wwPDB X-ray Structure Validation Summary Report (i)

Apr 1, 2025 – 10:46 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

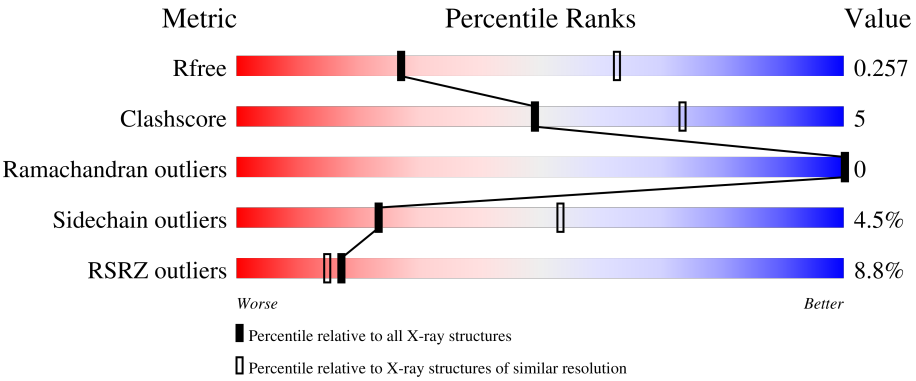
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 >=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 <=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	3% 64% 5% 32%
1	C	152	15% 52% 14% · 33%
1	E	152	2% 64% · 33%
1	G	152	10% 54% 11% · 34%
1	I	152	17% 59% 8% · 33%

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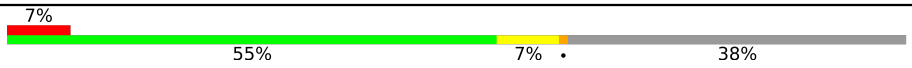
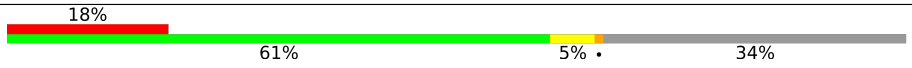
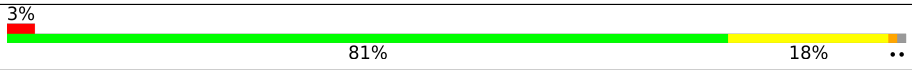
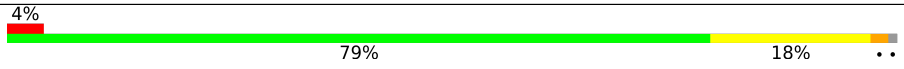
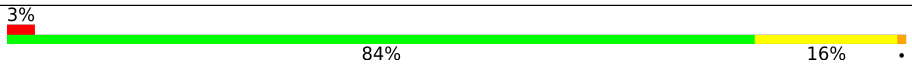
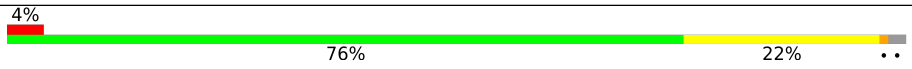
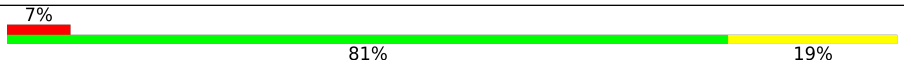
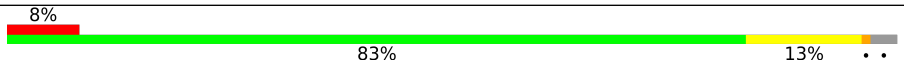
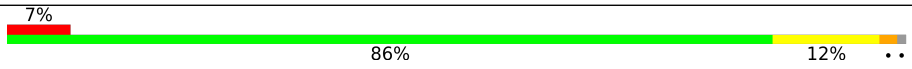
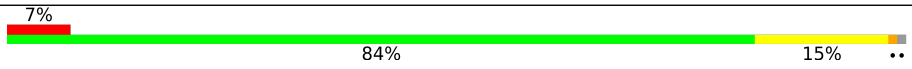
Mol	Chain	Length	Quality of chain
1	K	152	
1	M	152	
1	O	152	
2	B	195	
2	D	195	
2	F	195	
2	H	195	
2	J	195	
2	L	195	
2	N	195	
2	P	195	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	

2 Entry composition (i)

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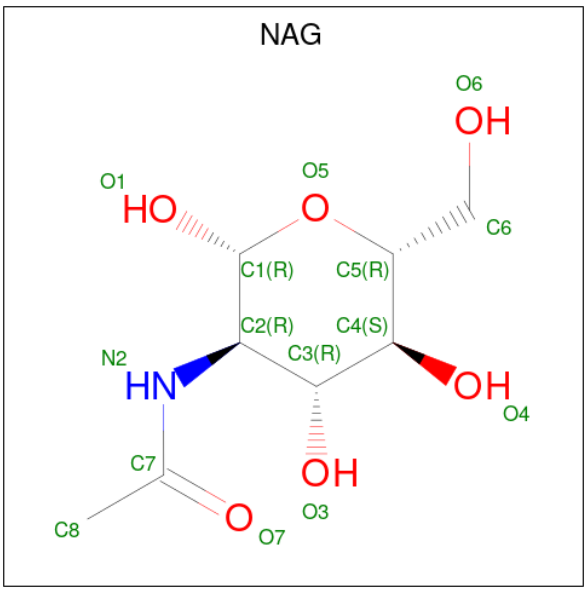
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	193	Total	C	N	O	S	0	0	0
			1492	941	256	287	8			
2	P	194	Total	C	N	O	S	0	0	0
			1501	947	258	288	8			

- 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: $C_8H_{15}NO_6$).



