



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 AM UTC

PDB ID : 7NP1 / pdb_00007np1
Title : Crystal Structure of the SARS-CoV-2 Receptor Binding Domain in Complex with Antibody ION-360
Authors : Hall, G.; Cowan, R.; Carr, M.
Deposited on : 2021-02-26
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

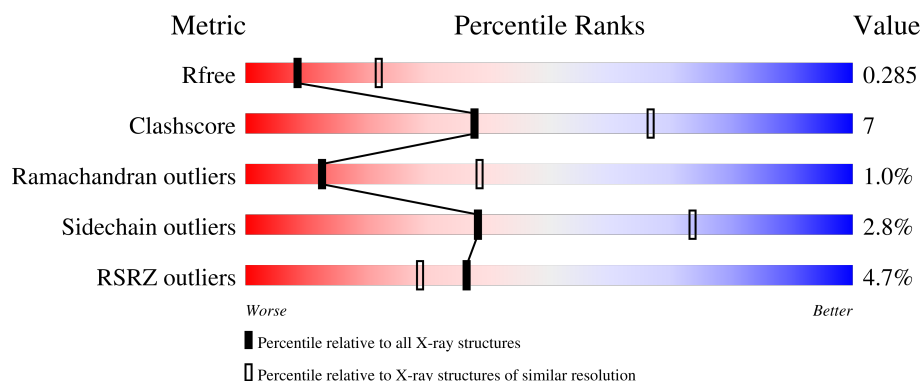
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	2% 58% 15% 26%
1	B	232	5% 64% 8% 28%
1	C	232	% 65% 17% 18%
1	D	232	4% 63% 15% 22%
2	H	224	3% 84% 14% .

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Mol	Chain	Length	Quality of chain
2	I	224	4% 79% 17% .
2	J	224	6% 79% 18% ..
2	K	224	7% 75% 19% ..
3	L	217	% 84% 13% ..
3	M	217	3% 77% 19% ..
3	N	217	12% 79% 17% ..
3	O	217	2% 84% 14% .
4	E	2	100%
4	F	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18843 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1368	879	228	255	6			
1	B	168	Total	C	N	O	S	0	0	0
			1346	865	225	251	5			
1	C	190	Total	C	N	O	S	0	0	0
			1508	967	250	283	8			
1	D	181	Total	C	N	O	S	0	0	0
			1445	927	239	272	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	540	ALA	-	expression tag	UNP P0DTC2
A	541	ALA	-	expression tag	UNP P0DTC2
A	542	ALA	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	SER	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	540	ALA	-	expression tag	UNP P0DTC2
B	541	ALA	-	expression tag	UNP P0DTC2
B	542	ALA	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	SER	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2
B	550	HIS	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	542	ALA	-	expression tag	UNP P0DTC2
C	543	ALA	-	expression tag	UNP P0DTC2
C	544	ALA	-	expression tag	UNP P0DTC2
C	545	GLY	-	expression tag	UNP P0DTC2
C	546	SER	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
C	548	HIS	-	expression tag	UNP P0DTC2
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
D	?	-	HIS	deletion	UNP P0DTC2
D	?	-	ALA	deletion	UNP P0DTC2
D	542	ALA	-	expression tag	UNP P0DTC2
D	543	ALA	-	expression tag	UNP P0DTC2
D	544	ALA	-	expression tag	UNP P0DTC2
D	545	GLY	-	expression tag	UNP P0DTC2
D	546	SER	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2
D	548	HIS	-	expression tag	UNP P0DTC2
D	549	HIS	-	expression tag	UNP P0DTC2
D	550	HIS	-	expression tag	UNP P0DTC2
D	551	HIS	-	expression tag	UNP P0DTC2
D	552	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1615	1014	272	323	6			
2	I	216	Total	C	N	O	S	0	1	0
			1597	1004	270	317	6			
2	J	218	Total	C	N	O	S	0	0	0
			1602	1007	270	319	6			
2	K	217	Total	C	N	O	S	0	0	0
			1598	1005	269	318	6			

- Molecule 3 is a protein called Immunoglobulin light chain.

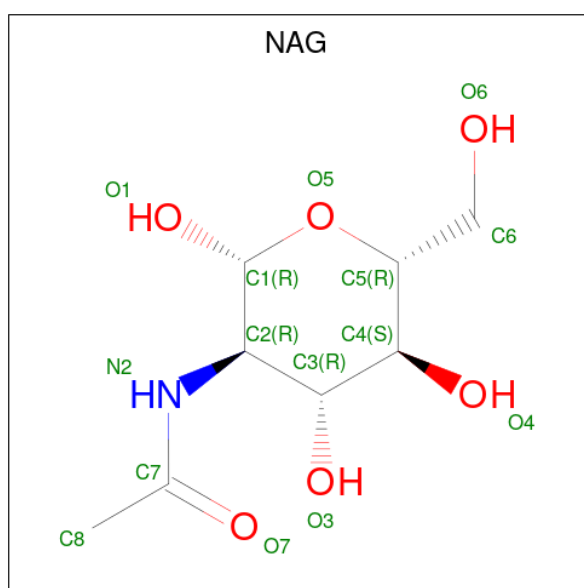
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	1	0
			1657	1036	278	338	5			
3	M	214	Total	C	N	O	S	0	0	0
			1652	1033	277	337	5			
3	N	214	Total	C	N	O	S	0	1	0
			1656	1035	279	337	5			
3	O	214	Total	C	N	O	S	0	0	0
			1652	1033	277	337	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

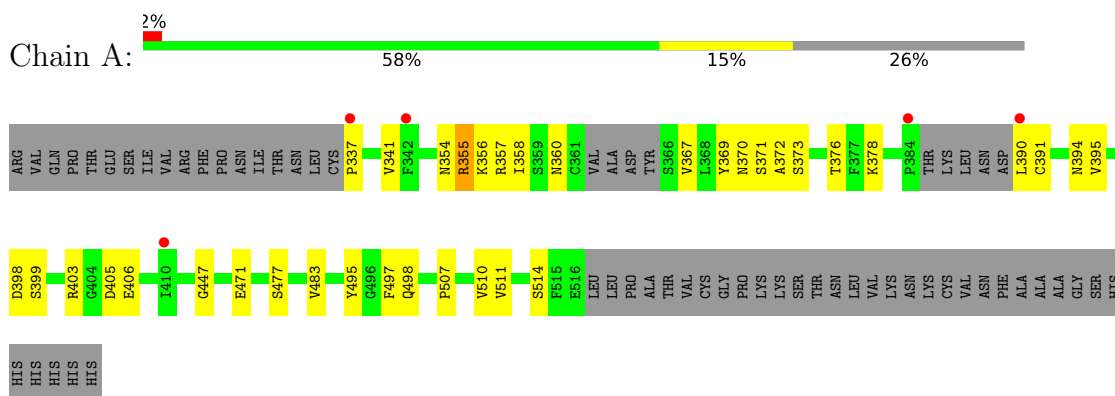
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	10	Total	O	0	0
			10	10		
6	C	7	Total	O	0	0
			7	7		
6	D	4	Total	O	0	0
			4	4		
6	H	3	Total	O	0	0
			3	3		
6	I	4	Total	O	0	0
			4	4		
6	J	3	Total	O	0	0
			3	3		
6	K	6	Total	O	0	0
			6	6		
6	L	5	Total	O	0	0
			5	5		
6	M	6	Total	O	0	0
			6	6		
6	N	6	Total	O	0	0
			6	6		
6	O	11	Total	O	0	0
			11	11		

