HE3	1.57	0.87
4:D:301:NAG:C1	4:D:301:NAG:H82	2.11	0.80
4:F:301:NAG:H3	4:F:301:NAG:C8	2.16	0.76
2:H:63:GLU:HA	2:H:67:ASN:HB3	1.69	0.74
2:L:140:LEU:HD12	2:P:171:LEU:HD21	1.67	0.73
2:N:62:ARG:O	2:N:67:ASN:HB3	1.89	0.73
2:H:103:SER:HB2	2:H:108:PRO:HB3	1.71	0.71
2:F:138:THR:HG22	2:F:219:SER:HB2	1.71	0.71
1:O:253:GLN:HB3	2:P:73:ILE:HG13	1.74	0.68
2:D:32:LEU:HD11	2:D:34:HIS:NE2	2.09	0.68
3:Q:1:NAG:H62	3:Q:2:FUC:H5	1.75	0.67
2:P:144:ASN:OD1	4:P:301:NAG:H2	1.95	0.65
1:G:189:THR:HB	1:G:196:LYS:HB2	1.79	0.65
1:E:254:ARG:HB2	2:F:73:ILE:HD12	1.78	0.64
2:N:105:THR:HB	2:N:108:PRO:CG	2.28	0.64
2:J:191:THR:HG22	2:J:192:HIS:CD2	2.33	0.64
2:B:61:HIS:CD2	3:Q:2:FUC:H62	2.33	0.64
2:D:47:LEU:HD21	2:D:120:ILE:HD11	1.80	0.63
2:L:163:GLU:HG3	2:L:195:THR:HB	1.81	0.63
2:H:150:SER:HB3	2:H:182:GLN:HB3	1.81	0.63
2:H:191:THR:HG22	2:H:192:HIS:ND1	2.15	0.61
4:D:301:NAG:C1	4:D:301:NAG:C8	2.77	0.61
1:C:245:ALA:O	2:D:71:ARG:NH2	2.34	0.61
2:N:124:GLY:HA2	2:N:211:LYS:HA	1.81	0.61
2:B:145:VAL:HG23	2:B:187:LEU:HB2	1.82	0.60
2:B:125:LEU:HD12	2:B:208:GLU:HB3	1.82	0.60
2:D:133:ALA:HB2	2:D:216:LEU:HD21	1.82	0.60
1:C:253:GLN:HG3	2:D:73:ILE:HD13	1.84	0.59
1:I:213:ALA:O	1:I:217:GLU:HG2	2.01	0.59
1:A:219:LYS:HG2	3:Q:1:NAG:H82	1.86	0.58
1:G:248:ILE:HD12	1:G:249:PRO:HD2	1.86	0.57
2:J:104:VAL:HB	2:J:107:SER:HB3	1.86	0.57
2:J:145:VAL:HG23	2:J:187:LEU:HB2	1.87	0.57
2:J:147:LEU:HD12	2:J:160:LEU:HD21	1.87	0.56
2:P:145:VAL:HG23	2:P:187:LEU:HB2	1.87	0.56
2:J:32:LEU:HD11	2:J:34:HIS:NE2	2.20	0.56
2:F:56:GLU:HG3	2:F:105:THR:H	1.69	0.56
1:K:248:ILE:HD13	1:K:257:VAL:HG11	1.87	0.56
1:C:224:LEU:HB2	3:R:2:FUC:H62	1.86	0.55
2:F:124:GLY:HA2	2:F:211:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:ALA:HB2	2:L:216:LEU:HD21	1.88	0.55
2:N:133:ALA:HB2	2:N:216:LEU:HD21	1.88	0.55
2:P:133:ALA:HB2	2:P:216:LEU:HD21	1.89	0.55
1:C:192:VAL:HG13	1:C:217:GLU:HG3	1.88	0.55
2:D:30:SER:HB3	2:D:50:TRP:HD1	1.71	0.55
1:C:252:ILE:HG23	1:I:255:GLU:HG3	1.89	0.54
1:O:247:LYS:HD2	1:O:251:PHE:HA	1.88	0.54
2:H:121:VAL:HG11	2:H:209:TRP:CD2	2.43	0.54
2:J:133:ALA:HB2	2:J:216:LEU:HD21	1.90	0.54
2:N:121:VAL:HG11	2:N:209:TRP:CD2	2.42	0.54
1:K:166:GLU:O	1:K:170:ILE:HG12	2.08	0.53
2:D:158:TYR:HE1	2:D:173:ALA:HB2	1.73	0.53
2:N:33:ALA:HB2	2:N:118:LEU:HD21	1.91	0.53
2:B:39:VAL:HG11	2:B:45:VAL:HB	1.90	0.53
2:N:105:THR:HB	2:N:108:PRO:CD	2.38	0.53
2:N:158:TYR:HE1	2:N:173:ALA:HB2	1.71	0.53
1:O:248:ILE:HG13	1:O:249:PRO:HD2	1.89	0.53
2:B:133:ALA:HB2	2:B:216:LEU:HD21	1.91	0.53
2:B:124:GLY:HA2	2:B:211:LYS:HA	1.90	0.52
2:B:175:PRO:HD2	2:B:182:GLN:O	2.08	0.52
1:K:200:THR:O	1:K:204:TYR:HB3	2.09	0.52
2:L:99:ARG:HD2	2:L:117:PRO:HB3	1.91	0.52
2:L:121:VAL:HG11	2:L:209:TRP:CD2	2.44	0.52
2:H:123:ILE:HD11	2:H:209:TRP:CE3	2.44	0.52
2:N:145:VAL:HG23	2:N:187:LEU:HB2	1.90	0.52
2:L:124:GLY:HA2	2:L:211:LYS:HA	1.90	0.52
2:N:126:TYR:H	2:N:210:SER:HA	1.75	0.52
1:A:166:GLU:O	1:A:170:ILE:HG12	2.09	0.52
2:D:140:LEU:O	2:D:143:GLU:HB2	2.10	0.52
1:C:259:MET:O	1:C:263:ILE:HG13	2.09	0.52
2:L:63:GLU:HB3	4:L:301:NAG:H61	1.92	0.52
2:H:62:ARG:O	2:H:67:ASN:HB2	2.11	0.51
1:I:166:GLU:O	1:I:170:ILE:HG12	2.10	0.51
2:L:30:SER:HB2	2:L:50:TRP:HB3	1.91	0.51
2:F:145:VAL:HG23	2:F:187:LEU:HB2	1.92	0.51
2:D:30:SER:HB3	2:D:50:TRP:CD1	2.45	0.51
2:F:158:TYR:HE1	2:F:173:ALA:HB2	1.76	0.51
2:H:124:GLY:HA2	2:H:211:LYS:HA	1.91	0.51
2:J:108:PRO:HB2	2:J:109:TYR:CD2	2.45	0.50
2:P:176:LYS:HB2	2:P:180:THR:HG22	1.94	0.50
1:M:166:GLU:O	1:M:170:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:VAL:HG11	2:P:209:TRP:CD2	2.45	0.50
4:F:301:NAG:H83	4:F:301:NAG:C3	2.34	0.50
2:H:133:ALA:HB2	2:H:216:LEU:HD21	1.94	0.50
1:K:218:TYR:HB3	1:K:234:ILE:CG1	2.33	0.50
4:F:301:NAG:C8	4:F:301:NAG:C3	2.90	0.49
1:G:252:ILE:HG13	1:G:254:ARG:H	1.76	0.49
1:M:238:ALA:O	1:M:242:PHE:HB2	2.12	0.49
1:C:261:ASP:O	1:C:265:LYS:HG2	2.13	0.49
2:H:57:HIS:CE1	2:H:71:ARG:HH21	2.31	0.49
2:D:72:LEU:HD23	2:D:83:ALA:HB1	1.93	0.49
2:H:47:LEU:HD21	2:H:120:ILE:HD11	1.96	0.48
2:N:71:ARG:NH2	2:N:106:HIS:NE2	2.61	0.48
2:B:33:ALA:HB2	2:B:118:LEU:HD21	1.96	0.48
1:G:243:PHE:HE1	2:H:69:THR:HG21	1.79	0.48
2:J:191:THR:HG22	2:J:192:HIS:NE2	2.29	0.48
2:D:67:ASN:N	2:D:67:ASN:OD1	2.46	0.47
2:F:104:VAL:HG11	2:F:106:HIS:CD2	2.49	0.47
2:J:121:VAL:HG11	2:J:209:TRP:CD2	2.49	0.47
2:F:125:LEU:HD12	2:F:208:GLU:HB3	1.97	0.47
2:H:77:HIS:O	2:H:80:VAL:HG12	2.14	0.47
2:H:191:THR:HG22	2:H:192:HIS:CE1	2.50	0.47
1:C:185:PHE:HA	1:C:237:TRP:CD1	2.50	0.47
1:C:246:ARG:HA	2:D:106:HIS:CE1	2.50	0.47
2:H:101:TYR:CZ	2:H:114:PRO:HB3	2.50	0.47
2:L:168:GLU:HG2	2:L:209:TRP:HH2	1.80	0.47
1:I:249:PRO:HB2	1:I:251:PHE:HD2	1.79	0.47
1:C:248:ILE:HD12	1:C:249:PRO:HD2	1.96	0.47
1:G:193:LEU:O	1:G:197:SER:HB2	2.15	0.47
2:D:121:VAL:HG11	2:D:209:TRP:CD2	2.50	0.47
2:D:108:PRO:HG2	2:D:110:GLN:HB2	1.96	0.46
2:H:33:ALA:HB2	2:H:118:LEU:HD21	1.97	0.46
2:J:101:TYR:CZ	2:J:114:PRO:HB3	2.51	0.46
1:E:209:LYS:HD3	4:E:301:NAG:O6	2.15	0.46
