



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 05:42 PM JST

PDB ID : 9XAW / pdb_00009xaw
Title : Structure of the SARS-CoV-2 Spike N-terminal domain(NTD) in complex with the BLN8 Fab
Authors : Zhou, J.J.; Gao, G.F.
Deposited on : 2025-10-23
Resolution : 3.13 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:

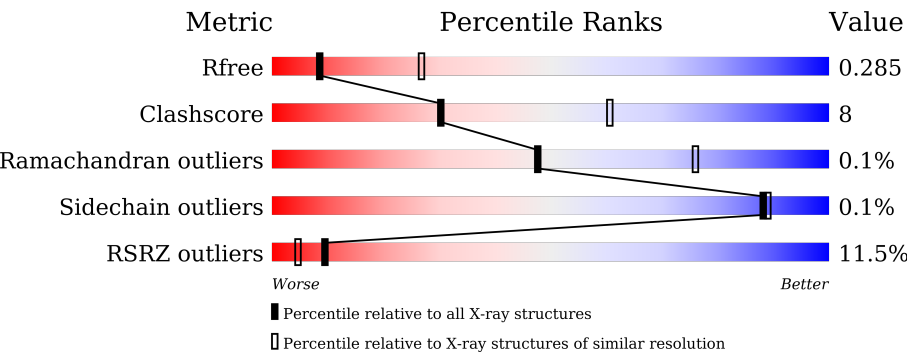
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	229	7% 78% 20% .
1	C	229	7% 77% 20% .
1	E	229	7% 81% 16% .
1	G	229	10% 72% 24% .
2	I	298	13% 74% 18% 7%
2	J	298	19% 73% 20% 7%

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Mol	Chain	Length	Quality of chain
2	K	298	
2	L	298	
3	B	212	
3	D	212	
3	F	212	
3	H	212	
4	M	2	
4	O	2	
4	P	2	
5	N	5	
6	Q	5	
7	R	4	
7	T	4	
8	S	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22383 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 BLN8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	C	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	E	223	Total	C	N	O	S	0	0	0
			1674	1054	286	327	7			
1	G	221	Total	C	N	O	S	0	0	0
			1658	1044	283	324	7			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	277	Total	C	N	O	S	0	0	0
			2226	1443	362	413	8			
2	I	276	Total	C	N	O	S	0	0	0
			2212	1434	358	412	8			
2	J	277	Total	C	N	O	S	0	0	0
			2228	1445	361	414	8			
2	L	279	Total	C	N	O	S	0	0	0
			2250	1461	366	415	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	306	HIS	-	expression tag	UNP P0DTC2
K	307	HIS	-	expression tag	UNP P0DTC2
K	308	HIS	-	expression tag	UNP P0DTC2
K	309	HIS	-	expression tag	UNP P0DTC2
K	310	HIS	-	expression tag	UNP P0DTC2
K	311	HIS	-	expression tag	UNP P0DTC2
I	306	HIS	-	expression tag	UNP P0DTC2
I	307	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	308	HIS	-	expression tag	UNP P0DTC2
I	309	HIS	-	expression tag	UNP P0DTC2
I	310	HIS	-	expression tag	UNP P0DTC2
I	311	HIS	-	expression tag	UNP P0DTC2
J	306	HIS	-	expression tag	UNP P0DTC2
J	307	HIS	-	expression tag	UNP P0DTC2
J	308	HIS	-	expression tag	UNP P0DTC2
J	309	HIS	-	expression tag	UNP P0DTC2
J	310	HIS	-	expression tag	UNP P0DTC2
J	311	HIS	-	expression tag	UNP P0DTC2
L	306	HIS	-	expression tag	UNP P0DTC2
L	307	HIS	-	expression tag	UNP P0DTC2
L	308	HIS	-	expression tag	UNP P0DTC2
L	309	HIS	-	expression tag	UNP P0DTC2
L	310	HIS	-	expression tag	UNP P0DTC2
L	311	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called BLN8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	212	Total	C	N	O	S	0	0	0
			1584	988	260	329	7			
3	D	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			
3	F	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			
3	H	211	Total	C	N	O	S	0	0	0
			1577	985	259	326	7			

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



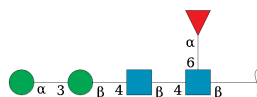
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	O	2	Total	C	N	O	0	0	0
			24	14	1	9			

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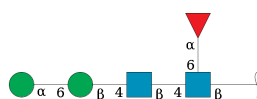
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



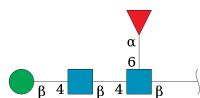
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Q	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