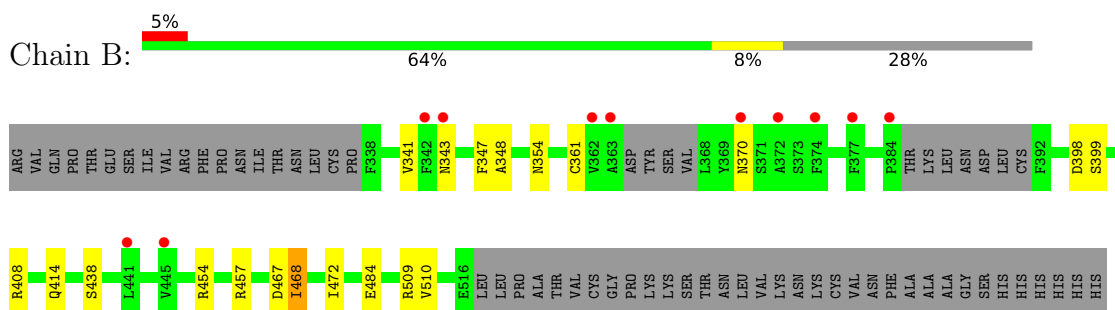
3 Residue-property plots [i](#)

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.

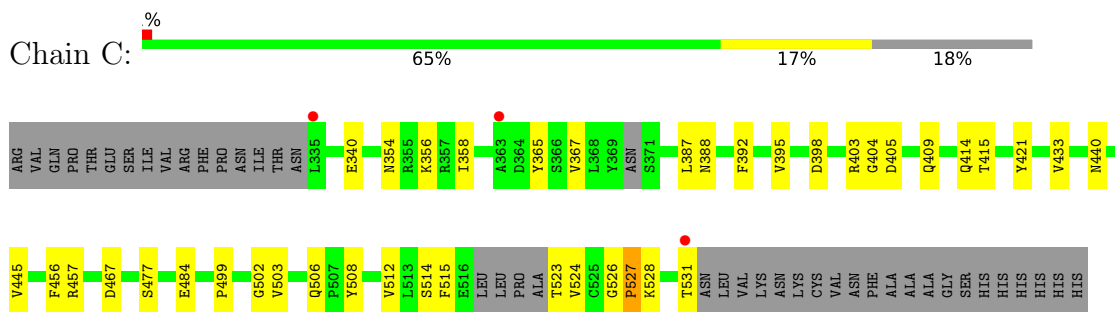
• Molecule 1: Spike protein S1



• Molecule 1: Spike protein S1

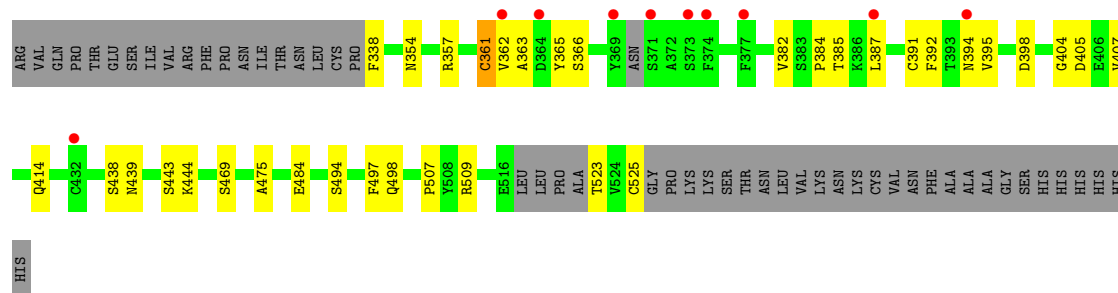


• Molecule 1: Spike protein S1

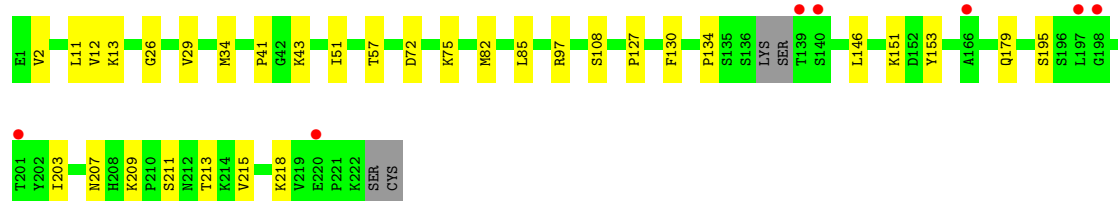
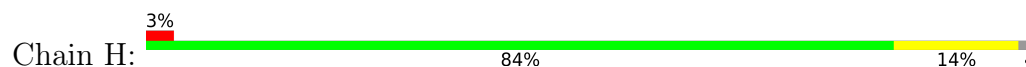


• Molecule 1: Spike protein S1

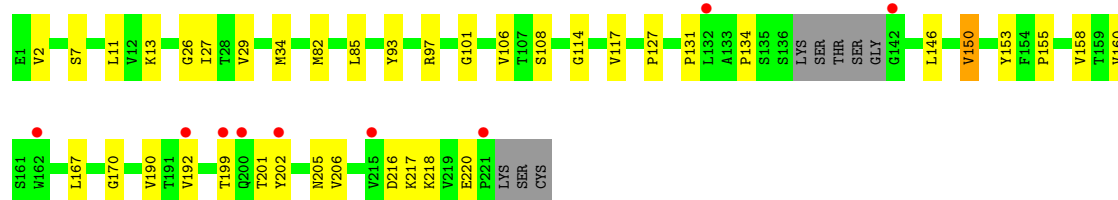
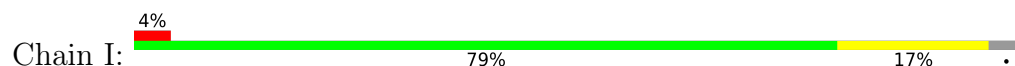




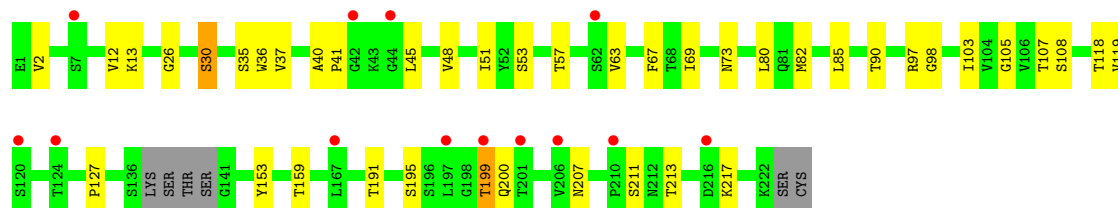
- Molecule 2: Immunoglobulin gamma-1 heavy chain



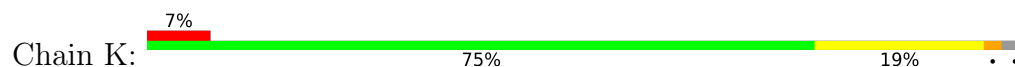
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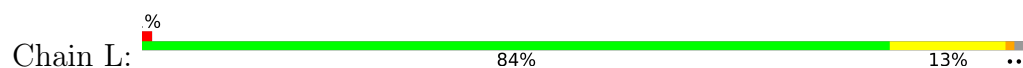