2:B:104:VAL:HB	2:B:106:HIS:ND1	2.30	0.46
2:J:72:LEU:HB3	2:J:83:ALA:HB1	1.98	0.46
2:B:192:HIS:HA	2:B:220:VAL:HG21	1.98	0.46
2:D:105:THR:HB	2:D:108:PRO:HD2	1.98	0.46
2:B:61:HIS:CD2	3:Q:2:FUC:C6	2.98	0.46
1:C:215:ILE:HA	1:C:220:PRO:CD	2.46	0.46
2:L:33:ALA:HB2	2:L:118:LEU:HD21	1.98	0.46
2:B:101:TYR:CZ	2:B:114:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LEU:HB2	2:B:185:PHE:CE2	2.52	0.45
2:D:77:HIS:HA	2:J:43:GLU:HG2	1.97	0.45
2:D:125:LEU:HD12	2:D:208:GLU:HB3	1.99	0.45
1:C:237:TRP:CH2	1:C:263:ILE:HG12	2.52	0.45
2:L:47:LEU:HD21	2:L:120:ILE:HD11	1.98	0.45
2:H:63:GLU:HA	2:H:67:ASN:CB	2.43	0.45
2:L:126:TYR:H	2:L:210:SER:HA	1.82	0.45
1:I:252:ILE:HG21	2:L:99:ARG:HH12	1.81	0.45
2:H:126:TYR:H	2:H:210:SER:HA	1.80	0.45
1:G:175:ASP:HA	1:G:178:ILE:HD12	1.99	0.45
1:G:252:ILE:HD11	1:G:254:ARG:HB2	1.99	0.44
2:J:158:TYR:HD2	2:J:183:ALA:HB2	1.82	0.44
2:D:101:TYR:CZ	2:D:114:PRO:HB3	2.51	0.44
2:F:33:ALA:HB2	2:F:118:LEU:HD21	2.00	0.44
1:O:222:SER:HA	3:U:2:FUC:C6	2.48	0.44
1:C:196:LYS:HA	1:C:196:LYS:HD2	1.80	0.44
2:H:38:LEU:HB3	2:H:123:ILE:HD13	2.00	0.44
2:B:61:HIS:NE2	3:Q:2:FUC:H5	2.33	0.44
2:H:62:ARG:O	2:H:67:ASN:CB	2.65	0.44
1:E:239:MET:HE2	2:F:109:TYR:HD1	1.82	0.43
1:G:245:ALA:O	2:H:71:ARG:NH2	2.51	0.43
2:J:38:LEU:HB3	2:J:123:ILE:HD11	1.99	0.43
2:F:101:TYR:CZ	2:F:114:PRO:HB3	2.53	0.43
1:I:252:ILE:HG12	2:L:117:PRO:HD3	2.01	0.43
1:O:253:GLN:CB	2:P:73:ILE:HG13	2.47	0.43
2:B:175:PRO:HG2	2:B:182:GLN:HG2	1.99	0.43
1:C:246:ARG:NH2	1:I:264:GLU:OE2	2.50	0.43
1:O:253:GLN:HB3	2:P:73:ILE:CG1	2.46	0.43
2:L:125:LEU:HD12	2:L:208:GLU:HB3	2.01	0.43
2:P:47:LEU:HD21	2:P:120:ILE:HD11	2.01	0.43
2:P:101:TYR:CZ	2:P:114:PRO:HB3	2.54	0.43
2:P:158:TYR:HD2	2:P:183:ALA:HB2	1.84	0.43
2:B:47:LEU:HD21	2:B:120:ILE:HD11	2.00	0.43
2:H:139:VAL:HG21	2:H:145:VAL:CG2	2.49	0.42
2:P:161:SER:HB2	2:P:168:GLU:HG3	2.02	0.42
1:A:219:LYS:HG2	3:Q:1:NAG:C8	2.48	0.42
2:D:150:SER:HB3	2:D:182:GLN:HG3	2.01	0.42
2:F:54:MET:HG3	2:F:76:HIS:ND1	2.35	0.42
1:M:200:THR:O	1:M:204:TYR:HB3	2.20	0.42
2:D:128:LYS:HG3	2:D:212:SER:O	2.20	0.42
2:P:33:ALA:HB2	2:P:118:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:30:SER:HG	2:P:50:TRP:HE1	1.68	0.42
2:P:139:VAL:HG21	2:P:145:VAL:CG1	2.50	0.42
2:F:67:ASN:HD22	3:S:1:NAG:H83	1.85	0.41
1:K:224:LEU:HG	1:K:243:PHE:CE1	2.54	0.41
2:B:30:SER:HB2	2:B:50:TRP:NE1	2.35	0.41
1:O:200:THR:O	1:O:204:TYR:HB3	2.20	0.41
1:G:219:LYS:HG2	4:H:301:NAG:H5	2.01	0.41
2:H:199:PHE:CE2	2:H:212:SER:HB2	2.55	0.41
2:H:128:LYS:HG3	2:H:213:SER:HA	2.02	0.41
3:Q:1:NAG:H62	3:Q:2:FUC:C5	2.45	0.41
1:G:242:PHE:HE2	1:G:257:VAL:HG12	1.86	0.41
2:D:147:LEU:HG	2:D:187:LEU:HD11	2.02	0.41
1:G:166:GLU:O	1:G:170:ILE:HG12	2.21	0.41
2:J:47:LEU:HD21	2:J:120:ILE:HD11	2.01	0.41
2:B:54:MET:HB3	2:B:76:HIS:CE1	2.56	0.41
2:J:27:ARG:HG3	2:N:175:PRO:HG3	2.03	0.41
2:J:32:LEU:CD1	2:J:34:HIS:NE2	2.83	0.41
2:N:105:THR:HB	2:N:108:PRO:HG3	2.00	0.41
1:O:247:LYS:HE3	1:O:248:ILE:O	2.21	0.41
2:H:121:VAL:HG11	2:H:209:TRP:CE2	2.56	0.41
2:L:90:MET:HG3	2:L:122:ILE:HD12	2.02	0.41
2:F:121:VAL:HG11	2:F:209:TRP:CD2	2.56	0.40
1:I:200:THR:O	1:I:204:TYR:HB3	2.22	0.40
1:C:224:LEU:HG	1:C:243:PHE:CZ	2.57	0.40
4:H:301:NAG:O7	4:H:301:NAG:C1	2.69	0.40
2:F:128:LYS:HG3	2:F:212:SER:O	2.22	0.40
2:D:121:VAL:HG22	2:D:207:TYR:HA	2.02	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	100/152 (66%)	98 (98%)	2 (2%)	0	100	100
1	C	98/152 (64%)	97 (99%)	1 (1%)	0	100	100
1	E	98/152 (64%)	95 (97%)	3 (3%)	0	100	100
1	G	96/152 (63%)	92 (96%)	4 (4%)	0	100	100
1	I	98/152 (64%)	93 (95%)	5 (5%)	0	100	100
1	K	89/152 (59%)	87 (98%)	2 (2%)	0	100	100
1	M	81/152 (53%)	81 (100%)	0	0	100	100
1	O	97/152 (64%)	93 (96%)	4 (4%)	0	100	100
2	B	192/195 (98%)	184 (96%)	8 (4%)	0	100	100
2	D	192/195 (98%)	185 (96%)	7 (4%)	0	100	100
2	F	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
2	H	188/195 (96%)	185 (98%)	3 (2%)	0	100	100
2	J	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
2	L	185/195 (95%)	179 (97%)	6 (3%)	0	100	100
2	N	191/195 (98%)	182 (95%)	9 (5%)	0	100	100
2	P	192/195 (98%)	185 (96%)	7 (4%)	0	100	100
All	All	2283/2776 (82%)	2208 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	79/110 (72%)	75 (95%)	4 (5%)	20	48
1	C	82/110 (74%)	77 (94%)	5 (6%)	15	40
1	E	78/110 (71%)	77 (99%)	1 (1%)	65	86
1	G	79/110 (72%)	76 (96%)	3 (4%)	28	60
1	I	81/110 (74%)	78 (96%)	3 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	75/110 (68%)	71 (95%)	4 (5%)	19	46
1	M	70/110 (64%)	66 (94%)	4 (6%)	17	43
1	O	81/110 (74%)	78 (96%)	3 (4%)	29	61
2	B	168/169 (99%)	159 (95%)	9 (5%)	18	46
2	D	168/169 (99%)	159 (95%)	9 (5%)	18	46
2	F	169/169 (100%)	163 (96%)	6 (4%)	30	62
2	H	166/169 (98%)	158 (95%)	8 (5%)	21	51
2	J	169/169 (100%)	160 (95%)	9 (5%)	19	46
2	L	163/169 (96%)	158 (97%)	5 (3%)	35	67
2	N	167/169 (99%)	159 (95%)	8 (5%)	21	51
2	P	168/169 (99%)	160 (95%)	8 (5%)	21	51
All	All	1963/2232 (88%)	1874 (96%)	89 (4%)	23	53