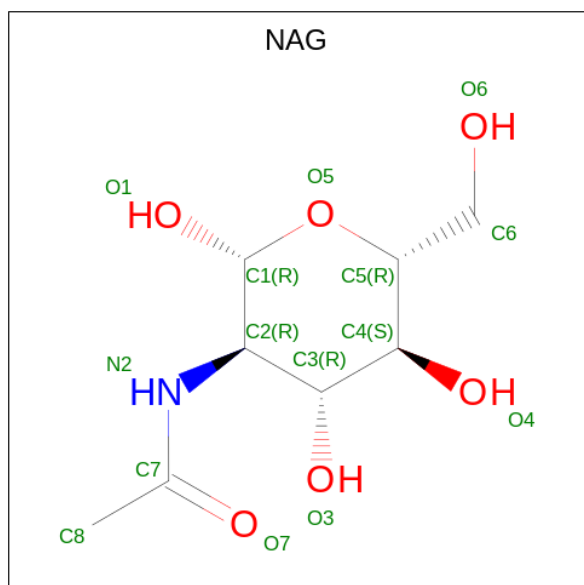
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	R	4	Total	C	N	O	0	0	0
			49	28	2	19			
7	T	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

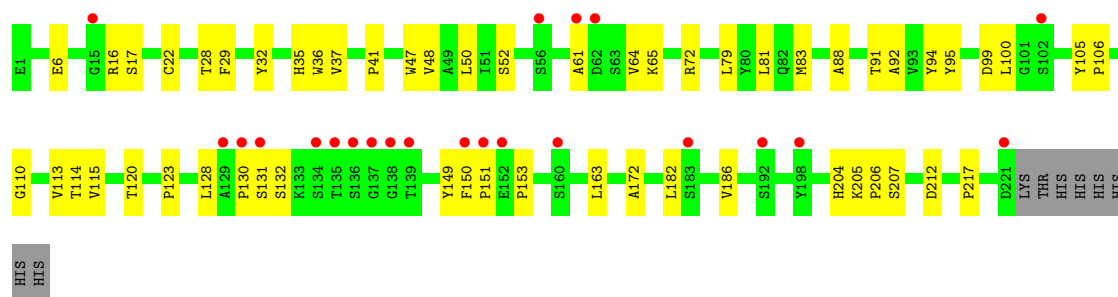


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	J	1	Total	C	N	O	0	0
			14	8	1	5		

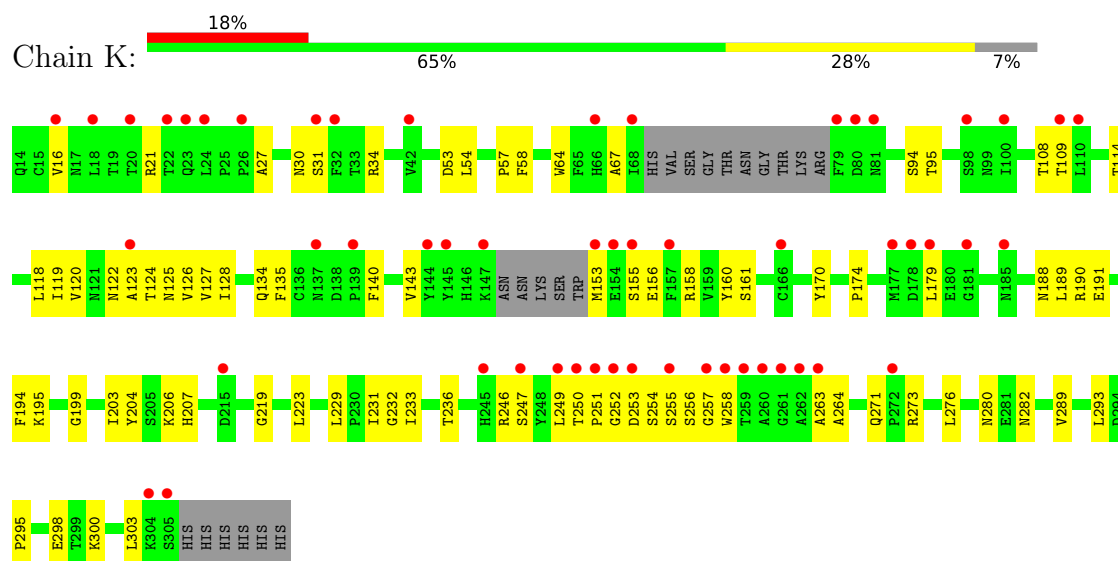
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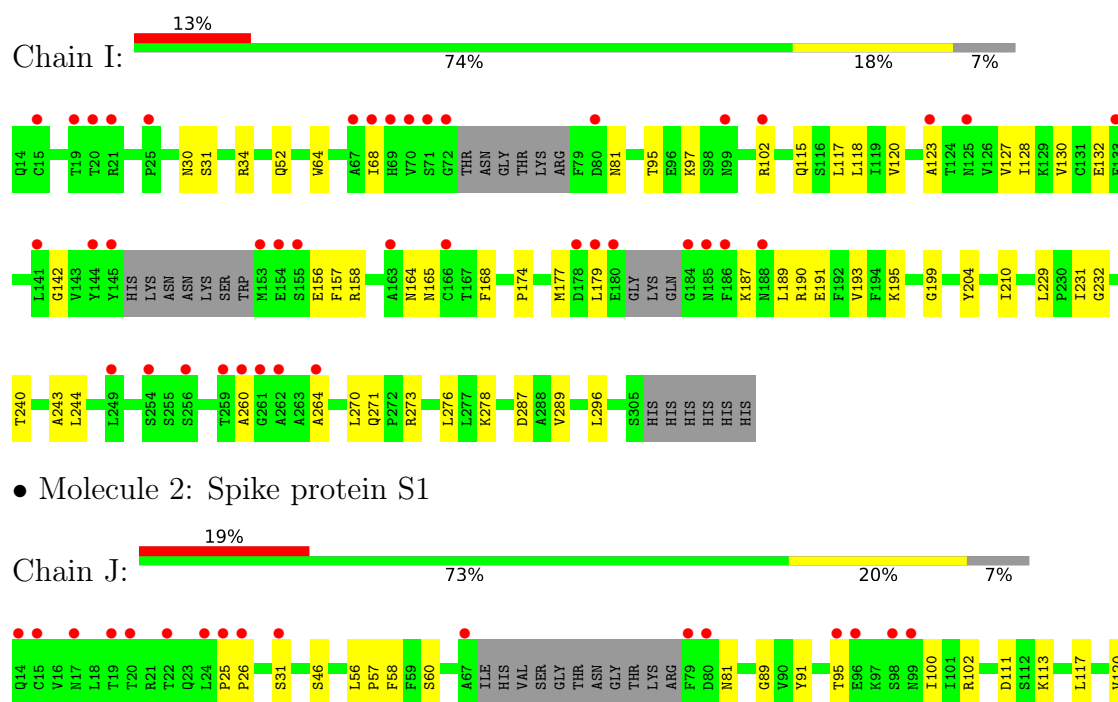
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	J	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		