- Molecule 2: Immunoglobulin gamma-1 heavy chain

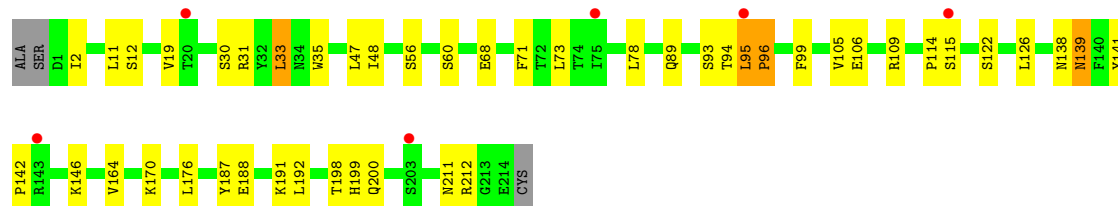
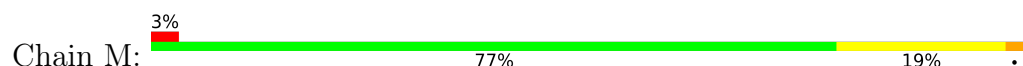




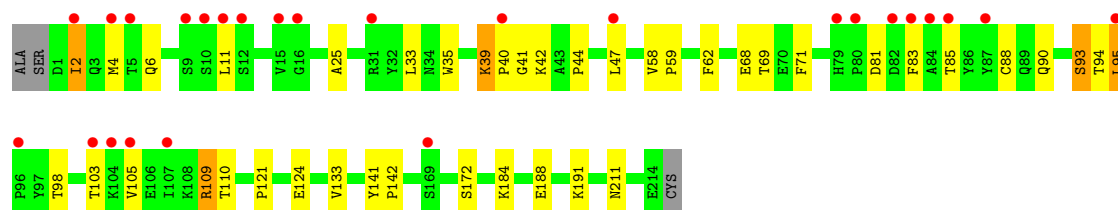
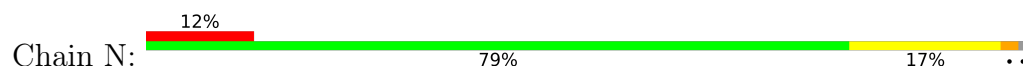
- Molecule 3: Immunoglobulin light chain



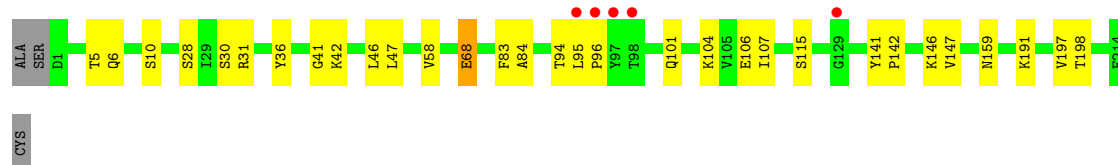
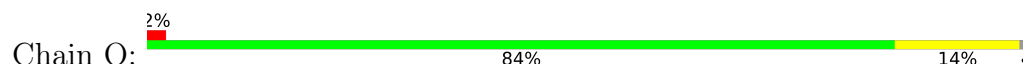
- Molecule 3: Immunoglobulin light chain



- Molecule 3: Immunoglobulin light chain



- Molecule 3: Immunoglobulin light chain



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



MAG1
FUC2

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

Chain F:

50%

50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.05Å 107.90Å 181.63Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	48.28 – 2.80 48.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.28-2.80) 99.8 (48.28-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.81Å)	Xtriage
Refinement program	PDB-REDO v1.0, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.232 , 0.281 0.237 , 0.285	Depositor DCC
R_{free} test set	8477 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18843	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 28.53 % 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 1.8134e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.16	0/1406	0.40	0/1906
1	B	0.20	0/1383	0.44	0/1875
1	C	0.19	0/1548	0.41	0/2100
1	D	0.18	0/1483	0.43	2/2012 (0.1%)
2	H	0.17	0/1649	0.40	0/2245
2	I	0.17	0/1634	0.41	0/2225
2	J	0.19	0/1636	0.47	0/2227
2	K	0.20	0/1632	0.46	0/2222
3	L	0.18	0/1696	0.44	0/2302
3	M	0.17	0/1688	0.44	0/2291
3	N	0.19	0/1695	0.48	0/2301
3	O	0.17	0/1688	0.43	0/2291
All	All	0.18	0/19138	0.44	2/25997 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1
3	M	0	1
3	N	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	CYS	CA-C-N	6.28	133.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	CYS	C-N-CA	6.28	133.00	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	1	ASP	Peptide
3	M	95	LEU	Peptide
3	N	83	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1368	0	1288	23	0
1	B	1346	0	1264	15	0
1	C	1508	0	1432	22	0
1	D	1445	0	1361	20	1
2	H	1615	0	1594	18	1
2	I	1597	0	1579	22	0
2	J	1602	0	1582	27	0
2	K	1598	0	1579	31	0
3	L	1657	0	1610	20	0
3	M	1652	0	1604	23	0
3	N	1656	0	1606	29	0
3	O	1652	0	1604	19	0
4	E	24	0	22	0	0
4	F	24	0	22	0	0
5	B	14	0	13	1	0
5	D	14	0	13	0	0
6	A	6	0	0	0	0
6	B	10	0	0	0	0
6	C	7	0	0	1	0
6	D	4	0	0	0	0
6	H	3	0	0	0	0
6	I	4	0	0	0	0
6	J	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	6	0	0	0	0
6	L	5	0	0	0	0
6	M	6	0	0	0	0
6	N	6	0	0	0	0
6	O	11	0	0	1	0
All	All	18843	0	18173	260	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:109:ARG:HG3	3:N:109:ARG:HH11	1.39	0.87
2:K:90:THR:HG22	2:K:119:VAL:H	1.40	0.85
3:O:6:GLN:H	3:O:101:GLN:HE22	1.26	0.83
2:K:164:SER:H	2:K:205:ASN:HD21	1.22	0.82
1:D:365:TYR:HD1	1:D:387:LEU:HB3	1.45	0.80
2:J:40:ALA:HB1	2:J:41:PRO:HD2	1.63	0.80
3:O:104:LYS:NZ	6:O:301:HOH:O	2.18	0.76
3:L:2:ILE:O	3:L:26:SER:OG	2.02	0.76
1:C:484:GLU:OE2	2:I:13:LYS:NZ	2.18	0.75
2:I:134:PRO:HG3	2:I:146:LEU:HB3	1.68	0.75
2:J:45:LEU:HD21	3:N:44:PRO:HG2	1.69	0.74
2:I:205:ASN:ND2	2:I:216:ASP:OD1	2.15	0.73
3:N:6:GLN:OE1	3:N:103:THR:OG1	2.07	0.73
1:D:438:SER:HB3	1:D:509:ARG:HD2	1.71	0.72
2:J:90:THR:HG23	2:J:118:THR:HA	1.71	0.72
2:I:82:MET:HB3	2:I:85:LEU:HD21	1.73	0.70
3:M:19:VAL:HG21	3:M:78:LEU:HD13	1.73	0.70
2:H:203:ILE:HD11	2:H:218:LYS:HE2	1.74	0.69
3:N:109:ARG:HD2	3:N:172:SER:HB2	1.74	0.69
2:K:11:LEU:HD12	2:K:12:VAL:H	1.59	0.68
3:N:2:ILE:HD12	3:N:2:ILE:H	1.60	0.67
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.76	0.67
1:D:365:TYR:CD1	1:D:387:LEU:HB3	2.30	0.66
3:N:90:GLN:HE21	3:N:98:THR:HG22	1.60	0.66
2:I:29:VAL:HG22	2:I:34:MET:HE2	1.78	0.66
2:H:211:SER:HG	2:H:213:THR:HG1	1.40	0.66
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.29	0.65
1:C:433:VAL:HG12	1:C:512:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:164:SER:H	2:K:205:ASN:ND2	1.93	0.65
2:H:134:PRO:HG3	2:H:146:LEU:HB3	1.77	0.64
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.79	0.63
2:K:194:SER:O	2:K:197:LEU:HG	2.00	0.62
3:L:6:GLN:HB2	3:L:101:GLN:NE2	2.14	0.62
2:I:2:VAL:HG22	2:I:26:GLY:HA3	1.82	0.61
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.82	0.61
2:J:35:SER:OG	2:J:98:GLY:O	2.18	0.61
1:A:355:ARG:HD3	1:A:398:ASP:OD1	2.01	0.60
2:I:218:LYS:HD2	2:I:220:GLU:OE1	2.02	0.60
1:C:340:GLU:OE1	1:C:356:LYS:NZ	2.35	0.60
3:M:11:LEU:HD22	3:M:105:VAL:HG22	1.83	0.60
2:H:72:ASP:OD2	2:H:75:LYS:HE2	2.02	0.60
1:C:456:PHE:CZ	2:J:105:GLY:HA3	2.36	0.59
2:H:151:LYS:NZ	2:H:179:GLN:HE22	1.99	0.59
3:M:146:LYS:HB3	3:M:198:THR:HB	1.85	0.59
2:I:192:VAL:HG21	2:I:202:TYR:OH	2.03	0.59
2:J:159:THR:HG22	2:J:207:ASN:HB3	1.84	0.59
2:I:27:ILE:HD12	2:I:97:ARG:HG3	1.84	0.59
1:B:454:ARG:HD3	1:B:457:ARG:HG3	1.85	0.58
3:L:147:VAL:HG22	3:L:197:VAL:HG22	1.84	0.58
3:O:147:VAL:HG12	3:O:197:VAL:HG22	1.84	0.58
2:K:97:ARG:O	2:K:108:SER:HA	2.04	0.58
3:L:11:LEU:HD22	3:L:105:VAL:HG22	1.85	0.58
2:K:164:SER:N	2:K:205:ASN:HD21	1.99	0.57
3:M:170:LYS:HA	3:M:170:LYS:HE2	1.85	0.57
3:O:6:GLN:N	3:O:101:GLN:HE22	1.99	0.57
1:C:409:GLN:HA	1:C:414:GLN:HG2	1.85	0.57
1:C:526:GLY:O	1:C:528:LYS:N	2.37	0.57
3:O:5:THR:HA	3:O:101:GLN:HE22	1.70	0.57
1:A:372:ALA:O	1:A:373:SER:OG	2.20	0.57
1:D:363:ALA:HB1	1:D:365:TYR:CZ	2.39	0.56
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.41	0.56
1:D:361:CYS:HA	1:D:362:VAL:HB	1.88	0.56
1:D:357:ARG:HE	1:D:394:ASN:HD21	1.53	0.55
2:J:13:LYS:N	2:J:13:LYS:HD2	2.21	0.55
3:L:6:GLN:HB2	3:L:101:GLN:HE22	1.70	0.55
3:N:39:LYS:NZ	3:N:81:ASP:O	2.37	0.55
2:I:27:ILE:CD1	2:I:97:ARG:HG3	2.37	0.55
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.88	0.55
3:N:109:ARG:HG3	3:N:109:ARG:NH1	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:5:THR:HA	3:O:101:GLN:NE2	2.21	0.55
1:A:403:ARG:HB2	1:A:406:GLU:HG3	1.89	0.54
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.88	0.54
2:K:134:PRO:HG3	2:K:146:LEU:HB3	1.90	0.54
2:H:41:PRO:O	2:H:43:LYS:HE2	2.07	0.54
2:I:82:MET:HE1	2:I:117:VAL:HG11	1.89	0.54
3:N:25:ALA:HB3	3:N:69:THR:HA	1.89	0.54
2:H:11:LEU:HD12	2:H:12:VAL:H	1.73	0.54
2:K:82:MET:HE1	2:K:117:VAL:HG21	1.89	0.54
3:O:6:GLN:H	3:O:101:GLN:NE2	2.02	0.54
2:H:29:VAL:HG22	2:H:34:MET:HE2	1.90	0.54
1:A:356:LYS:HD3	1:A:357:ARG:N	2.23	0.53
2:I:101:GLY:HA3	2:I:106:VAL:HG12	1.90	0.53
1:D:363:ALA:HB1	1:D:365:TYR:CE2	2.44	0.53
1:D:361:CYS:HB3	1:D:362:VAL:C	2.34	0.52
2:K:197:LEU:HD12	2:K:198:GLY:H	1.75	0.52
1:C:445:VAL:HG12	1:C:499:PRO:HG2	1.90	0.52
2:K:20:LEU:HG	2:K:82:MET:HE2	1.91	0.52
3:N:47:LEU:HA	3:N:58:VAL:HG21	1.91	0.52
1:A:367:VAL:HA	1:A:370:ASN:ND2	2.24	0.52
2:K:11:LEU:HD12	2:K:12:VAL:N	2.22	0.52
3:O:47:LEU:HA	3:O:58:VAL:HG21	1.90	0.52
1:B:408:ARG:NH1	1:B:414:GLN:OE1	2.43	0.52
3:L:19:VAL:HG21	3:L:78:LEU:HD13	1.91	0.52
1:C:354:ASN:O	1:C:398:ASP:HA	2.10	0.51
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.91	0.51
2:J:127:PRO:HB3	2:J:153:TYR:HB3	1.92	0.51
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.45	0.51
1:C:388:ASN:HB3	1:C:527:PRO:HD2	1.91	0.51
3:L:2:ILE:HG13	3:L:93:SER:HB3	1.92	0.51
1:D:354:ASN:O	1:D:398:ASP:HA	2.10	0.51
2:K:47:TRP:HE1	2:K:50:VAL:HG13	1.74	0.51
2:K:88:GLU:OE2	2:K:88:GLU:N	2.30	0.51
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.74	0.51
3:M:199:HIS:CD2	3:M:200:GLN:H	2.27	0.51
3:O:94:THR:C	3:O:96:PRO:HD2	2.35	0.51
1:B:467:ASP:O	1:B:468:ILE:HG12	2.10	0.51