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	TYR
1	A	224	LEU
1	A	246	ARG
1	A	254	ARG
2	B	43	GLU
2	B	65	MET
2	B	93	ASP
2	B	99	ARG
2	B	110	GLN
2	B	170	ARG
2	B	182	GLN
2	B	197	ARG
2	B	198	CYS
1	C	196	LYS
1	C	200	THR
1	C	204	TYR
1	C	255	GLU
1	C	258	SER
2	D	28	LYS
2	D	32	LEU
2	D	50	TRP
2	D	65	MET

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Mol	Chain	Res	Type
2	D	71	ARG
2	D	81	SER
2	D	100	CYS
2	D	105	THR
2	D	119	ASP
1	E	224	LEU
2	F	43	GLU
2	F	48	GLN
2	F	54	MET
2	F	99	ARG
2	F	176	LYS
2	F	197	ARG
1	G	198	LEU
1	G	219	LYS
1	G	252	ILE
2	H	42	GLU
2	H	48	GLN
2	H	89	ARG
2	H	99	ARG
2	H	104	VAL
2	H	123	ILE
2	H	152	ARG
2	H	203	HIS
1	I	204	TYR
1	I	240	GLU
1	I	254	ARG
2	J	48	GLN
2	J	81	SER
2	J	84	ASN
2	J	89	ARG
2	J	93	ASP
2	J	100	CYS
2	J	106	HIS
2	J	110	GLN
2	J	128	LYS
1	K	187	VAL
1	K	204	TYR
1	K	205	ASN
1	K	224	LEU
2	L	54	MET
2	L	99	ARG
2	L	100	CYS

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Mol	Chain	Res	Type
2	L	167	HIS
2	L	168	GLU
1	M	204	TYR
1	M	205	ASN
1	M	219	LYS
1	M	242	PHE
2	N	67	ASN
2	N	100	CYS
2	N	105	THR
2	N	106	HIS
2	N	116	ASP
2	N	165	GLU
2	N	169	ARG
2	N	170	ARG
1	O	193	LEU
1	O	204	TYR
1	O	251	PHE
2	P	42	GLU
2	P	48	GLN
2	P	100	CYS
2	P	109	TYR
2	P	125	LEU
2	P	127	GLU
2	P	167	HIS
2	P	180	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

10 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	0.45	0	19,19,21	0.80	1 (5%)
3	FUC	Q	2	3	10,10,11	0.48	0	14,14,16	1.34	2 (14%)
3	NAG	R	1	2,3	14,14,15	0.41	0	17,19,21	0.60	0
3	FUC	R	2	3	10,10,11	0.32	0	14,14,16	0.86	0
3	NAG	S	1	2,3	14,14,15	0.36	0	17,19,21	0.93	0
3	FUC	S	2	3	10,10,11	0.31	0	14,14,16	0.64	0
3	NAG	T	1	2,3	14,14,15	0.29	0	17,19,21	0.55	0
3	FUC	T	2	3	10,10,11	0.84	0	14,14,16	1.21	3 (21%)
3	NAG	U	1	2,3	14,14,15	0.25	0	17,19,21	0.35	0
3	FUC	U	2	3	10,10,11	0.28	0	14,14,16	0.73	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	-	0/6/22/26	1/1/1/1
3	FUC	Q	2	3	-	-	0/1/1/1
3	NAG	R	1	2,3	-	5/6/23/26	0/1/1/1
3	FUC	R	2	3	-	-	0/1/1/1
3	NAG	S	1	2,3	-	2/6/23/26	0/1/1/1
3	FUC	S	2	3	-	-	0/1/1/1
3	NAG	T	1	2,3	-	2/6/23/26	0/1/1/1
3	FUC	T	2	3	-	-	0/1/1/1
3	NAG	U	1	2,3	-	1/6/23/26	0/1/1/1
3	FUC	U	2	3	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2	FUC	C1-C2-C3	3.73	114.26	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2	FUC	O5-C1-C2	2.39	114.46	110.77
3	Q	1	NAG	C4-C5-C6	2.24	116.54	112.60
3	T	2	FUC	C1-C2-C3	2.20	112.38	109.67
3	T	2	FUC	C1-O5-C5	2.12	117.58	112.78
3	T	2	FUC	C2-C3-C4	2.06	114.46	110.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	T	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6