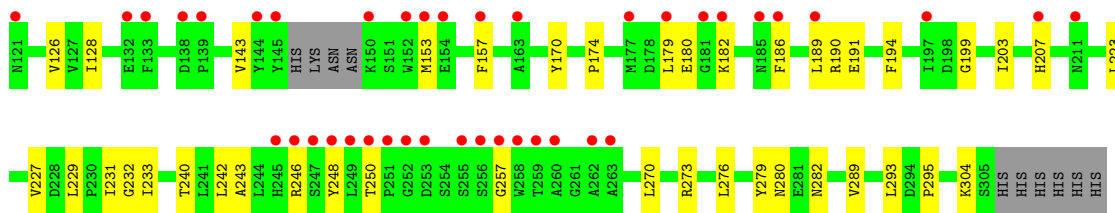


• Molecule 2: Spike protein S1

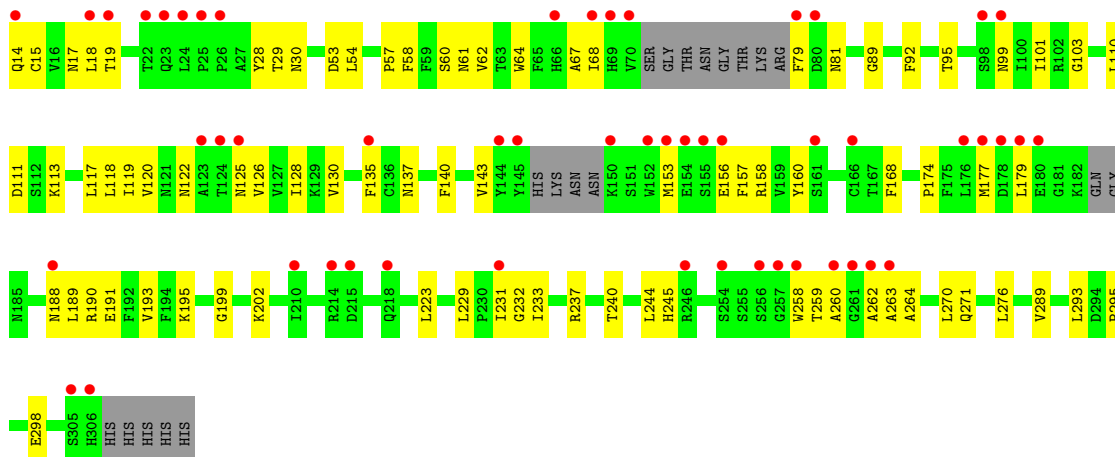


• Molecule 2: Spike protein S1

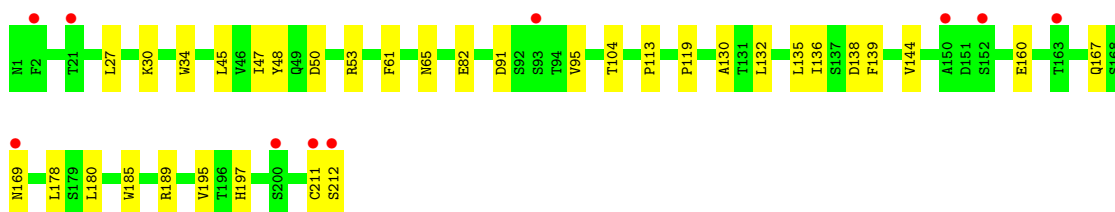
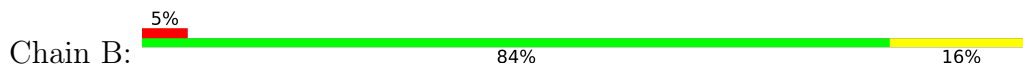