1:C:421:TYR:OH	2:J:53:SER:O	2.19	0.51
2:J:199:THR:HG23	2:J:200:GLN:OE1	2.09	0.51
3:M:114:PRO:HD3	3:M:199:HIS:ND1	2.25	0.51
3:L:164:VAL:HG22	3:L:176:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:109:ARG:NH1	3:N:110:THR:O	2.44	0.51
1:B:343:ASN:OD1	5:B:601:NAG:N2	2.44	0.50
1:A:403:ARG:HH21	1:A:405:ASP:HB2	1.76	0.50
3:N:94:THR:O	3:N:95:LEU:HB2	2.10	0.50
3:N:11:LEU:HD22	3:N:105:VAL:HG22	1.93	0.50
2:K:50:VAL:CG2	2:K:58:TYR:HB2	2.42	0.50
1:D:392:PHE:O	1:D:523:THR:N	2.45	0.49
3:N:59:PRO:HG2	3:N:62:PHE:HE2	1.78	0.49
3:O:30:SER:OG	3:O:31:ARG:N	2.46	0.49
3:M:35:TRP:CE2	3:M:73:LEU:HB2	2.48	0.49
2:K:156:GLU:HB3	2:K:157:PRO:HA	1.94	0.49
2:H:82:MET:HE2	2:H:85:LEU:HD21	1.93	0.49
3:M:89:GLN:HB2	3:M:99:PHE:CD1	2.48	0.49
1:B:408:ARG:HH22	1:B:414:GLN:HE22	1.61	0.49
3:M:30:SER:OG	3:M:31:ARG:N	2.41	0.49
3:N:184:LYS:O	3:N:188:GLU:HG2	2.12	0.49
1:B:347:PHE:CE1	1:B:509:ARG:HB3	2.48	0.48
3:L:1:ASP:O	3:L:3:GLN:NE2	2.46	0.48
1:D:405:ASP:OD1	1:D:405:ASP:N	2.44	0.48
1:D:384:PRO:HA	1:D:387:LEU:HD23	1.96	0.48
2:H:97:ARG:O	2:H:108:SER:HA	2.14	0.48
2:J:51:ILE:HD12	2:J:57:THR:HG22	1.95	0.48
3:M:47:LEU:O	3:M:48:ILE:HD13	2.14	0.48
1:D:365:TYR:CE1	1:D:387:LEU:HD12	2.48	0.47
3:L:6:GLN:NE2	3:L:88:CYS:H	2.12	0.47
2:K:127:PRO:HB3	2:K:153:TYR:HB3	1.96	0.47
3:N:124:GLU:OE1	3:N:124:GLU:N	2.43	0.47
1:C:523:THR:HG23	1:C:524:VAL:HG13	1.97	0.47
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.95	0.47
2:K:2:VAL:HG22	2:K:26:GLY:HA3	1.97	0.47
3:L:6:GLN:HE21	3:L:88:CYS:H	1.63	0.47
1:C:503:VAL:HA	1:C:506:GLN:HE21	1.80	0.47
2:I:127:PRO:HB2	2:I:150:VAL:HG23	1.96	0.47
1:C:456:PHE:HZ	2:J:105:GLY:HA3	1.77	0.46
1:C:523:THR:N	6:C:601:HOH:O	2.47	0.46
3:N:141:TYR:CD1	3:N:142:PRO:HA	2.50	0.46
1:B:438:SER:CB	1:B:509:ARG:HG3	2.45	0.46
2:K:35:SER:OG	2:K:50:VAL:HG12	2.15	0.46
3:O:101:GLN:CD	3:O:101:GLN:H	2.22	0.46
1:B:472:ILE:HD12	1:B:484:GLU:HG2	1.97	0.46
2:J:211:SER:OG	2:J:213:THR:OG1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.50	0.46
2:J:63:VAL:HB	2:J:67:PHE:CD2	2.51	0.46
2:K:167:LEU:HD21	2:K:190:VAL:HG21	1.98	0.46
3:M:138:ASN:OD1	3:M:139:ASN:ND2	2.49	0.46
2:J:2:VAL:HG22	2:J:26:GLY:HA3	1.98	0.46
1:A:471:GLU:OE2	1:A:471:GLU:N	2.49	0.46
2:I:127:PRO:HB3	2:I:153:TYR:HB3	1.97	0.46
2:I:217:LYS:HD2	2:I:217:LYS:HA	1.86	0.46
2:K:38:ARG:HG2	2:K:48:VAL:CG2	2.45	0.46
3:L:210:PHE:CD1	3:L:210:PHE:C	2.94	0.46
1:D:497:PHE:CE2	1:D:507:PRO:HB3	2.51	0.45
2:K:72:ASP:OD2	2:K:75:LYS:N	2.40	0.45
2:K:116:LEU:HD12	2:K:117:VAL:N	2.31	0.45
1:C:502:GLY:O	1:C:506:GLN:HG3	2.17	0.45
3:M:93:SER:OG	3:M:94:THR:O	2.35	0.45
2:J:103:ILE:O	2:J:107:THR:HG23	2.16	0.45
3:M:141:TYR:CG	3:M:142:PRO:HA	2.52	0.45
3:O:141:TYR:CG	3:O:142:PRO:HA	2.52	0.45
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.45
2:I:131:PRO:O	3:M:122:SER:OG	2.35	0.45
3:N:4:MET:HE2	3:N:25:ALA:HA	1.98	0.45
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.52	0.45
1:A:399:SER:HA	1:A:510:VAL:O	2.16	0.45
1:B:348:ALA:HB2	1:B:354:ASN:OD1	2.16	0.45
2:J:82:MET:HB3	2:J:85:LEU:HD21	1.99	0.45
1:A:370:ASN:OD1	1:A:371:SER:N	2.50	0.44
2:K:156:GLU:HG3	2:K:184:TYR:CE2	2.51	0.44
3:L:184:LYS:O	3:L:188:GLU:HG3	2.16	0.44
3:M:187:TYR:O	3:M:212:ARG:NH1	2.49	0.44
3:N:94:THR:O	3:N:94:THR:OG1	2.32	0.44
2:K:18:LEU:HD12	2:K:19:ARG:H	1.81	0.44
2:J:217:LYS:HD2	2:J:217:LYS:HA	1.66	0.44
3:M:33:LEU:HD22	3:M:71:PHE:CG	2.52	0.44
3:M:191:LYS:HG3	3:M:211:ASN:OD1	2.17	0.44
2:J:45:LEU:HD21	3:N:44:PRO:CG	2.45	0.44
3:N:2:ILE:HD12	3:N:2:ILE:N	2.29	0.44
3:N:2:ILE:HD13	3:N:90:GLN:NE2	2.33	0.44
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.53	0.44
1:A:367:VAL:HA	1:A:370:ASN:HD21	1.81	0.44
1:A:369:TYR:O	1:A:372:ALA:HB2	2.18	0.44
1:C:392:PHE:CD2	1:C:515:PHE:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:LYS:HA	2:H:43:LYS:HD3	1.88	0.44
3:M:109:ARG:HE	3:M:109:ARG:HB2	1.62	0.44
1:A:376:THR:HG23	1:A:378:LYS:HE3	1.99	0.44
2:J:12:VAL:O	2:J:119:VAL:HA	2.17	0.44
2:K:50:VAL:HG23	2:K:58:TYR:HB2	2.00	0.44
2:J:36:TRP:NE1	2:J:80:LEU:HB2	2.33	0.43
3:O:41:GLY:O	3:O:42:LYS:HD2	2.18	0.43
1:A:356:LYS:HG3	1:A:358:ILE:HD11	2.00	0.43
3:N:2:ILE:HD11	3:N:93:SER:HB2	2.00	0.43
3:M:164:VAL:HG22	3:M:176:LEU:HD12	2.01	0.43
1:A:398:ASP:O	1:A:511:VAL:HA	2.18	0.43
3:O:36:TYR:CE1	3:O:46:LEU:HD13	2.54	0.43
3:O:83:PHE:C	3:O:83:PHE:CD1	2.96	0.43
1:B:399:SER:HA	1:B:510:VAL:O	2.18	0.43
3:N:121:PRO:HD3	3:N:133:VAL:HG22	2.01	0.43
1:D:338:PHE:HE2	1:D:365:TYR:CD2	2.37	0.43
2:H:213:THR:HG22	2:H:215:VAL:HG23	2.01	0.43
2:J:103:ILE:C	2:J:107:THR:HG23	2.44	0.43
2:H:130:PHE:CE2	3:L:125:GLN:HG3	2.54	0.43
3:O:106:GLU:HG2	3:O:107:ILE:N	2.34	0.43
3:L:116:VAL:O	3:L:208:LYS:HE2	2.18	0.43
1:A:354:ASN:O	1:A:398:ASP:HA	2.18	0.43
2:K:107:THR:O	2:K:108:SER:HB2	2.19	0.43
2:I:97:ARG:O	2:I:108:SER:HA	2.17	0.43
2:K:36:TRP:HD1	2:K:69:ILE:HD12	1.83	0.43
1:A:356:LYS:HD3	1:A:356:LYS:C	2.44	0.42
2:J:36:TRP:O	2:J:48:VAL:HG12	2.19	0.42
3:L:2:ILE:CG1	3:L:93:SER:HB3	2.49	0.42
1:B:408:ARG:NH2	1:B:414:GLN:HE22	2.17	0.42
1:C:440:ASN:OD1	1:C:440:ASN:N	2.50	0.42
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.54	0.42
3:M:212:ARG:HG3	3:M:212:ARG:HH11	1.84	0.42
2:J:13:LYS:HD2	2:J:13:LYS:H	1.84	0.42
1:A:403:ARG:NH2	1:A:405:ASP:HB2	2.35	0.42
2:J:36:TRP:HD1	2:J:69:ILE:HD12	1.85	0.42
3:N:2:ILE:HD11	3:N:93:SER:CB	2.49	0.42
3:N:41:GLY:O	3:N:42:LYS:HD3	2.20	0.42
1:A:337:PRO:HD2	1:A:360:ASN:HD21	1.85	0.42
2:H:207:ASN:HD21	2:H:209:LYS:HG3	1.84	0.42
2:I:11:LEU:HB2	2:I:155:PRO:HG3	2.01	0.42
2:J:30:SER:HB3	2:J:73:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:SER:O	1:D:444:LYS:HD2	2.19	0.41
3:O:146:LYS:HB3	3:O:198:THR:HB	2.01	0.41
1:A:358:ILE:HB	1:A:395:VAL:CG1	2.50	0.41
2:K:99:GLU:O	2:K:99:GLU:HG2	2.21	0.41
3:N:191:LYS:HE2	3:N:211:ASN:HB3	2.02	0.41
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.55	0.41
2:H:2:VAL:HG22	2:H:26:GLY:HA3	2.03	0.41
2:I:160:VAL:HG12	2:I:206:VAL:HG22	2.02	0.41
1:D:475:ALA:HB1	2:K:32:ASN:HD21	1.84	0.41
2:I:192:VAL:HG21	2:I:202:TYR:CZ	2.55	0.41
3:O:159:ASN:OD1	3:O:159:ASN:N	2.52	0.41
3:M:188:GLU:HA	3:M:212:ARG:NH1	2.35	0.41
1:A:447:GLY:HA2	1:A:498:GLN:HG2	2.03	0.41
2:I:170:GLY:C	2:I:190:VAL:HG23	2.46	0.41
3:O:28:SER:OG	3:O:68:GLU:HG3	2.21	0.41
1:C:403:ARG:NH2	1:C:405:ASP:OD1	2.54	0.41
1:D:438:SER:O	1:D:507:PRO:HG2	2.21	0.41
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.56	0.40
2:K:27:ILE:HD13	2:K:27:ILE:HA	1.98	0.40
3:M:2:ILE:HD12	3:M:2:ILE:N	2.36	0.40
3:M:199:HIS:CD2	3:M:200:GLN:N	2.89	0.40
1:B:472:ILE:CD1	1:B:484:GLU:HG2	2.52	0.40
1:D:404:GLY:O	1:D:407:VAL:HG23	2.22	0.40
2:I:93:TYR:O	2:I:114:GLY:HA2	2.21	0.40
2:J:97:ARG:O	2:J:108:SER:HA	2.21	0.40
1:D:382:VAL:HG22	1:D:387:LEU:HD22	2.03	0.40
3:L:42:LYS:HA	3:L:42:LYS:HD2	1.89	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:GLU:OE1	2:H:13:LYS:NZ[2_556]	2.09	0.11