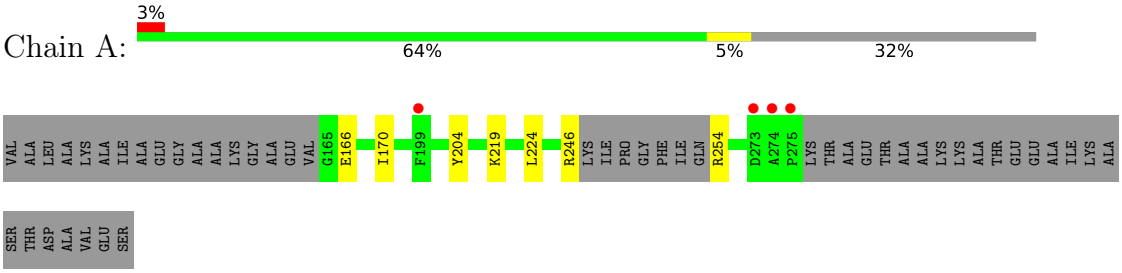
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1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

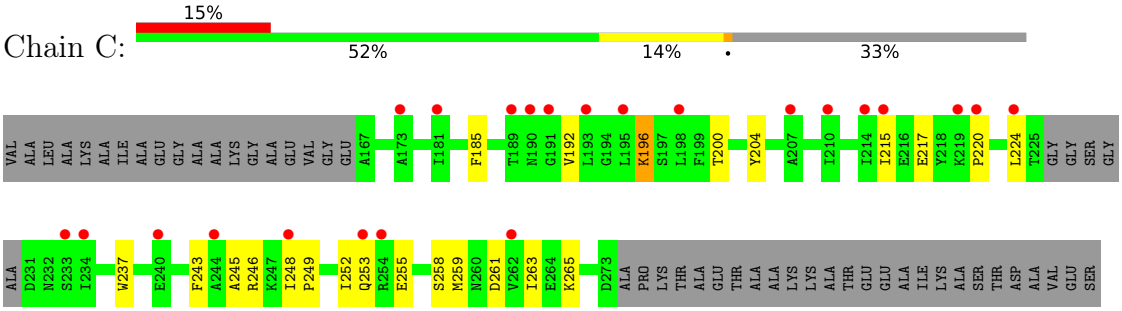
• Molecule 1: RIFIN RBK21

Chain A:



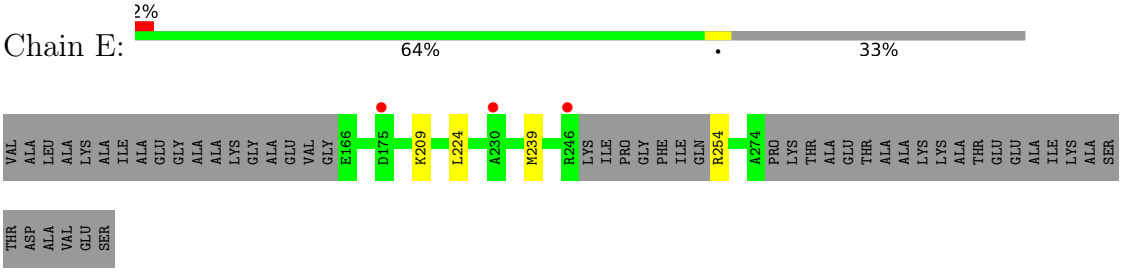
• Molecule 1: RIFIN RBK21

Chain C:



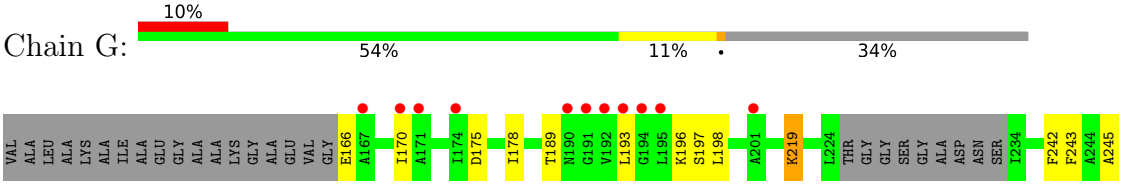
• Molecule 1: RIFIN RBK21

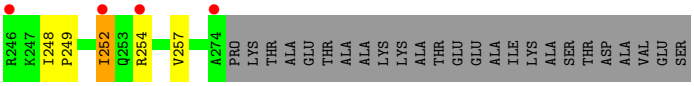
Chain E:



• Molecule 1: RIFIN RBK21

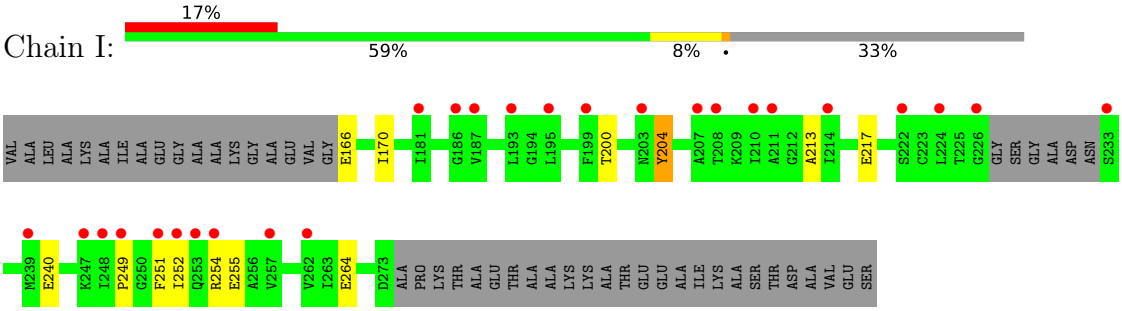
Chain G:





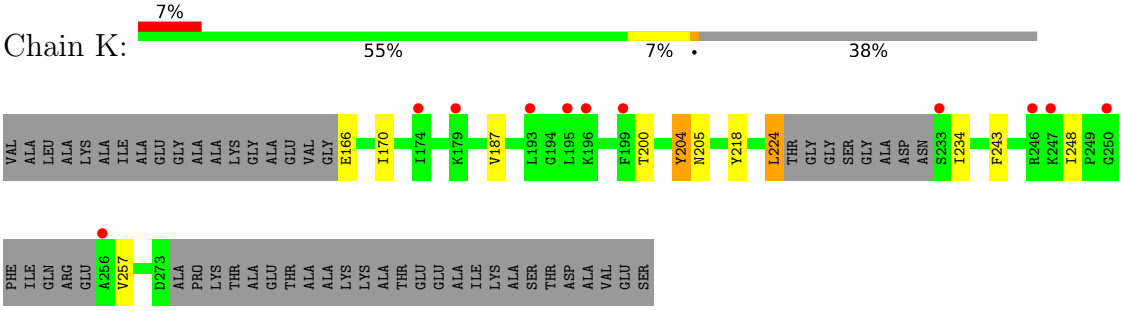
• Molecule 1: RIFIN RBK21

Chain I:



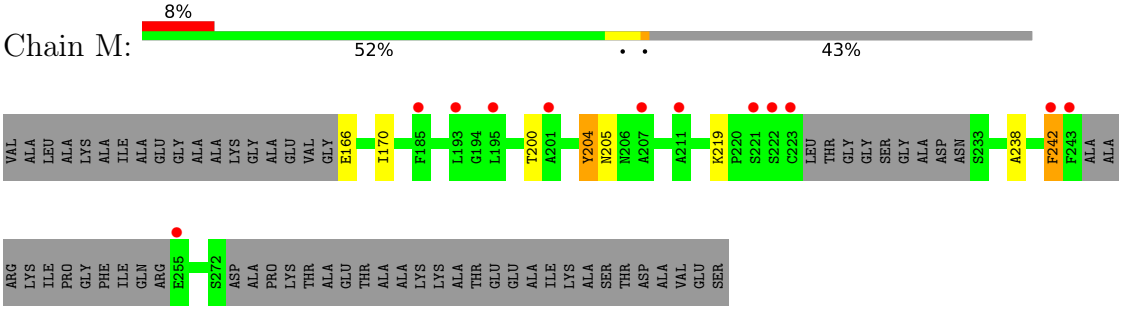
• Molecule 1: RIFIN RBK21

Chain K:



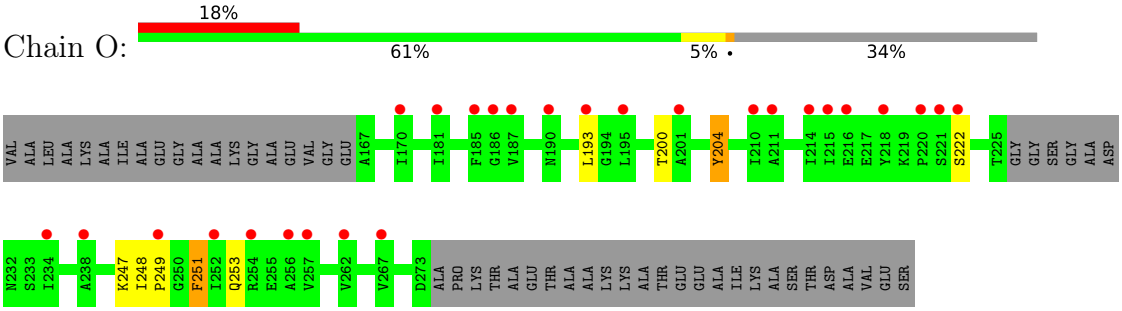
• Molecule 1: RIFIN RBK21

Chain M:



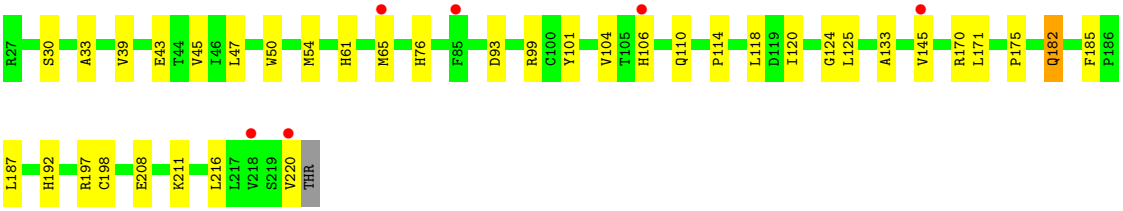
• Molecule 1: RIFIN RBK21

Chain O:

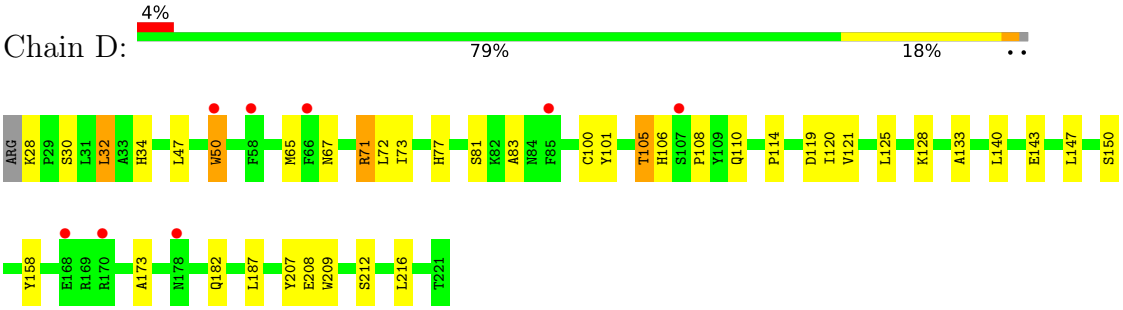


• Molecule 2: KIR2DL protein

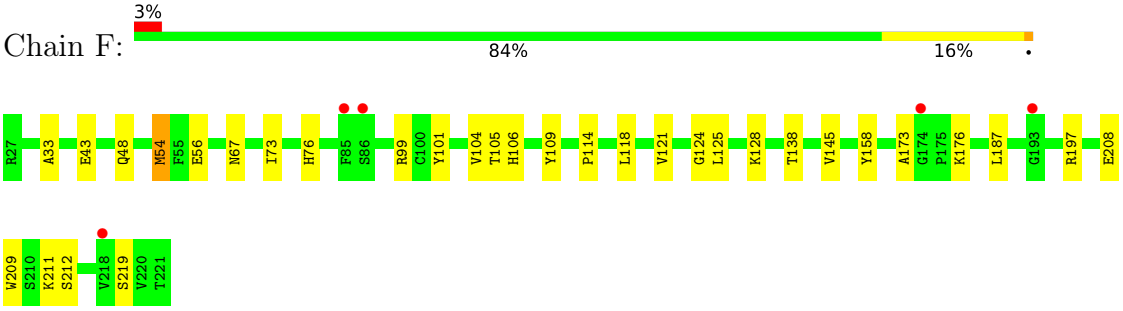
Chain B:



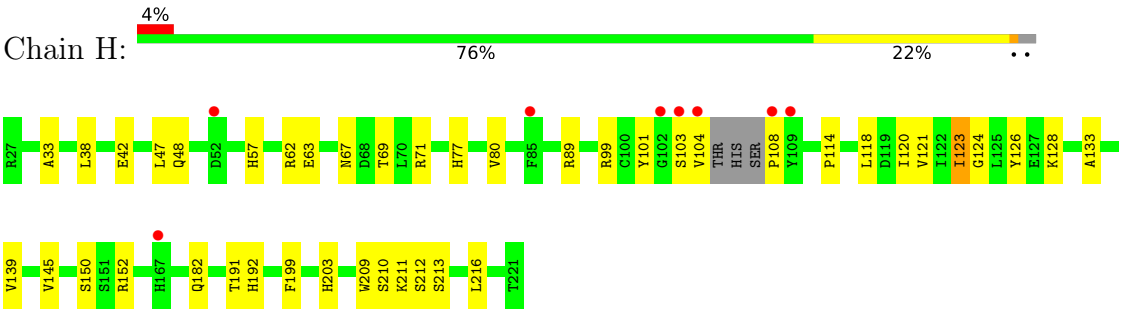
• Molecule 2: KIR2DL protein



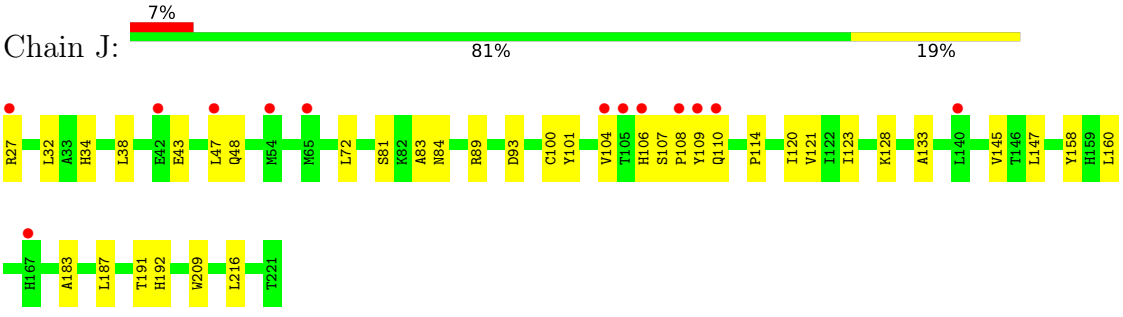
• Molecule 2: KIR2DL protein



• Molecule 2: KIR2DL protein

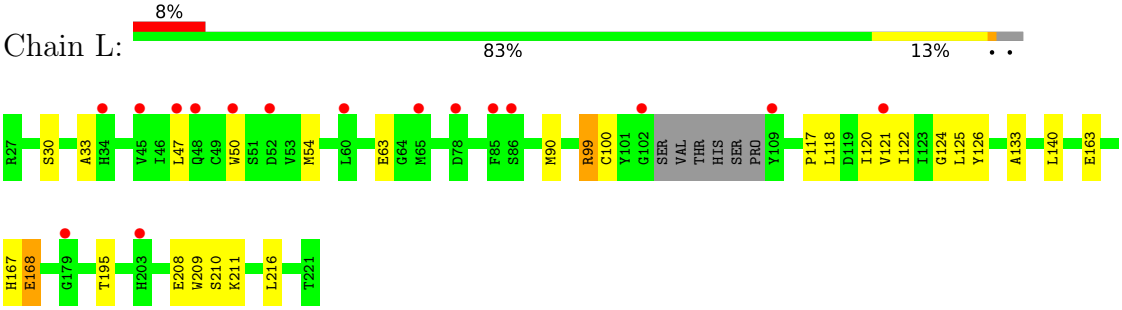


• Molecule 2: KIR2DL protein



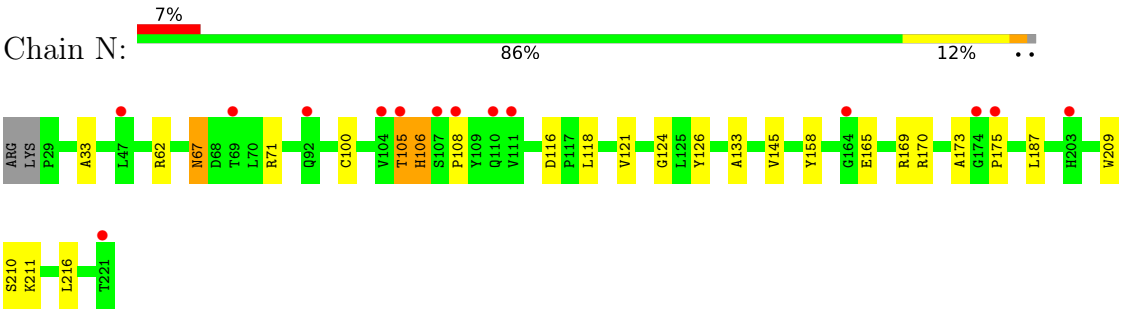
• Molecule 2: KIR2DL protein

Chain L:



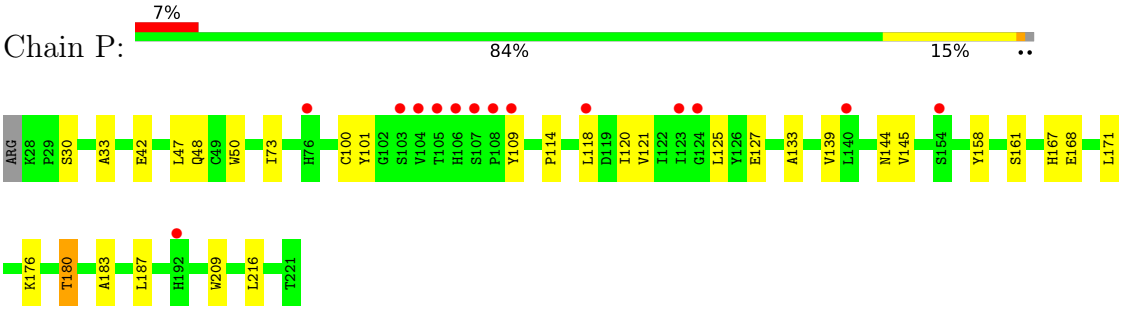
• Molecule 2: KIR2DL protein

Chain N:



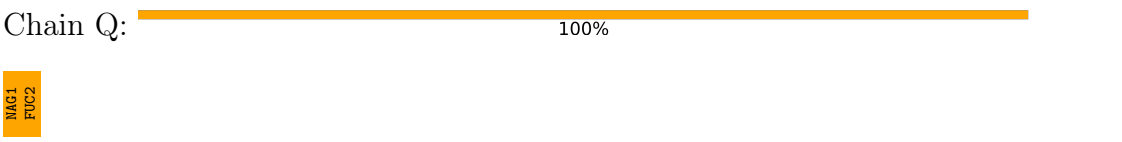
• Molecule 2: KIR2DL protein

Chain P:



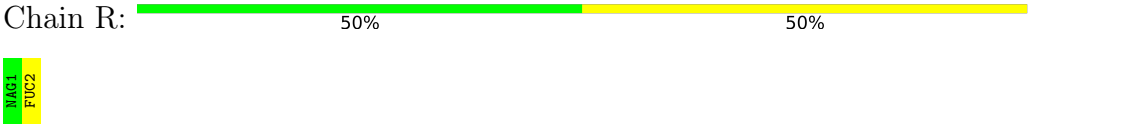
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:



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

Chain S:

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

Chain T:

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

Chain U:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.80 (at 2.91Å)	Xtriage
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^2)	75.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18222	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2283/2776 (82%)	2208 (97%)	75 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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
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

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	187	VAL

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Mol	Chain	Res	Type
2	N	100	CYS
1	K	205	ASN
2	L	168	GLU
2	N	165	GLU

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.