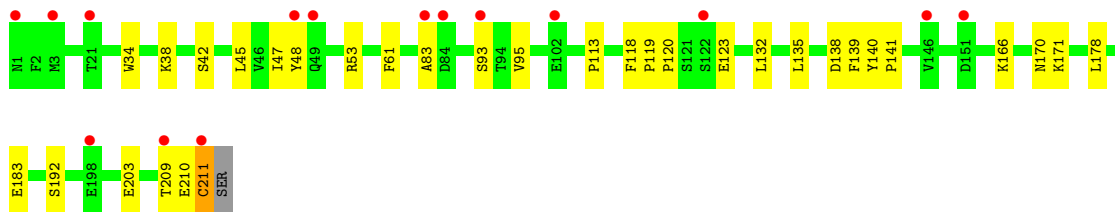
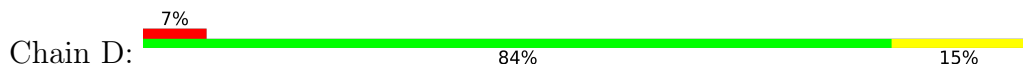
• Molecule 2: Spike protein S1



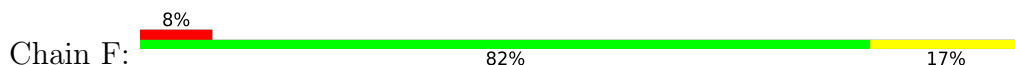
• Molecule 3: BLN8 light chain

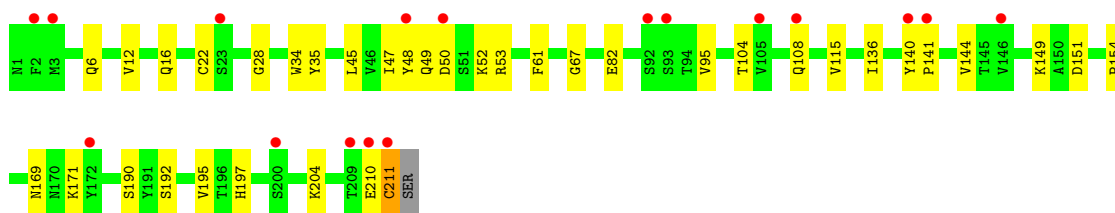


• Molecule 3: BLN8 light chain



• Molecule 3: BLN8 light chain





- Molecule 3: BLN8 light chain



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



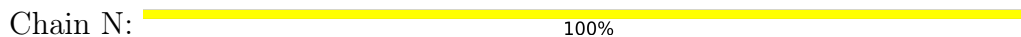
- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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





- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

100%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

25%

75%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.94Å 117.49Å 138.05Å 110.91° 90.27° 96.37°	Depositor
Resolution (Å)	64.40 – 3.13 64.40 – 3.13	Depositor EDS
% Data completeness (in resolution range)	98.4 (64.40-3.13) 98.4 (64.40-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.232 , 0.285 0.232 , 0.285	Depositor DCC
R_{free} test set	3618 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22383	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1715	0.29	0/2335
1	C	0.10	0/1715	0.31	0/2335
1	E	0.12	0/1715	0.35	0/2335
1	G	0.09	0/1699	0.30	0/2314
2	I	0.15	0/2272	0.33	0/3093
2	J	0.09	0/2290	0.30	0/3117
2	K	0.17	0/2287	0.37	0/3112
2	L	0.11	0/2313	0.34	0/3148
3	B	0.09	0/1623	0.31	0/2216
3	D	0.10	0/1616	0.30	0/2208
3	F	0.10	0/1616	0.34	0/2208
3	H	0.11	0/1616	0.30	0/2208
All	All	0.11	0/22477	0.32	0/30629

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	1674	0	1641	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1674	0	1640	32	0
1	E	1674	0	1640	26	0
1	G	1658	0	1620	37	0
2	I	2212	0	2132	37	0
2	J	2228	0	2150	42	0
2	K	2226	0	2154	60	0
2	L	2250	0	2172	56	0
3	B	1584	0	1523	23	0
3	D	1577	0	1517	23	0
3	F	1577	0	1517	25	0
3	H	1577	0	1517	11	0
4	M	24	0	22	0	0
4	O	24	0	22	0	0
4	P	24	0	22	0	0
5	N	60	0	52	0	0
6	Q	60	0	52	0	0
7	R	49	0	43	0	0
7	T	49	0	43	0	0
8	S	28	0	25	0	0
9	I	28	0	26	1	0
9	J	56	0	52	0	0
9	K	28	0	26	0	0
9	L	42	0	39	0	0
All	All	22383	0	21647	370	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 8.