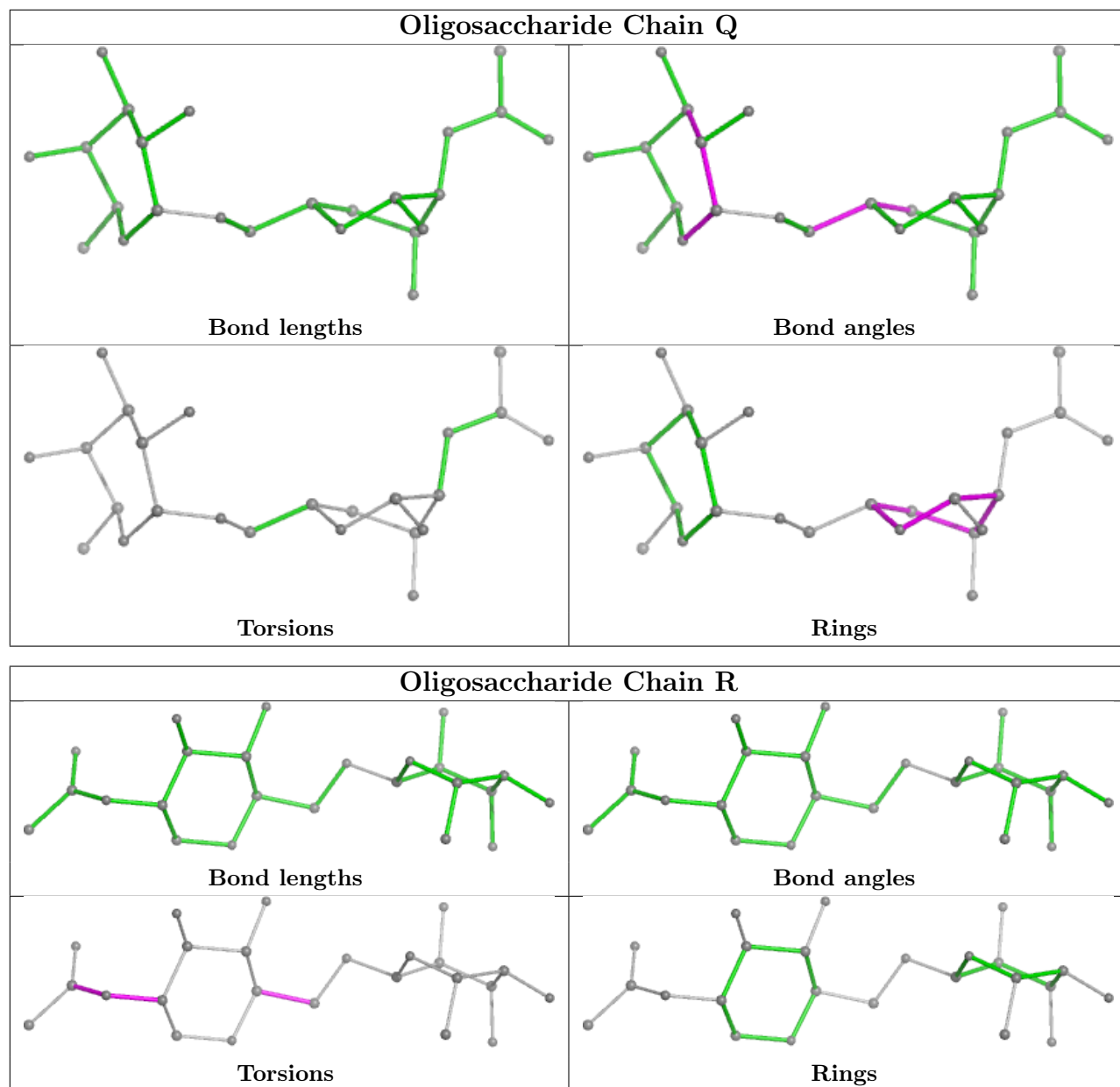
All (1) ring outliers are listed below:

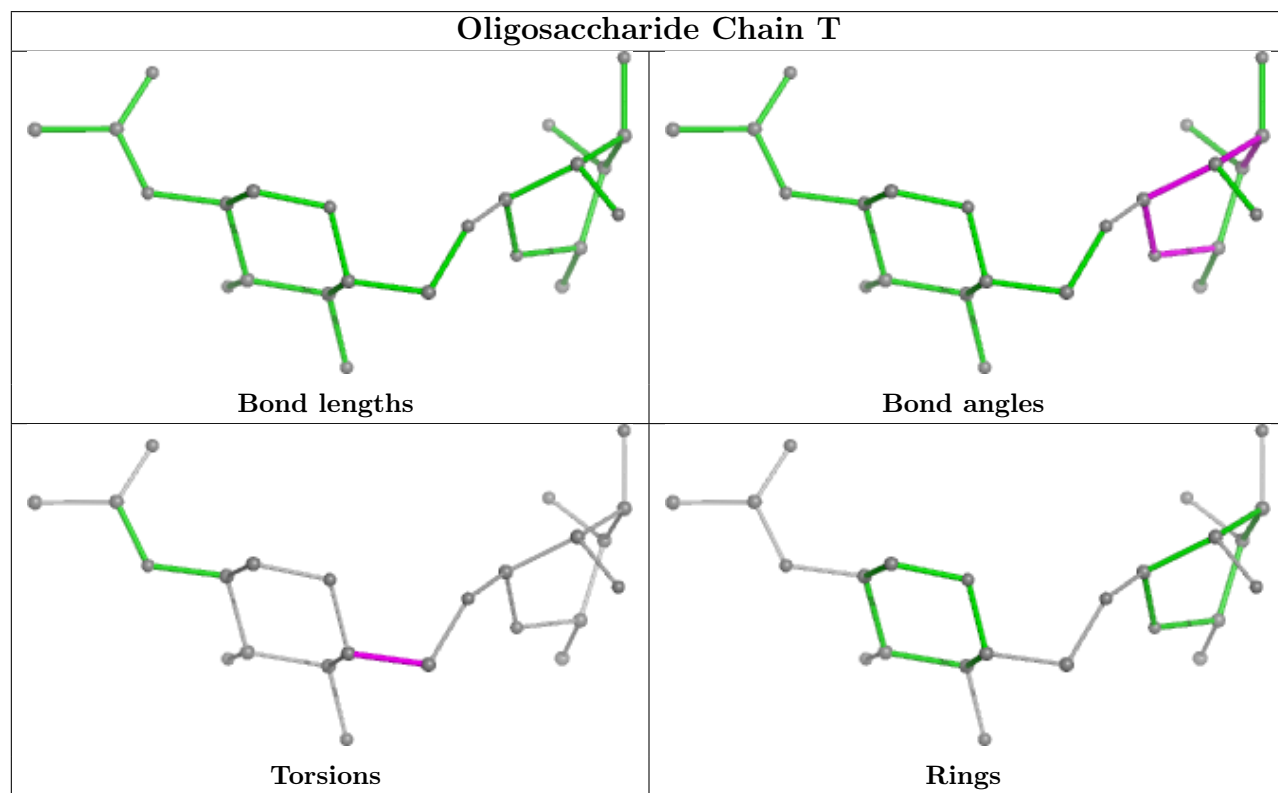
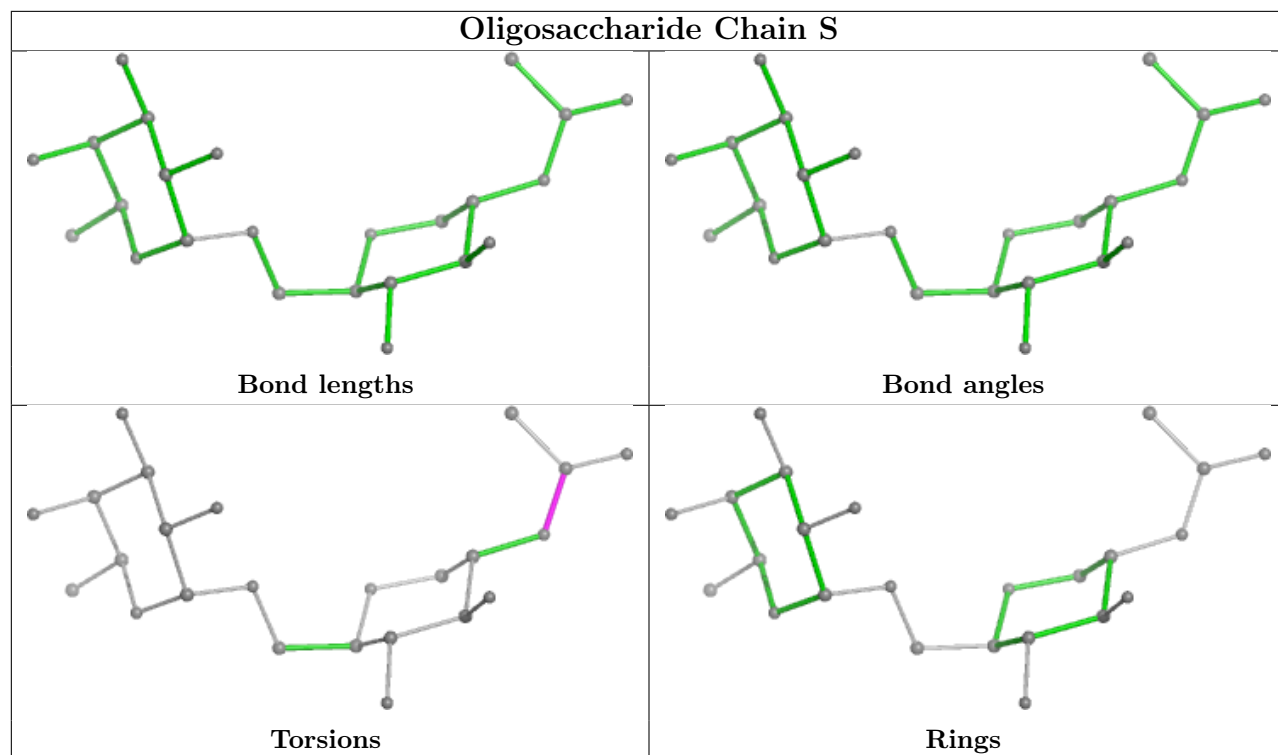
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C1-C2-C3-C4-C5-O5