The worst 5 of 6 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 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

All (1) ring outliers are listed below:

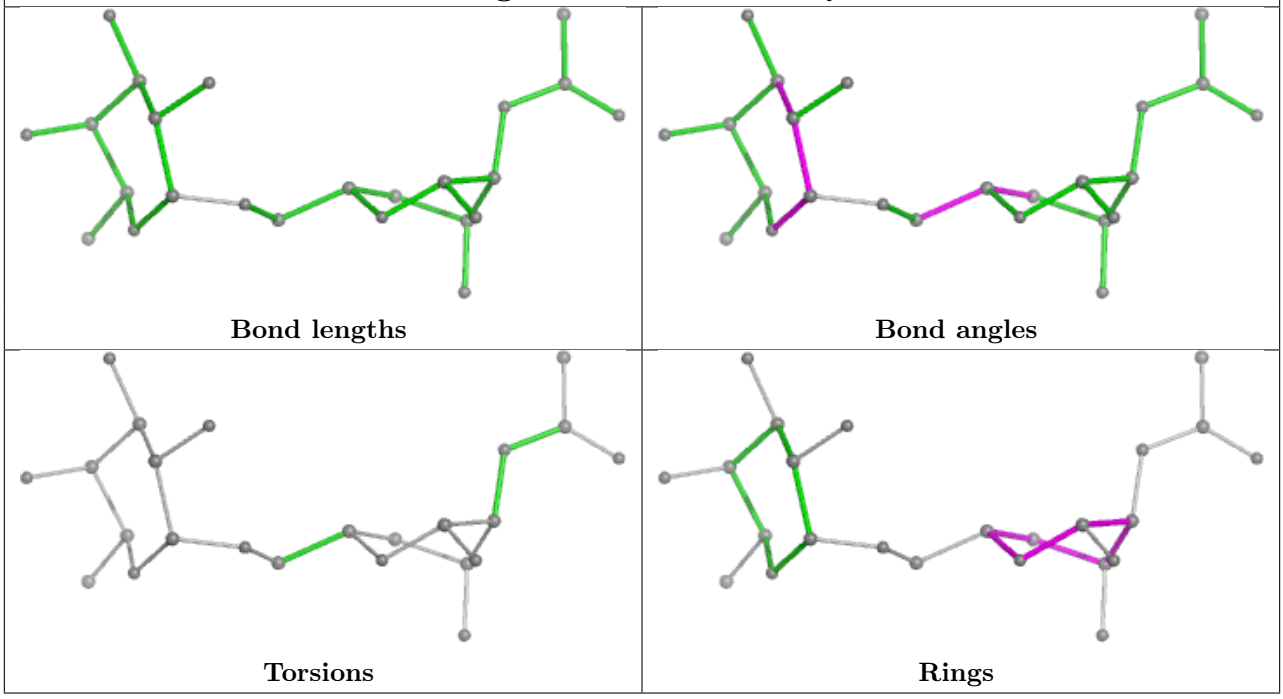
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

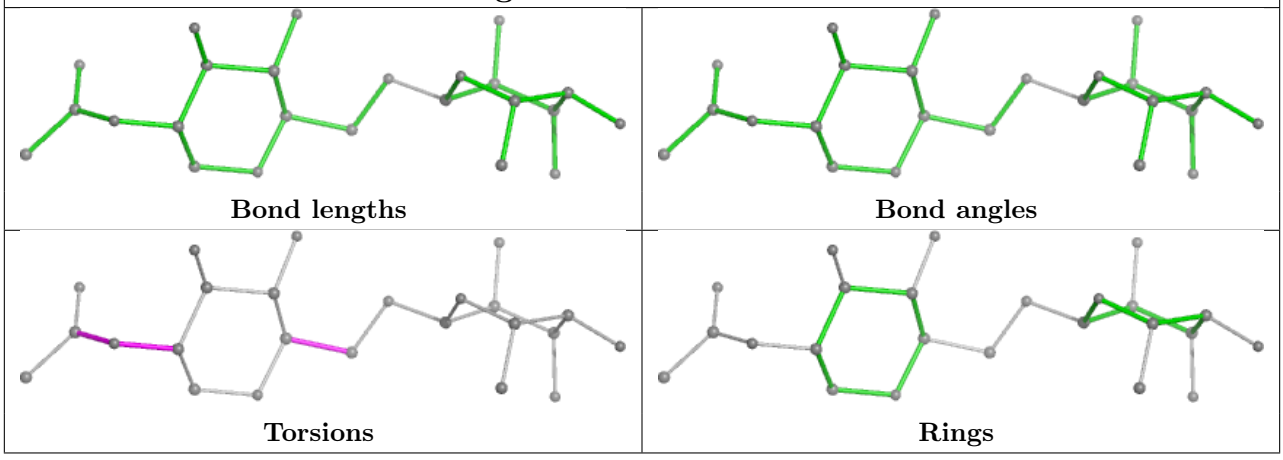
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	FUC	1	0
3	S	1	NAG	1	0
3	Q	2	FUC	5	0
3	Q	1	NAG	4	0
3	U	2	FUC	1	0