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	165/232 (71%)	156 (94%)	9 (6%)	0	100	100
1	B	162/232 (70%)	148 (91%)	12 (7%)	2 (1%)	10	34
1	C	184/232 (79%)	174 (95%)	9 (5%)	1 (0%)	24	55
1	D	175/232 (75%)	163 (93%)	11 (6%)	1 (1%)	21	51
2	H	216/224 (96%)	209 (97%)	7 (3%)	0	100	100
2	I	213/224 (95%)	206 (97%)	7 (3%)	0	100	100
2	J	214/224 (96%)	204 (95%)	9 (4%)	1 (0%)	24	55
2	K	213/224 (95%)	204 (96%)	6 (3%)	3 (1%)	9	30
3	L	213/217 (98%)	201 (94%)	9 (4%)	3 (1%)	9	30
3	M	212/217 (98%)	200 (94%)	7 (3%)	5 (2%)	4	17
3	N	213/217 (98%)	197 (92%)	12 (6%)	4 (2%)	6	22
3	O	212/217 (98%)	199 (94%)	10 (5%)	3 (1%)	9	30
All	All	2392/2692 (89%)	2261 (94%)	108 (4%)	23 (1%)	12	38

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	ASN
2	J	199	THR
3	M	96	PRO
3	N	40	PRO
3	N	95	LEU
3	O	95	LEU
1	B	468	ILE
1	C	527	PRO
2	K	158	VAL
3	M	68	GLU
3	M	192	LEU
3	N	68	GLU
1	D	439	ASN
3	L	3	GLN
3	M	139	ASN
3	O	68	GLU
3	O	84	ALA
2	K	108	SER

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Mol	Chain	Res	Type
3	L	68	GLU
3	M	95	LEU
3	L	40	PRO
3	N	39	LYS
2	K	157	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/202 (73%)	140 (95%)	8 (5%)	20	51
1	B	144/202 (71%)	142 (99%)	2 (1%)	59	85
1	C	165/202 (82%)	160 (97%)	5 (3%)	36	72
1	D	157/202 (78%)	148 (94%)	9 (6%)	18	49
2	H	182/186 (98%)	181 (100%)	1 (0%)	81	93
2	I	180/186 (97%)	174 (97%)	6 (3%)	33	69
2	J	180/186 (97%)	176 (98%)	4 (2%)	45	78
2	K	180/186 (97%)	173 (96%)	7 (4%)	28	64
3	L	190/191 (100%)	189 (100%)	1 (0%)	81	93
3	M	189/191 (99%)	181 (96%)	8 (4%)	26	61
3	N	189/191 (99%)	185 (98%)	4 (2%)	47	79
3	O	189/191 (99%)	186 (98%)	3 (2%)	55	83
All	All	2093/2316 (90%)	2035 (97%)	58 (3%)	38	73

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	VAL
1	A	355	ARG
1	A	390	LEU
1	A	391	CYS
1	A	394	ASN