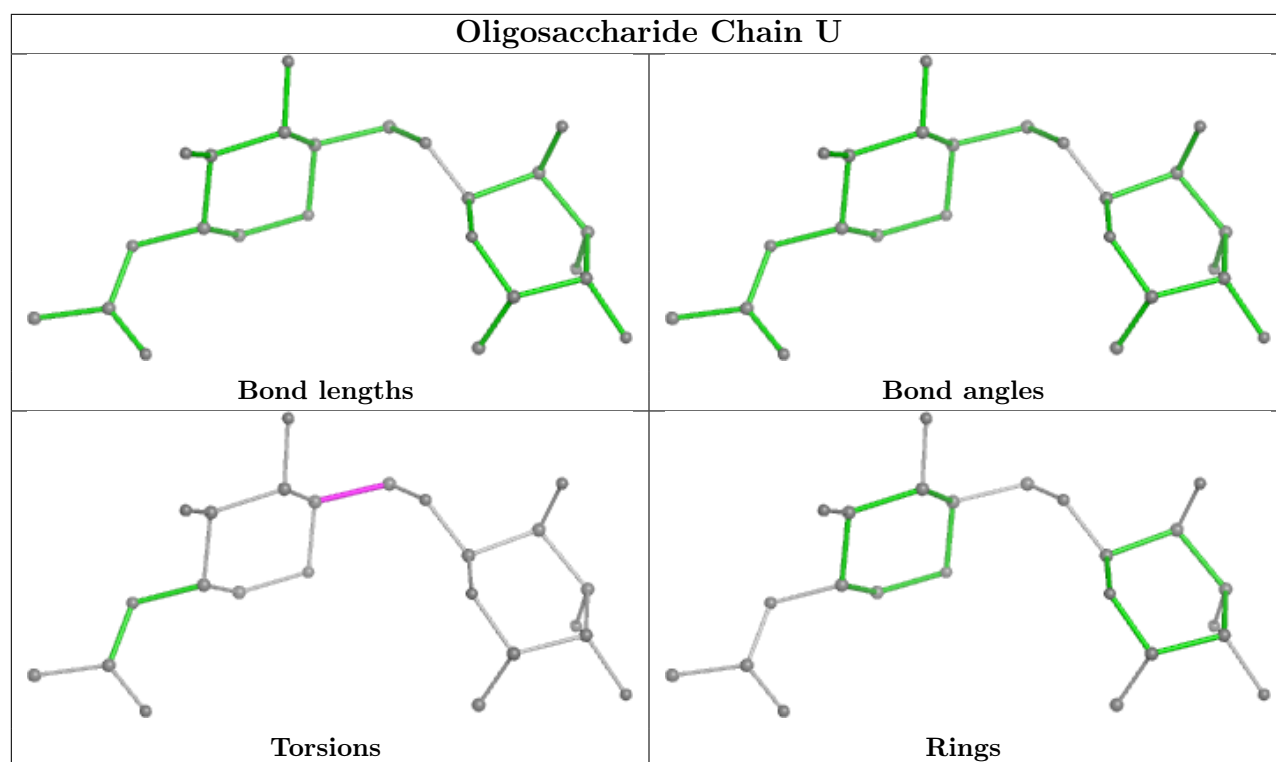
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	FUC	1	0
3	S	1	NAG	1	0
3	Q	2	FUC	5	0
3	Q	1	NAG	4	0
3	U	2	FUC	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](#)