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

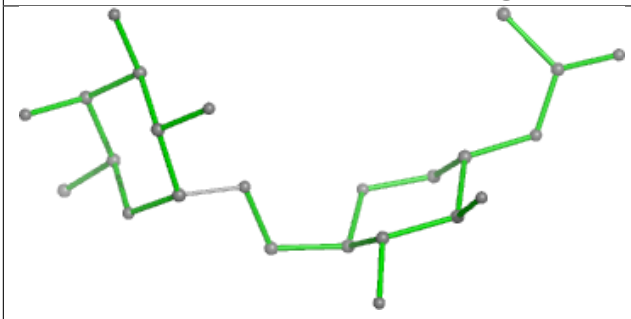
Oligosaccharide Chain Q



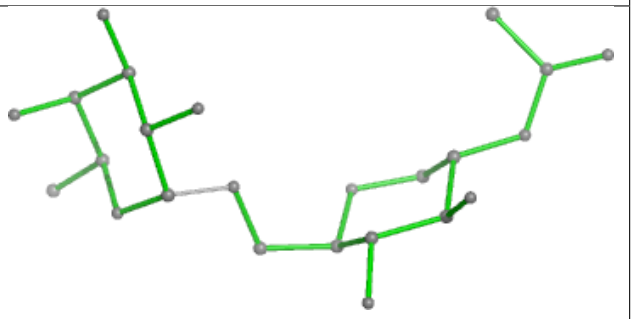
Oligosaccharide Chain R



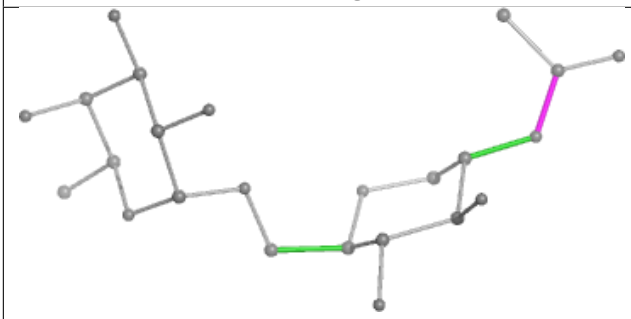
Oligosaccharide Chain S



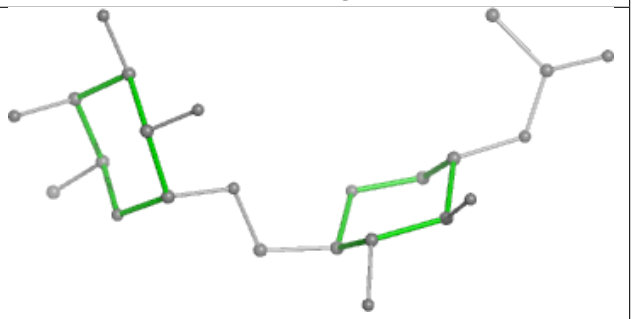
Bond lengths



Bond angles

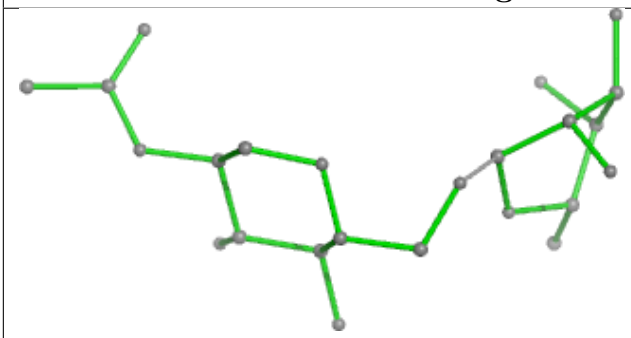


Torsions

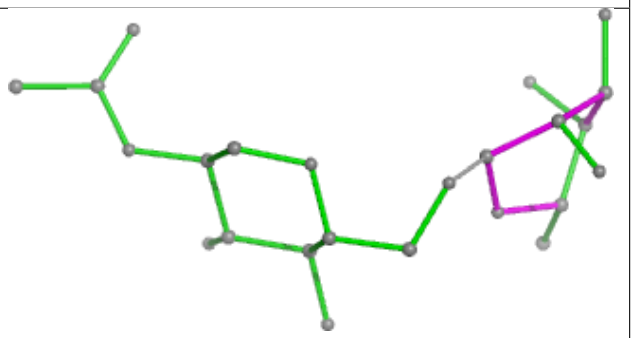


Rings

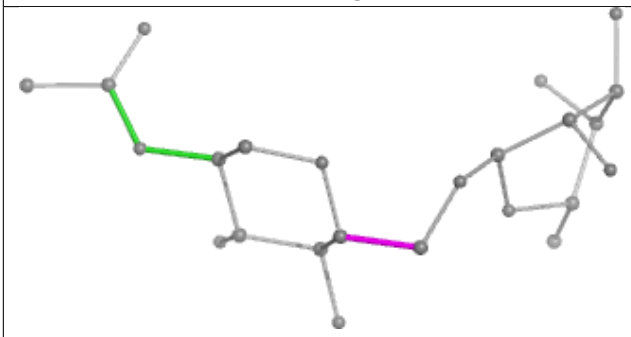
Oligosaccharide Chain T



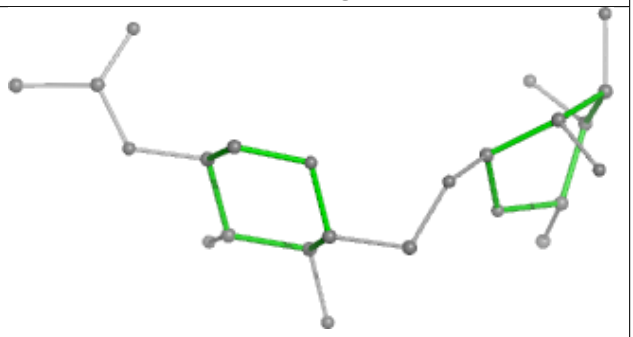
Bond lengths



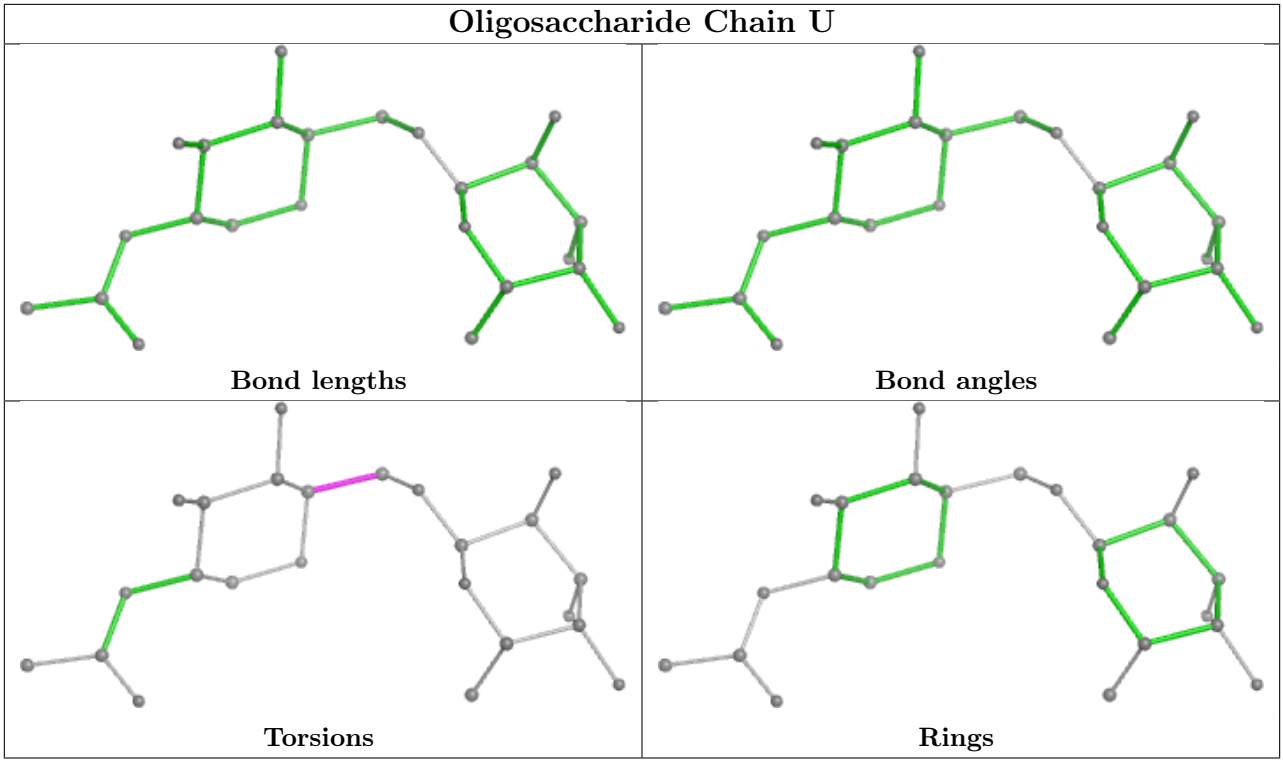
Bond angles



Torsions



Rings



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.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

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^{th} 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	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