All (370) 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)
2:L:189:LEU:HD22	2:L:191:GLU:HG2	1.25	1.10
2:J:189:LEU:HD22	2:J:191:GLU:HG3	1.26	1.06
2:L:189:LEU:HD22	2:L:191:GLU:CG	2.00	0.91
2:J:189:LEU:CD2	2:J:191:GLU:HG3	2.04	0.87
2:L:67:ALA:O	2:L:263:ALA:HB3	1.76	0.85
2:L:189:LEU:CD2	2:L:191:GLU:HG2	2.07	0.81
3:H:45:LEU:HD21	3:H:48:TYR:HB3	1.63	0.81
1:E:130:PRO:HG3	1:E:142:LEU:HB3	1.67	0.75
2:I:102:ARG:HG3	2:I:243:ALA:HB2	1.68	0.75
2:K:246:ARG:HE	2:K:251:PRO:HB2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:135:PHE:HA	2:K:160:TYR:HA	1.68	0.75
2:K:179:LEU:O	2:K:188:ASN:ND2	2.22	0.73
2:I:68:ILE:HD13	2:I:260:ALA:HB1	1.69	0.73
3:F:45:LEU:HD21	3:F:48:TYR:HB3	1.71	0.73
2:K:280:ASN:ND2	2:K:282:ASN:OD1	2.22	0.73
2:K:246:ARG:NE	2:K:251:PRO:HB2	2.03	0.72
3:B:189:ARG:HH12	1:C:89:GLU:H	1.36	0.72
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.71	0.71
1:C:218:LYS:HE2	3:D:211:CYS:HB3	1.71	0.71
2:J:280:ASN:ND2	2:J:282:ASN:OD1	2.24	0.71
2:J:111:ASP:OD2	2:J:113:LYS:NZ	2.24	0.71
1:G:130:PRO:HD2	1:G:217:PRO:HA	1.73	0.70
1:G:16:ARG:HE	1:G:17:SER:H	1.40	0.69
2:J:189:LEU:HD22	2:J:191:GLU:CG	2.16	0.68
2:K:231:ILE:HD12	2:K:233:ILE:HG12	1.74	0.68
1:C:130:PRO:HG3	1:C:142:LEU:HB3	1.75	0.68
1:A:91:THR:HG23	1:A:114:THR:HA	1.74	0.68
1:A:210:LYS:HB3	1:E:212:ASP:HB2	1.75	0.67
1:G:17:SER:HA	1:G:83:MET:O	1.94	0.67
1:E:130:PRO:HD2	1:E:217:PRO:HA	1.76	0.67
1:E:91:THR:HG23	1:E:114:THR:HA	1.77	0.66
2:L:122:ASN:HB2	2:L:125:ASN:H	1.61	0.66
1:A:123:PRO:HB3	1:A:149:TYR:HB3	1.76	0.66
2:K:153:MET:HE3	2:K:155:SER:HB3	1.76	0.66
1:E:52:SER:O	1:E:72:ARG:NH1	2.28	0.66
2:L:231:ILE:HD12	2:L:233:ILE:HG12	1.76	0.65
2:L:276:LEU:HB2	2:L:289:VAL:HB	1.78	0.65
3:B:34:TRP:HB2	3:B:47:ILE:HB	1.77	0.65
2:K:16:VAL:HG22	2:K:253:ASP:HA	1.78	0.65
2:L:143:VAL:HG13	2:L:153:MET:HG3	1.79	0.64
2:I:276:LEU:HB2	2:I:289:VAL:HB	1.79	0.64
2:I:34:ARG:HD3	2:I:191:GLU:OE2	1.98	0.64
2:J:81:ASN:ND2	2:J:240:THR:O	2.30	0.64
2:K:58:PHE:HB2	2:K:293:LEU:HD11	1.80	0.63
3:B:185:TRP:HE1	3:B:212:SER:HB2	1.64	0.63
2:L:120:VAL:HG21	2:L:157:PHE:HE2	1.63	0.63
3:B:82:GLU:HG3	3:B:104:THR:HA	1.80	0.63
1:G:151:PRO:HD2	1:G:204:HIS:CE1	2.34	0.63
2:J:143:VAL:HG13	2:J:153:MET:HG3	1.81	0.63
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.81	0.62
1:E:166:GLY:O	1:E:186:VAL:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:GLN:HB2	3:F:52:LYS:HD3	1.81	0.62
2:J:276:LEU:HB2	2:J:289:VAL:HB	1.82	0.62
1:G:91:THR:HG23	1:G:114:THR:HA	1.82	0.61
2:L:119:ILE:HG12	2:L:128:ILE:HG12	1.82	0.61
1:E:163:LEU:HD21	1:E:186:VAL:HG21	1.81	0.61
2:L:156:GLU:OE2	2:L:158:ARG:NH1	2.33	0.61
1:A:192:SER:HB2	1:A:196:GLN:HB3	1.83	0.61