15 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	$\# Z  > 2$
4	NAG	D	301	2	14,14,15	0.45	0	17,19,21	1.40	3 (17%)
4	NAG	P	301	2	14,14,15	0.49	0	17,19,21	0.77	1 (5%)
4	NAG	A	301	1	14,14,15	0.46	0	17,19,21	0.62	0
4	NAG	L	302	2	14,14,15	0.26	0	17,19,21	0.77	1 (5%)
4	NAG	E	301	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	F	301	2	14,14,15	0.58	0	17,19,21	2.11	3 (17%)
4	NAG	B	301	2	14,14,15	0.45	0	17,19,21	0.63	1 (5%)
4	NAG	H	301	2	14,14,15	0.44	0	17,19,21	1.43	3 (17%)
4	NAG	H	302	2	14,14,15	0.30	0	17,19,21	1.45	3 (17%)
4	NAG	L	301	2	14,14,15	0.60	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	N	302	2	14,14,15	0.29	0	17,19,21	1.04	2 (11%)
4	NAG	N	301	2	14,14,15	0.28	0	17,19,21	1.12	2 (11%)
4	NAG	O	301	1	14,14,15	0.46	0	17,19,21	0.47	0
4	NAG	J	301	2	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	I	301	1	14,14,15	0.47	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	301	2	-	5/6/23/26	0/1/1/1
4	NAG	P	301	2	-	2/6/23/26	0/1/1/1
4	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	NAG	L	302	2	-	4/6/23/26	0/1/1/1
4	NAG	E	301	1	-	0/6/23/26	0/1/1/1
4	NAG	F	301	2	-	3/6/23/26	0/1/1/1
4	NAG	B	301	2	-	2/6/23/26	0/1/1/1
4	NAG	H	301	2	-	1/6/23/26	0/1/1/1
4	NAG	H	302	2	-	2/6/23/26	0/1/1/1
4	NAG	L	301	2	-	2/6/23/26	0/1/1/1
4	NAG	N	302	2	-	2/6/23/26	0/1/1/1
4	NAG	N	301	2	-	2/6/23/26	0/1/1/1
4	NAG	O	301	1	-	0/6/23/26	0/1/1/1
4	NAG	J	301	2	-	0/6/23/26	0/1/1/1
4	NAG	I	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	301	NAG	C1-O5-C5	5.49	119.64	112.19
4	F	301	NAG	C2-N2-C7	4.55	129.38	122.90
4	D	301	NAG	C2-N2-C7	4.24	128.94	122.90
4	H	301	NAG	C1-O5-C5	3.68	117.18	112.19
4	F	301	NAG	C3-C4-C5	3.55	116.57	110.24
4	H	301	NAG	C2-N2-C7	3.25	127.53	122.90
4	H	302	NAG	C1-O5-C5	3.14	116.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	302	NAG	C1-O5-C5	3.07	116.35	112.19
4	H	302	NAG	C4-C3-C2	-3.06	106.53	111.02
4	H	302	NAG	C2-N2-C7	2.74	126.80	122.90
4	N	301	NAG	C2-N2-C7	2.72	126.78	122.90
4	D	301	NAG	C1-O5-C5	2.41	115.46	112.19
4	H	301	NAG	C1-C2-N2	2.32	114.46	110.49
4	N	301	NAG	C1-C2-N2	2.14	114.14	110.49
4	P	301	NAG	C2-N2-C7	2.09	125.89	122.90
4	N	302	NAG	O5-C5-C6	-2.07	103.97	107.20
4	D	301	NAG	C1-C2-N2	2.06	114.01	110.49
4	B	301	NAG	C2-N2-C7	2.03	125.80	122.90
4	L	302	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	NAG	C1-C2-N2-C7
4	D	301	NAG	C8-C7-N2-C2
4	D	301	NAG	O7-C7-N2-C2
4	F	301	NAG	C3-C2-N2-C7
4	H	301	NAG	C1-C2-N2-C7
4	B	301	NAG	C8-C7-N2-C2
4	B	301	NAG	O7-C7-N2-C2
4	L	302	NAG	O7-C7-N2-C2
4	A	301	NAG	C8-C7-N2-C2
4	A	301	NAG	O7-C7-N2-C2
4	F	301	NAG	C8-C7-N2-C2
4	F	301	NAG	O7-C7-N2-C2
4	L	302	NAG	C8-C7-N2-C2
4	P	301	NAG	C8-C7-N2-C2
4	P	301	NAG	O7-C7-N2-C2
4	N	301	NAG	O5-C5-C6-O6
4	L	301	NAG	C4-C5-C6-O6
4	L	302	NAG	O5-C5-C6-O6
4	N	301	NAG	C3-C2-N2-C7
4	L	301	NAG	O5-C5-C6-O6
4	D	301	NAG	C4-C5-C6-O6
4	H	302	NAG	C3-C2-N2-C7
4	N	302	NAG	C4-C5-C6-O6
4	L	302	NAG	C4-C5-C6-O6
4	N	302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	301	NAG	O5-C5-C6-O6
4	H	302	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	NAG	2	0
4	P	301	NAG	1	0
4	E	301	NAG	1	0
4	F	301	NAG	4	0
4	H	301	NAG	2	0
4	L	301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	104/152 (68%)	0.37	4 (3%) 44 39	40, 61, 102, 123	0
1	C	102/152 (67%)	1.44	23 (22%) 3 3	111, 152, 179, 192	0
1	E	102/152 (67%)	0.28	3 (2%) 54 49	45, 64, 93, 112	0
1	G	100/152 (65%)	1.11	15 (15%) 6 6	92, 121, 188, 195	0
1	I	102/152 (67%)	1.46	26 (25%) 2 2	126, 160, 197, 206	0
1	K	95/152 (62%)	1.04	11 (11%) 11 10	120, 169, 191, 196	0
1	M	87/152 (57%)	1.01	12 (13%) 8 7	122, 178, 201, 205	0
1	O	101/152 (66%)	1.53	27 (26%) 2 2	135, 162, 221, 227	0
2	B	194/195 (99%)	0.18	6 (3%) 51 46	36, 55, 82, 97	0
2	D	194/195 (99%)	0.39	8 (4%) 42 36	40, 71, 100, 117	0
2	F	195/195 (100%)	0.42	5 (2%) 57 52	41, 66, 94, 108	0
2	H	192/195 (98%)	0.43	8 (4%) 41 35	39, 67, 92, 117	0
2	J	195/195 (100%)	0.72	13 (6%) 25 21	56, 80, 118, 132	0
2	L	189/195 (96%)	0.72	16 (8%) 18 16	58, 96, 132, 144	0
2	N	193/195 (98%)	0.66	14 (7%) 22 19	53, 91, 143, 157	0
2	P	194/195 (99%)	0.75	14 (7%) 23 19	58, 82, 120, 135	0
All	All	2339/2776 (84%)	0.70	205 (8%) 17 15	36, 84, 185, 227	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	195	LEU	6.9
1	G	195	LEU	5.9
1	C	210	ILE	5.6
1	O	193	LEU	5.3
1	G	191	GLY	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	195	LEU	5.1
2	D	178	ASN	4.8
2	J	108	PRO	4.6
2	N	174	GLY	4.6
2	P	124	GLY	4.5
2	D	107	SER	4.4
1	I	252	ILE	4.3
1	M	242	PHE	4.2
1	I	181	ILE	4.2
2	J	109	TYR	4.0
2	J	42	GLU	4.0
1	I	214	ILE	4.0
1	O	221	SER	3.9
2	P	104	VAL	3.9
2	N	108	PRO	3.8
2	J	110	GLN	3.8
1	A	274	ALA	3.7
1	O	211	ALA	3.7
1	C	191	GLY	3.6
2	N	105	THR	3.5
2	H	108	PRO	3.5
1	I	251	PHE	3.5
2	H	104	VAL	3.4
2	J	106	HIS	3.4
2	H	167	HIS	3.4
1	C	262	VAL	3.3
1	O	249	PRO	3.3
1	I	210	ILE	3.3
2	B	85	PHE	3.3
2	P	103	SER	3.2
2	L	34	HIS	3.2
2	J	104	VAL	3.2
2	P	192	HIS	3.2
1	C	193	LEU	3.2
1	G	201	ALA	3.1
1	C	190	ASN	3.1
1	G	193	LEU	3.1
2	F	193	GLY	3.1
1	A	199	PHE	3.1
1	I	211	ALA	3.1
2	H	102	GLY	3.1
1	G	170	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	203	HIS	3.1
2	L	85	PHE	3.1
2	P	109	TYR	3.0
2	J	167	HIS	3.0
1	O	210	ILE	3.0
2	P	105	THR	3.0
1	K	179	LYS	3.0
1	I	257	VAL	3.0
1	C	207	ALA	2.9
2	H	103	SER	2.9
1	K	250	GLY	2.9
1	M	193	LEU	2.9
1	C	220	PRO	2.9
1	K	193	LEU	2.9
1	G	274	ALA	2.9
1	I	239	MET	2.8
1	C	189	THR	2.8
1	M	195	LEU	2.8
1	C	234	ILE	2.8
1	I	248	ILE	2.8
2	L	102	GLY	2.8
1	I	208	THR	2.8
1	O	214	ILE	2.8
2	N	175	PRO	2.7
2	L	48	GLN	2.7
1	O	220	PRO	2.7
2	N	164	GLY	2.7
2	J	54	MET	2.7
1	O	254	ARG	2.7
1	G	192	VAL	2.7
1	C	240	GLU	2.7
2	J	105	THR	2.7
2	J	27	ARG	2.6
2	L	86	SER	2.6
1	I	247	LYS	2.6
2	B	145	VAL	2.6
1	O	238	ALA	2.6
1	O	170	ILE	2.6
2	D	85	PHE	2.6
1	K	196	LYS	2.6
2	F	86	SER	2.6
2	N	92	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	194	GLY	2.5
1	C	214	ILE	2.5
2	L	50	TRP	2.5
2	J	65	MET	2.5
1	I	203	ASN	2.5
2	L	47	LEU	2.5
1	G	167	ALA	2.5
2	H	52	ASP	2.5
1	O	257	VAL	2.5
2	L	109	TYR	2.5
2	N	110	GLN	2.4
2	P	108	PRO	2.4
1	M	223	CYS	2.4
1	O	218	TYR	2.4
1	I	254	ARG	2.4
1	M	207	ALA	2.4
2	P	118	LEU	2.4
2	P	140	LEU	2.4
1	I	186	GLY	2.4
2	D	168	GLU	2.4
1	O	215	ILE	2.4
2	D	66	PHE	2.4
1	I	193	LEU	2.4
2	N	107	SER	2.4
1	G	171	ALA	2.4
1	M	243	PHE	2.4
1	K	195	LEU	2.3
1	I	226	GLY	2.3
1	O	186	GLY	2.3
1	C	195	LEU	2.3
2	L	78	ASP	2.3
1	C	254	ARG	2.3
1	C	224	LEU	2.3
1	I	249	PRO	2.3
1	C	219	LYS	2.3
1	C	248	ILE	2.3
1	K	199	PHE	2.3
1	C	233	SER	2.3
1	C	244	ALA	2.3
1	I	233	SER	2.3
1	M	211	ALA	2.3
1	O	201	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	216	GLU	2.3
1	O	256	ALA	2.3
2	F	174	GLY	2.2
2	N	47	LEU	2.2
2	P	123	ILE	2.2
2	P	76	HIS	2.2
1	I	207	ALA	2.2
1	O	222	SER	2.2
1	A	275	PRO	2.2
2	L	121	VAL	2.2
1	M	185	PHE	2.2
2	D	58	PHE	2.2
2	H	85	PHE	2.2
1	M	201	ALA	2.2
1	I	224	LEU	2.2
1	O	187	VAL	2.2
2	N	111	VAL	2.2
1	C	253	GLN	2.2
1	I	253	GLN	2.2
2	B	106	HIS	2.2
2	N	203	HIS	2.2
2	H	109	TYR	2.2
2	B	65	MET	2.2
1	C	173	ALA	2.2
2	L	52	ASP	2.2
1	K	174	ILE	2.2
2	P	107	SER	2.2
2	F	85	PHE	2.1
2	L	65	MET	2.1
1	C	198	LEU	2.1
1	K	256	ALA	2.1
1	O	267	VAL	2.1
2	B	218	VAL	2.1
2	L	45	VAL	2.1
1	O	185	PHE	2.1
1	G	190	ASN	2.1
1	M	255	GLU	2.1
1	O	234	ILE	2.1
1	O	252	ILE	2.1
1	I	187	VAL	2.1
1	I	262	VAL	2.1
1	O	262	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	218	VAL	2.1
1	A	273	ASP	2.1
1	E	175	ASP	2.1
1	K	246	ARG	2.1
2	N	69	THR	2.1
2	J	47	LEU	2.1
1	E	230	ALA	2.1
1	O	190	ASN	2.1
2	N	104	VAL	2.1
2	D	170	ARG	2.1
2	L	179	GLY	2.1
1	I	199	PHE	2.1
2	J	140	LEU	2.1
2	P	154	SER	2.1
1	O	181	ILE	2.1
2	D	50	TRP	2.1
1	E	246	ARG	2.1
2	N	221	THR	2.0
1	I	222	SER	2.0
1	K	233	SER	2.0
1	M	221	SER	2.0
1	M	222	SER	2.0
1	C	215	ILE	2.0
1	G	252	ILE	2.0
1	G	246	ARG	2.0
1	G	254	ARG	2.0
2	B	220	VAL	2.0
1	K	247	LYS	2.0
2	L	60	LEU	2.0
1	C	181	ILE	2.0
1	G	174	ILE	2.0
2	P	106	HIS	2.0