The worst 5 of 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

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)

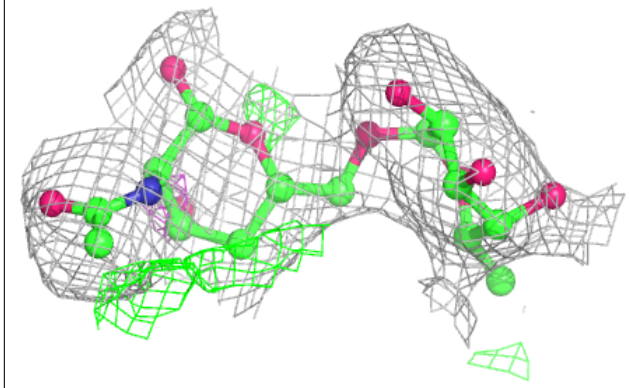
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

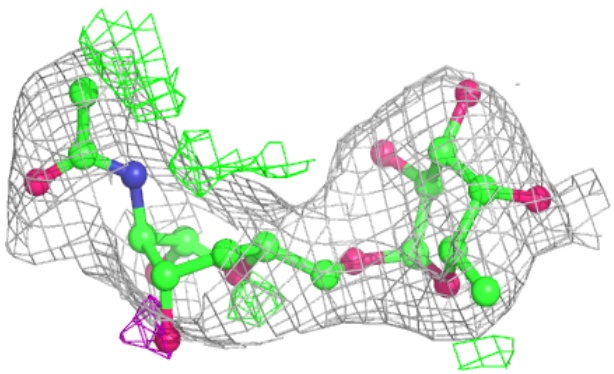
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	T	2	10/11	0.51	0.19	108,108,109,109	0
3	NAG	R	1	14/15	0.52	0.16	116,117,118,118	0
3	FUC	U	2	10/11	0.70	0.16	118,119,119,119	0
3	FUC	R	2	10/11	0.78	0.12	119,119,119,119	0
3	NAG	U	1	14/15	0.79	0.13	115,116,117,118	0
3	NAG	Q	1	14/15	0.83	0.14	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

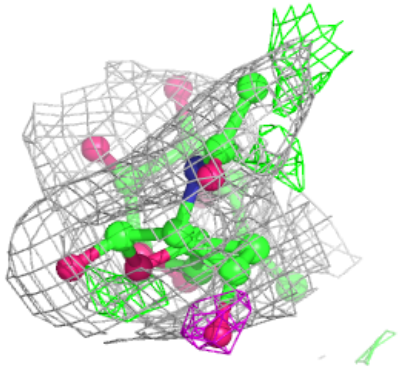
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

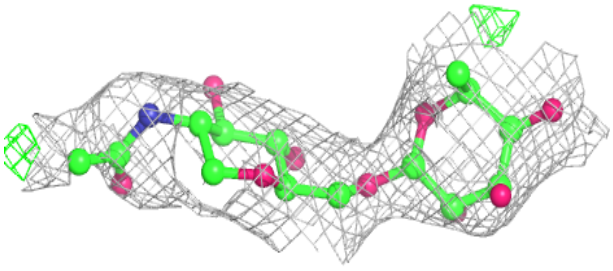


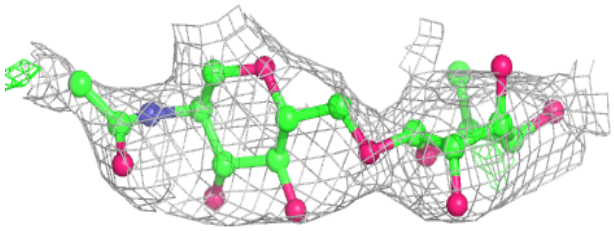


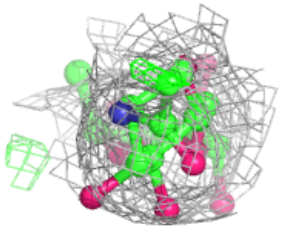


Electron density around Chain R:

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

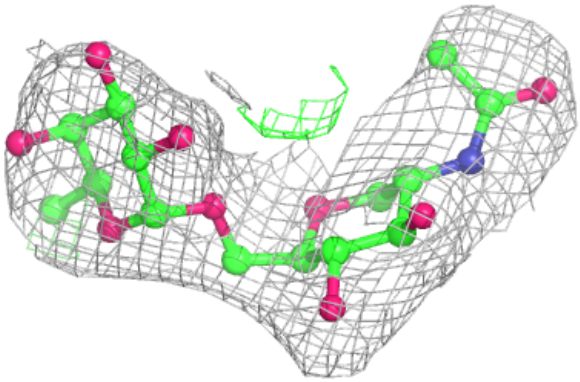


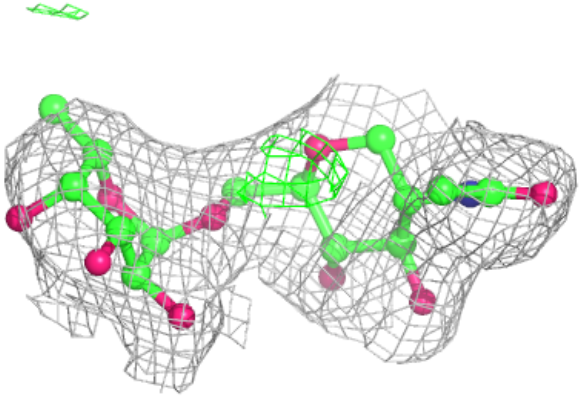


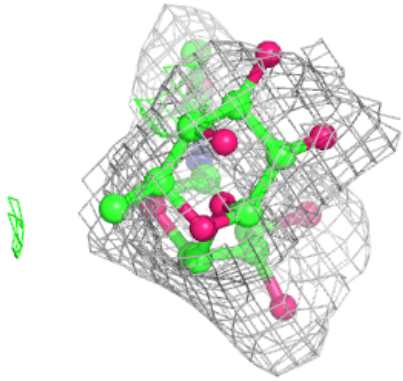


Electron density around Chain S:

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

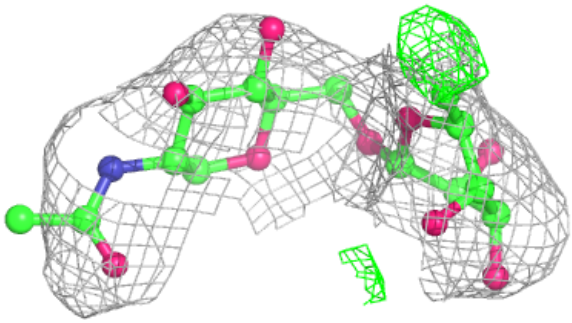


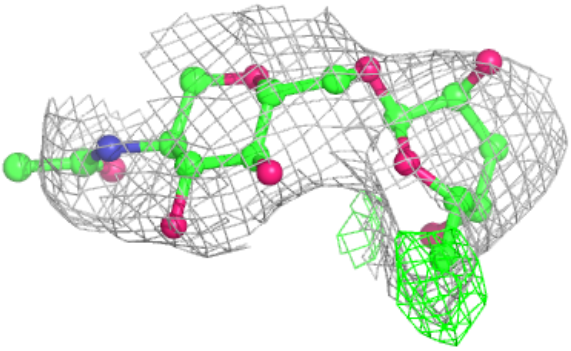


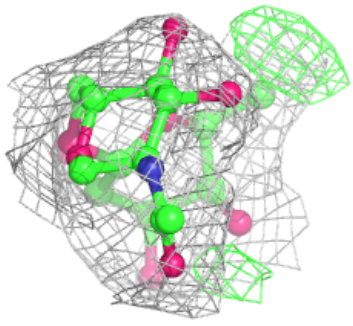


Electron density around Chain T:

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

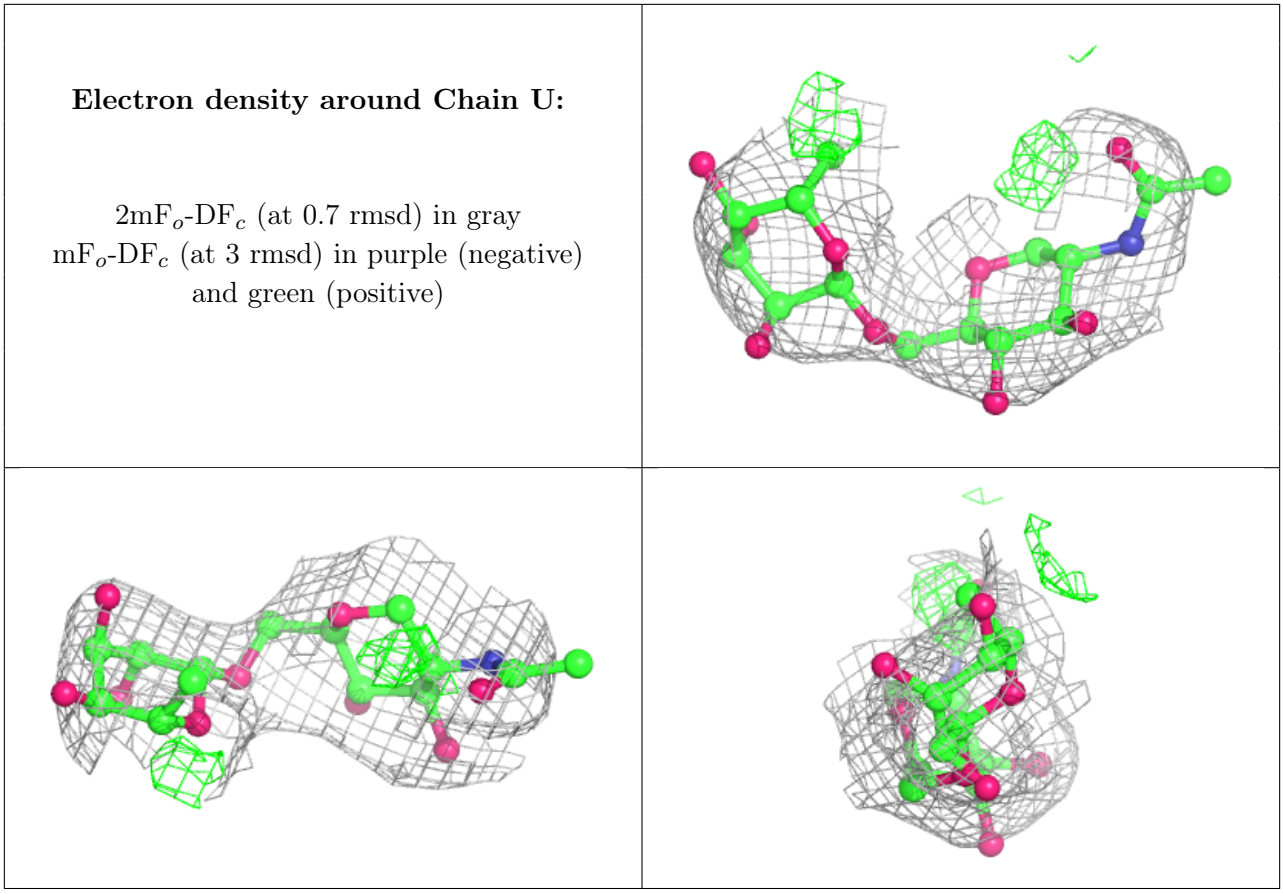






Electron density around Chain U:

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



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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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 (i)

There are no such residues in this entry.