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Mol	Chain	Res	Type
1	A	477	SER
1	A	483	VAL
1	A	514	SER
1	B	341	VAL
1	B	361	CYS
1	C	367	VAL
1	C	415	THR
1	C	477	SER
1	C	514	SER
1	C	531	THR
1	D	366	SER
1	D	385	THR
1	D	391	CYS
1	D	395	VAL
1	D	414	GLN
1	D	469	SER
1	D	494	SER
1	D	498	GLN
1	D	525	CYS
2	H	195	SER
2	I	7	SER
2	I	150	VAL
2	I	158	VAL
2	I	167	LEU
2	I	199	THR
2	I	201	THR
2	J	30	SER
2	J	37	VAL
2	J	191	THR
2	J	195	SER
2	K	97	ARG
2	K	106	VAL
2	K	107	THR
2	K	168	THR
2	K	191	THR
2	K	192	VAL
2	K	197	LEU
3	L	132	SER
3	M	12	SER
3	M	33	LEU
3	M	56	SER
3	M	60	SER

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Mol	Chain	Res	Type
3	M	96	PRO
3	M	106	GLU
3	M	115	SER
3	M	126	LEU
3	N	2	ILE
3	N	85	THR
3	N	93	SER
3	N	109	ARG
3	O	10	SER
3	O	115	SER
3	O	191	LYS

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

Mol	Chain	Res	Type
1	B	481	ASN
1	C	388	ASN
1	C	450	ASN
1	D	394	ASN
1	D	414	GLN
1	D	498	GLN
2	H	73	ASN
2	H	179	GLN
2	H	207	ASN
2	I	81	GLN
2	J	73	ASN
2	J	179	GLN
2	K	179	GLN
2	K	205	ASN
3	L	6	GLN
3	M	139	ASN
3	O	6	GLN
3	O	37	GLN
3	O	101	GLN
3	O	125	GLN
3	O	148	GLN
3	O	200	GLN
3	O	211	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	1	1,4	14,14,15	0.54	0	17,19,21	0.55	0
4	FUC	E	2	4	10,10,11	0.80	0	14,14,16	0.71	0
4	NAG	F	1	1,4	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
4	FUC	F	2	4	10,10,11	0.81	0	14,14,16	0.81	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	E	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.55	115.61	112.19

There are no chirality outliers.

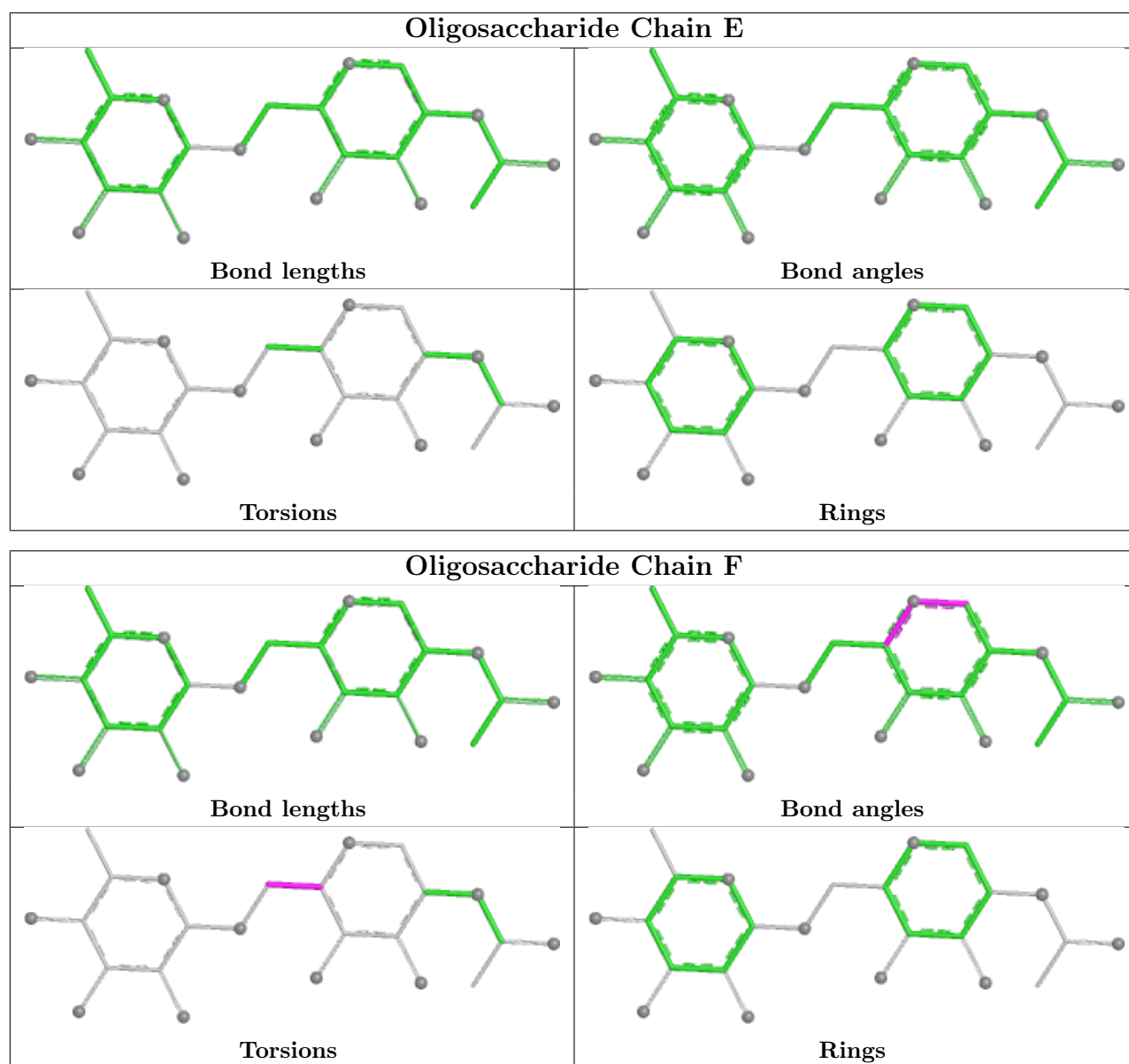
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