2:I:95:THR:HB	2:I:187:LYS:HE3	1.83	0.61
2:L:245:HIS:O	2:L:259:THR:N	2.24	0.61
2:K:64:TRP:HE1	2:K:264:ALA:HB1	1.65	0.60
2:K:295:PRO:HG3	1:G:99:ASP:OD2	2.01	0.60
2:K:122:ASN:HB3	2:K:124:THR:H	1.66	0.60
1:C:83:MET:HE1	1:C:113:VAL:HG21	1.84	0.59
2:I:123:ALA:O	2:I:174:PRO:HG3	2.01	0.59
1:A:130:PRO:HD2	1:A:217:PRO:HA	1.85	0.59
1:C:210:LYS:HB3	1:G:212:ASP:HB2	1.85	0.59
2:I:179:LEU:HB2	2:I:190:ARG:HH22	1.67	0.59
1:C:91:THR:HG23	1:C:114:THR:HA	1.83	0.59
2:J:250:THR:HG23	2:J:257:GLY:HA2	1.84	0.59
2:L:64:TRP:HE1	2:L:264:ALA:HB1	1.68	0.59
3:H:49:GLN:HB2	3:H:52:LYS:HD3	1.84	0.58
1:G:52:SER:O	1:G:72:ARG:NH1	2.36	0.58
2:K:276:LEU:HB2	2:K:289:VAL:HB	1.86	0.58
1:A:185:VAL:HG21	3:B:135:LEU:HD13	1.85	0.58
3:B:130:ALA:HB3	3:B:180:LEU:O	2.03	0.58
2:I:189:LEU:HG	2:I:191:GLU:HG3	1.86	0.57
3:B:119:PRO:HA	3:B:132:LEU:HD23	1.85	0.57
1:G:172:ALA:HB2	1:G:182:LEU:HD23	1.86	0.57
2:I:81:ASN:ND2	2:I:240:THR:O	2.37	0.57
1:A:173:VAL:HG21	3:B:160:GLU:HB3	1.87	0.57
2:I:156:GLU:OE2	2:I:158:ARG:NH1	2.37	0.57
2:J:95:THR:HG22	2:J:189:LEU:HA	1.85	0.57
1:G:29:PHE:O	1:G:72:ARG:NH2	2.37	0.57
2:L:143:VAL:HG22	2:L:153:MET:HE3	1.87	0.57
3:D:45:LEU:HD21	3:D:48:TYR:HB3	1.86	0.57
1:G:172:ALA:HA	1:G:182:LEU:HB3	1.87	0.57
2:I:244:LEU:HD22	2:I:260:ALA:HB2	1.86	0.57
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.85	0.56
3:D:113:PRO:HB3	3:D:139:PHE:HB3	1.87	0.56
3:F:149:LYS:HB2	3:F:192:SER:HB2	1.88	0.56
2:L:135:PHE:HA	2:L:160:TYR:HA	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:LYS:HE3	3:D:170:ASN:HA	1.88	0.56
3:D:192:SER:HB3	3:D:203:GLU:OE2	2.05	0.56
2:K:53:ASP:OD1	2:K:54:LEU:N	2.34	0.56
2:K:27:ALA:HB3	2:K:64:TRP:HB3	1.88	0.56
1:A:73:ASP:OD2	1:A:76:LYS:HE2	2.05	0.56
2:I:115:GLN:HG2	2:I:132:GLU:HG2	1.87	0.56
3:B:138:ASP:OD1	3:B:167:GLN:NE2	2.39	0.56
2:L:81:ASN:ND2	2:L:240:THR:O	2.39	0.55
1:A:210:LYS:NZ	1:A:212:ASP:OD1	2.39	0.55
3:B:50:ASP:OD2	2:J:304:LYS:NZ	2.28	0.55
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.88	0.55
2:J:179:LEU:HD12	2:J:207:HIS:CD2	2.42	0.55
1:A:29:PHE:O	1:A:72:ARG:NH2	2.40	0.55
2:K:57:PRO:HG3	2:K:273:ARG:HD2	1.89	0.55
2:J:58:PHE:HB2	2:J:293:LEU:HD11	1.89	0.55
1:C:48:VAL:HG13	1:C:64:VAL:HG11	1.89	0.54
2:K:122:ASN:HB2	2:K:125:ASN:H	1.72	0.54
2:L:126:VAL:HB	2:L:174:PRO:HA	1.89	0.54
2:J:89:GLY:HA3	2:J:270:LEU:HD12	1.89	0.54
1:C:121:LYS:NZ	1:C:148:ASP:O	2.32	0.54
2:I:64:TRP:HE1	2:I:264:ALA:HB1	1.74	0.53
1:A:212:ASP:HB2	1:E:210:LYS:HB3	1.90	0.53
2:I:132:GLU:HG3	2:I:165:ASN:HB2	1.90	0.53
2:L:140:PHE:CZ	2:L:158:ARG:HD3	2.44	0.53
2:K:67:ALA:HB3	2:K:263:ALA:HB3	1.92	0.52
2:J:57:PRO:O	2:J:60:SER:OG	2.24	0.52
2:K:16:VAL:HG13	2:K:253:ASP:O	2.09	0.52