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

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

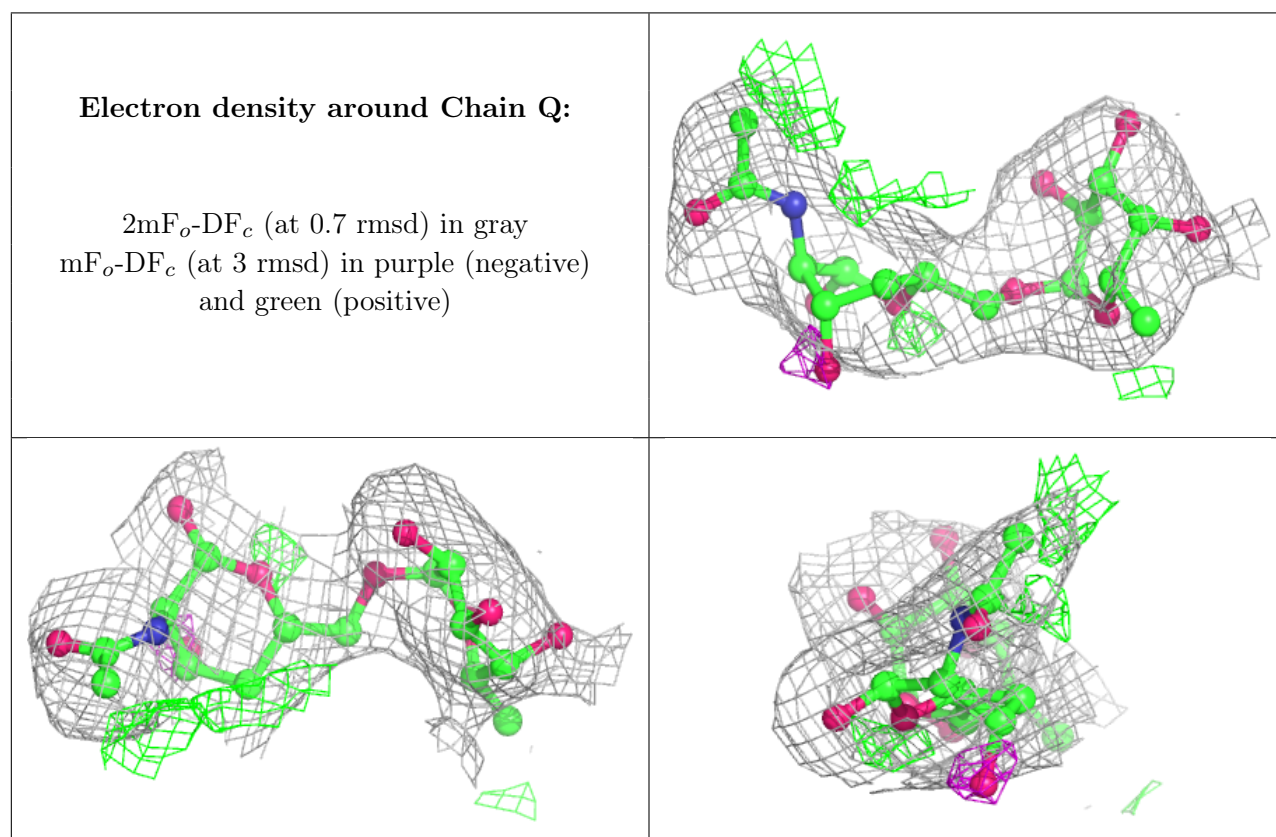
## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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.