2 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	$\# Z > 2$
5	NAG	D	601	1	14,14,15	0.44	0	17,19,21	0.52	0
5	NAG	B	601	1	14,14,15	0.66	1 (7%)	17,19,21	0.57	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
5	NAG	D	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	NAG	C1-C2	2.05	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/232 (73%)	0.44	5 (2%) 53 43	42, 59, 88, 106	0
1	B	168/232 (72%)	0.60	11 (6%) 25 18	39, 63, 92, 107	0
1	C	190/232 (81%)	0.28	3 (1%) 70 61	35, 59, 86, 100	0
1	D	181/232 (78%)	0.54	10 (5%) 30 23	40, 67, 108, 143	0
2	H	220/224 (98%)	0.27	7 (3%) 50 40	34, 55, 87, 119	0
2	I	216/224 (96%)	0.35	9 (4%) 40 32	34, 56, 91, 103	1 (0%)
2	J	218/224 (97%)	0.68	13 (5%) 27 21	41, 72, 94, 110	0
2	K	217/224 (96%)	0.71	16 (7%) 20 15	52, 69, 92, 114	0
3	L	214/217 (98%)	0.12	3 (1%) 73 64	33, 58, 73, 85	1 (0%)
3	M	214/217 (98%)	0.51	6 (2%) 55 45	46, 67, 85, 99	0
3	N	214/217 (98%)	0.75	26 (12%) 8 6	36, 64, 93, 117	1 (0%)
3	O	214/217 (98%)	0.28	5 (2%) 61 51	40, 59, 79, 93	0
All	All	2437/2692 (90%)	0.46	114 (4%) 36 29	33, 63, 92, 143	3 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	192	VAL	4.9
3	N	80	PRO	4.7
1	B	362	VAL	4.3
2	K	211	SER	4.2
3	O	95	LEU	4.2
3	N	83	PHE	4.2
2	K	197	LEU	4.1
3	N	87	TYR	4.1
3	N	107	ILE	4.1
2	H	201	THR	3.6
2	I	200	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	369	TYR	3.5
2	I	199	THR	3.4
3	N	96	PRO	3.3
2	I	202	TYR	3.3
1	A	390	LEU	3.3
2	J	120	SER	3.2
1	D	377	PHE	3.2
1	A	337	PRO	3.1
1	B	342	PHE	3.1
2	J	7	SER	3.1
3	N	15	VAL	3.1
2	K	144	ALA	3.0
3	M	20	THR	3.0
2	J	42	GLY	3.0
2	K	167	LEU	3.0
1	D	364	ASP	3.0
2	K	206	VAL	3.0
2	H	220	GLU	2.9
3	O	97	TYR	2.9
1	D	371	SER	2.9
1	B	370	ASN	2.8
1	D	387	LEU	2.8
2	J	167	LEU	2.8
2	H	140	SER	2.8
1	D	362	VAL	2.8
3	M	75	ILE	2.8
3	N	85	THR	2.8
2	K	41	PRO	2.8
1	B	374	PHE	2.6
2	I	162	TRP	2.6
1	B	445	VAL	2.6
3	N	40	PRO	2.6
3	N	2	ILE	2.6
2	J	216	ASP	2.6
1	B	377	PHE	2.6
2	H	166	ALA	2.6
3	M	115	SER	2.6
2	K	193	PRO	2.6
3	O	96	PRO	2.6
3	M	95	LEU	2.6
2	J	199	THR	2.6
3	M	203	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	394	ASN	2.5
1	B	441	LEU	2.5
1	B	363	ALA	2.5
2	I	132	LEU	2.4
3	N	82	ASP	2.4
2	K	190	VAL	2.4
3	N	16	GLY	2.4
3	N	11	LEU	2.4
3	O	129	GLY	2.4
2	K	198	GLY	2.4
3	N	31[A]	ARG	2.3
3	N	10	SER	2.3
2	H	139	THR	2.3
3	N	12	SER	2.3
3	M	143	ARG	2.3
1	B	343	ASN	2.3
1	B	372	ALA	2.3
1	C	363	ALA	2.3
1	D	432	CYS	2.3
2	J	62	SER	2.3
2	K	185	SER	2.3
2	J	197	LEU	2.2
1	A	384	PRO	2.2
2	J	206	VAL	2.2
2	K	142	GLY	2.2
3	N	169	SER	2.2
3	N	4	MET	2.2
3	N	95	LEU	2.2
1	C	531	THR	2.2
2	J	201	THR	2.2
3	O	98	THR	2.2
3	L	123	ASP	2.1
3	N	47	LEU	2.1
1	D	373	SER	2.1
3	N	9	SER	2.1
3	N	84	ALA	2.1
2	J	210	PRO	2.1
2	K	194	SER	2.1
2	K	199	THR	2.1
3	L	7	SER	2.1
3	L	77	SER	2.1
3	N	105	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	384	PRO	2.1
2	I	221	PRO	2.1
2	I	142	GLY	2.1
1	A	410	ILE	2.1
2	K	171	VAL	2.0
2	H	197	LEU	2.0
2	J	124	THR	2.0
3	N	5	THR	2.0
3	N	104	LYS	2.0
2	I	192	VAL	2.0
2	I	215	VAL	2.0
3	N	79	HIS	2.0
2	K	210	PRO	2.0
1	C	335	LEU	2.0
1	A	342	PHE	2.0
1	D	374	PHE	2.0
2	H	198	GLY	2.0
2	J	44	GLY	2.0
3	N	103	THR	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](#)

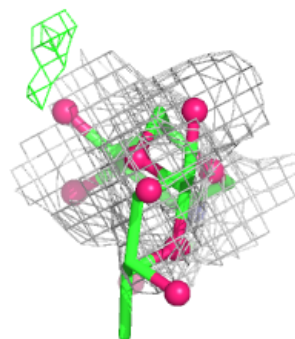
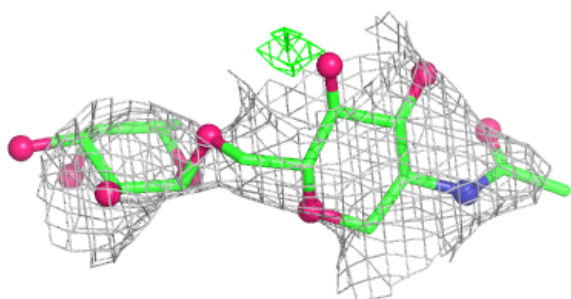
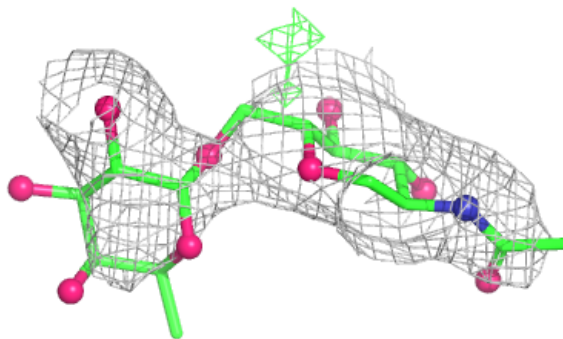
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	-	-	105,119,140,152	0
4	FUC	E	2	10/11	-	-	140,158,166,168	0
4	NAG	F	1	14/15	-	-	71,87,104,106	0
4	FUC	F	2	10/11	-	-	107,117,122,123	0

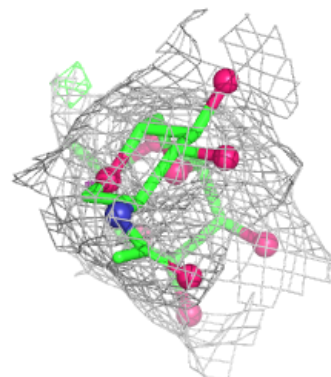
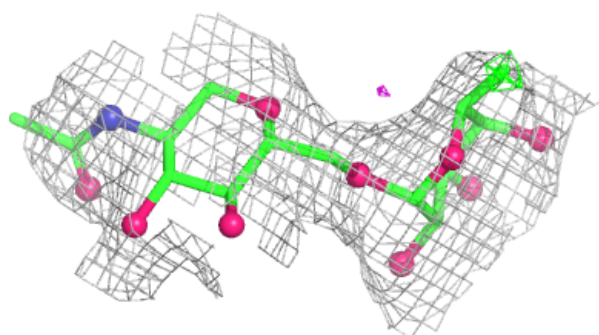
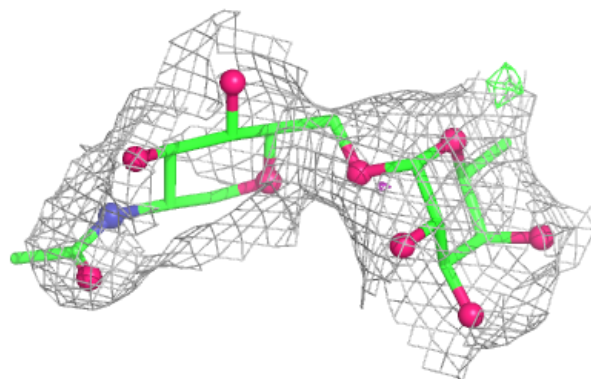
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	601	14/15	0.51	0.20	120,132,146,147	0
5	NAG	D	601	14/15	0.55	0.18	111,125,133,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.