2:J:246:ARG:HH21	2:J:248:TYR:HA	1.74	0.52
2:K:21:ARG:HE	2:K:21:ARG:HA	1.74	0.52
1:G:151:PRO:HD2	1:G:204:HIS:HE1	1.73	0.52
2:I:195:LYS:HE2	2:I:204:TYR:HE1	1.75	0.52
2:K:298:GLU:OE1	2:K:300:LYS:N	2.35	0.51
2:L:231:ILE:HG13	2:L:232:GLY:N	2.24	0.51
2:K:254:SER:C	2:K:256:SER:N	2.66	0.51
3:H:144:VAL:HG12	3:H:197:HIS:HB2	1.91	0.51
1:E:210:LYS:NZ	1:E:212:ASP:OD1	2.44	0.51
2:K:194:PHE:HD1	2:K:203:ILE:HG12	1.76	0.51
2:K:109:THR:O	2:K:114:THR:OG1	2.29	0.51
1:E:99:ASP:OD2	2:L:295:PRO:HG3	2.11	0.51
2:J:231:ILE:HD12	2:J:233:ILE:HG12	1.92	0.50
2:L:179:LEU:HD13	2:L:190:ARG:HE	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:MET:HE1	1:E:113:VAL:HG21	1.93	0.50
1:G:6:GLU:OE2	1:G:95:TYR:HA	2.10	0.50
3:H:113:PRO:HB3	3:H:139:PHE:HB3	1.93	0.50
2:I:164:ASN:HB2	9:I:402:NAG:H82	1.92	0.50
2:L:111:ASP:OD2	2:L:113:LYS:HG3	2.11	0.50
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.93	0.50
1:G:48:VAL:HG13	1:G:64:VAL:HG11	1.93	0.50
2:I:97:LYS:HD2	2:I:179:LEU:HD23	1.93	0.50
2:I:142:GLY:O	2:I:156:GLU:N	2.45	0.50
3:B:30:LYS:NZ	3:B:91:ASP:OD1	2.42	0.50
2:K:30:ASN:OD1	2:K:31:SER:N	2.45	0.50
2:L:92:PHE:HZ	2:L:101:ILE:HD13	1.77	0.49
2:K:179:LEU:HD23	2:K:207:HIS:HB3	1.95	0.49
2:K:247:SER:O	2:K:251:PRO:HB3	2.12	0.49
1:G:123:PRO:HB3	1:G:149:TYR:HB3	1.93	0.49
1:G:130:PRO:O	1:G:132:SER:N	2.43	0.49
2:K:249:LEU:O	2:K:250:THR:HG22	2.12	0.49
1:C:151:PRO:HD2	1:C:206:PRO:HB2	1.93	0.49
3:B:132:LEU:HD12	3:B:178:LEU:HD23	1.93	0.49
2:K:143:VAL:HG13	2:K:153:MET:HB2	1.94	0.49
2:K:128:ILE:HD13	2:K:229:LEU:HD11	1.94	0.49
2:L:199:GLY:HA2	2:L:232:GLY:HA2	1.95	0.49
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.48	0.48
1:A:151:PRO:HD2	1:A:206:PRO:HB2	1.95	0.48
3:D:138:ASP:HA	3:D:171:LYS:HB3	1.95	0.48
1:C:193:LEU:HD22	1:C:217:PRO:HG3	1.95	0.48
2:L:68:ILE:HG23	2:L:260:ALA:HB1	1.94	0.48
3:B:136:ILE:HG21	3:B:195:VAL:HG11	1.95	0.48
2:K:189:LEU:HG	2:K:191:GLU:HG3	1.96	0.48
1:G:163:LEU:HD21	1:G:186:VAL:HG21	1.95	0.48
2:K:126:VAL:HB	2:K:174:PRO:HA	1.94	0.48
2:K:195:LYS:HE2	2:K:204:TYR:HE1	1.77	0.48
1:E:29:PHE:O	1:E:72:ARG:NH2	2.46	0.48
1:G:35:HIS:CE1	1:G:50:LEU:HD13	2.49	0.48
2:L:128:ILE:HD13	2:L:229:LEU:HD11	1.94	0.48
2:K:303:LEU:HD22	3:H:30:LYS:HG2	1.95	0.48
2:L:19:THR:HB	2:L:79:PHE:HB3	1.96	0.48
2:K:199:GLY:HA2	2:K:232:GLY:HA2	1.95	0.48
1:E:2:VAL:HG13	1:E:27:PHE:CD1	2.48	0.48
3:F:144:VAL:HG12	3:F:197:HIS:HB2	1.96	0.48
1:C:205:LYS:N	1:C:206:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:120:VAL:HG23	2:K:127:VAL:HB	1.96	0.47
1:C:29:PHE:O	1:C:72:ARG:NH2	2.46	0.47
1:C:52:SER:O	1:C:72:ARG:NH1	2.47	0.47
1:C:130:PRO:HD2	1:C:217:PRO:HA	1.96	0.47
1:E:104:TRP:CH2	3:F:95:VAL:HG11	2.48	0.47