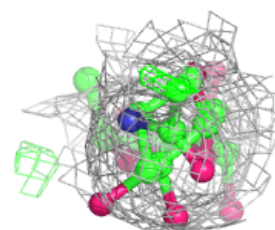
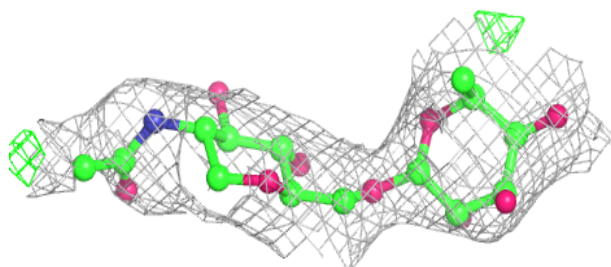
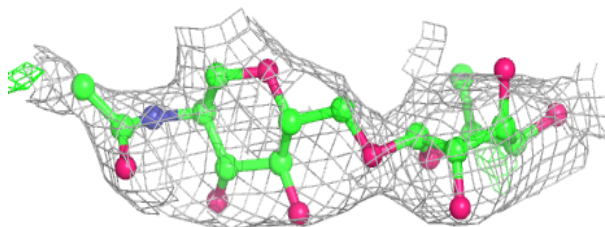
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	T	2	10/11	0.51	0.19	108,108,109,109	0
3	NAG	R	1	14/15	0.52	0.16	116,117,118,118	0
3	FUC	U	2	10/11	0.70	0.16	118,119,119,119	0
3	FUC	R	2	10/11	0.78	0.12	119,119,119,119	0
3	NAG	U	1	14/15	0.79	0.13	115,116,117,118	0
3	NAG	Q	1	14/15	0.83	0.14	59,60,61,61	0
3	NAG	T	1	14/15	0.85	0.10	107,107,108,108	0
3	FUC	Q	2	10/11	0.93	0.13	60,60,60,61	0
3	FUC	S	2	10/11	0.93	0.12	55,56,56,56	0
3	NAG	S	1	14/15	0.94	0.08	54,55,55,55	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.

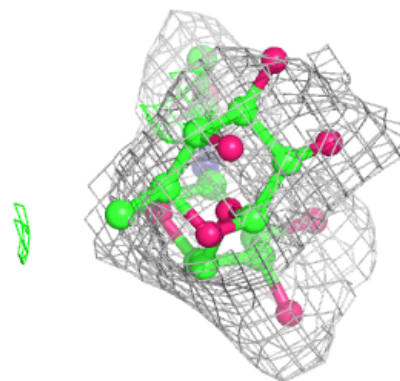
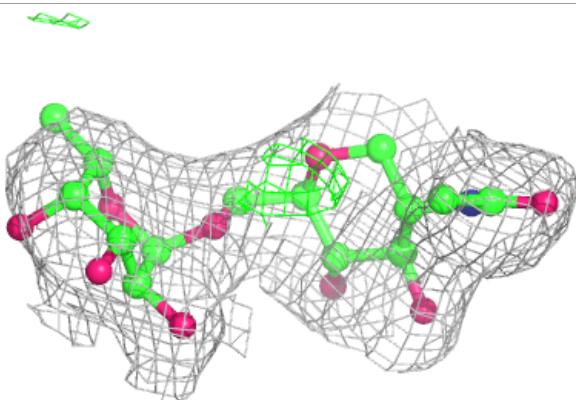
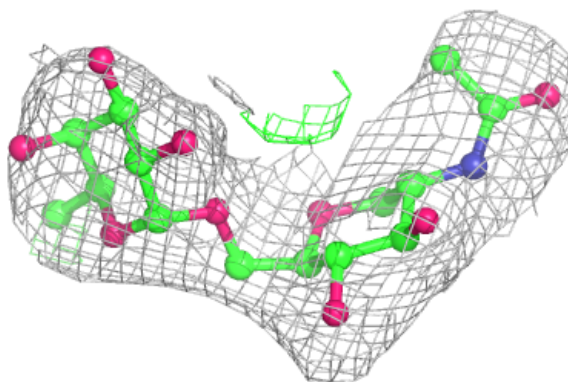


**Electron density around Chain R:**

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

**Electron density around Chain S:**

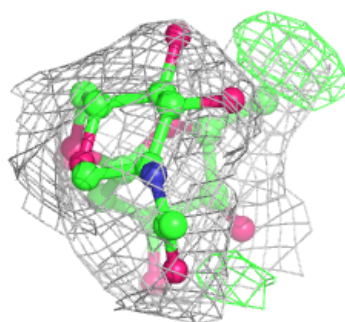
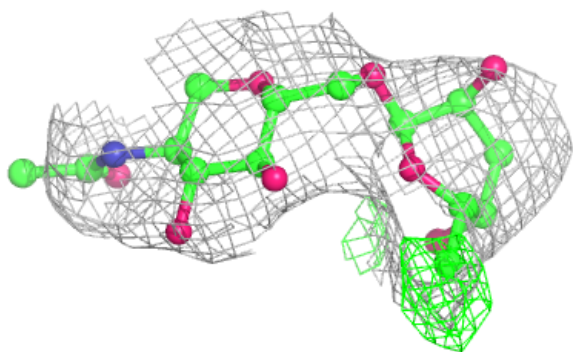
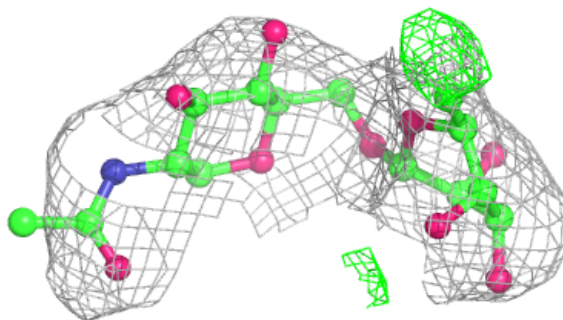
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



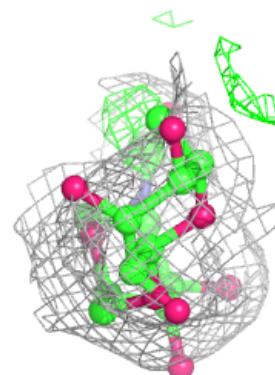
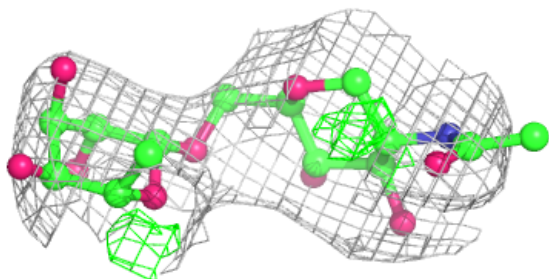
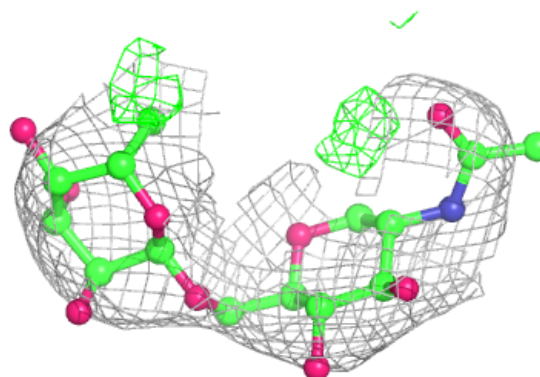


**Electron density around Chain T:**

$2mF_o-DF_c$  (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)





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	I	301	14/15	0.35	0.16	173,173,173,173	0
4	NAG	B	301	14/15	0.50	0.17	102,103,104,104	0
4	NAG	N	301	14/15	0.53	0.16	126,126,127,127	0
4	NAG	F	301	14/15	0.55	0.20	108,109,110,110	0
4	NAG	P	301	14/15	0.56	0.17	110,111,111,112	0
4	NAG	E	301	14/15	0.62	0.13	102,103,104,105	0
4	NAG	O	301	14/15	0.64	0.12	183,184,184,184	0
4	NAG	H	301	14/15	0.70	0.13	92,93,93,93	0
4	NAG	N	302	14/15	0.70	0.15	103,105,105,105	0
4	NAG	D	301	14/15	0.71	0.16	61,62,63,63	0
4	NAG	L	302	14/15	0.74	0.14	109,109,110,110	0
4	NAG	L	301	14/15	0.77	0.14	119,119,119,119	0
4	NAG	J	301	14/15	0.77	0.11	104,105,106,106	0
4	NAG	A	301	14/15	0.79	0.13	100,101,101,101	0
4	NAG	H	302	14/15	0.81	0.15	57,58,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.