2:J:57:PRO:HG3	2:J:273:ARG:HD2	1.96	0.47
3:F:6:GLN:HG2	3:F:22:CYS:HB2	1.96	0.47
1:A:104:TRP:CH2	3:B:95:VAL:HG11	2.48	0.47
1:E:6:GLU:OE2	1:E:95:TYR:HA	2.13	0.47
1:A:32:TYR:CD2	1:A:98:ARG:HD2	2.49	0.47
2:K:128:ILE:HB	2:K:170:TYR:HB3	1.96	0.47
2:K:231:ILE:HG13	2:K:232:GLY:H	1.79	0.47
1:E:28:THR:HB	2:L:271:GLN:HE22	1.80	0.47
2:L:118:LEU:HD11	2:L:120:VAL:HG13	1.96	0.47
3:B:27:LEU:HG	3:B:65:ASN:HD21	1.79	0.47
2:K:34:ARG:NH2	2:K:219:GLY:O	2.37	0.47
1:E:94:TYR:O	1:E:110:GLY:HA2	2.15	0.47
2:I:102:ARG:NH1	2:I:177:MET:SD	2.87	0.47
2:J:180:GLU:CD	2:J:180:GLU:H	2.22	0.47
2:L:130:VAL:HB	2:L:168:PHE:HB3	1.97	0.47
1:G:47:TRP:CG	3:H:95:VAL:HB	2.50	0.46
3:D:183:GLU:OE1	3:D:183:GLU:N	2.40	0.46
2:L:179:LEU:HD13	2:L:190:ARG:NE	2.30	0.46
3:D:45:LEU:HD11	3:D:48:TYR:HA	1.97	0.46
3:F:136:ILE:HG21	3:F:195:VAL:HG11	1.96	0.46
2:J:46:SER:HA	2:J:279:TYR:O	2.15	0.46
2:J:231:ILE:HG13	2:J:232:GLY:N	2.29	0.46
1:A:205:LYS:N	1:A:206:PRO:HD2	2.31	0.46
1:C:104:TRP:CH2	3:D:95:VAL:HG11	2.51	0.46
3:F:151:ASP:OD1	3:F:190:SER:N	2.48	0.46
2:I:193:VAL:HG13	2:I:270:LEU:HD11	1.97	0.46
2:L:103:GLY:HA3	2:L:119:ILE:O	2.14	0.46
1:C:28:THR:HB	2:I:271:GLN:HE22	1.81	0.46
1:G:120:THR:HG23	1:G:151:PRO:HG2	1.97	0.46
2:J:194:PHE:HD1	2:J:203:ILE:HG12	1.80	0.46
3:D:120:PRO:HD3	3:D:132:LEU:HD23	1.97	0.46
3:B:113:PRO:HB3	3:B:139:PHE:HB3	1.98	0.46
2:K:128:ILE:HG21	2:K:229:LEU:HD13	1.98	0.45
2:I:95:THR:HG21	2:I:210:ILE:HD11	1.98	0.45
1:A:48:VAL:HG13	1:A:64:VAL:HG21	1.98	0.45
1:A:99:ASP:OD2	2:J:295:PRO:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:VAL:HG13	1:C:27:PHE:CD1	2.51	0.45
2:J:100:ILE:HG22	2:J:242:LEU:HB3	1.98	0.45
2:J:128:ILE:HD13	2:J:229:LEU:HD11	1.97	0.45
2:L:99:ASN:ND2	2:L:177:MET:O	2.49	0.45
1:C:6:GLU:OE2	1:C:95:TYR:HA	2.16	0.45
1:C:20:LEU:HD12	1:C:81:LEU:HD23	1.98	0.45
3:D:119:PRO:HA	3:D:132:LEU:HD23	1.98	0.45
2:J:120:VAL:HG21	2:J:157:PHE:CE2	2.51	0.45
2:K:119:ILE:HG12	2:K:128:ILE:HG12	1.97	0.45
2:K:231:ILE:HG13	2:K:232:GLY:N	2.31	0.45
2:K:271:GLN:HB3	1:G:32:TYR:OH	2.16	0.45
1:G:205:LYS:N	1:G:206:PRO:HD2	2.32	0.45
3:F:115:VAL:O	3:F:204:LYS:NZ	2.39	0.45
2:L:193:VAL:HG23	2:L:223:LEU:HD22	1.97	0.45
2:I:130:VAL:HB	2:I:168:PHE:HB3	1.99	0.45
2:I:199:GLY:HA2	2:I:232:GLY:HA2	1.99	0.45
2:L:53:ASP:OD1	2:L:54:LEU:N	2.43	0.45
3:F:169:ASN:C	3:F:171:LYS:H	2.25	0.45
2:L:17:ASN:ND2	2:L:137:ASN:OD1	2.50	0.45
2:L:244:LEU:HB3	2:L:258:TRP:HB3	1.99	0.45
3:F:108:GLN:HB2	3:F:140:TYR:CD1	2.52	0.45
3:F:141:PRO:HB2	3:F:197:HIS:HE1	1.81	0.45
3:H:45:LEU:HD11	3:H:48:TYR:HA	1.99	0.45
2:J:189:LEU:HD23	2:J:189:LEU:O	2.17	0.45
2:I:117:LEU:HD22	2:I:231:ILE:HD13	1.98	0.44
2:J:179:LEU:HD23	2:J:190:ARG:NE	2.32	0.44
2:K:95:THR:HG22	2:K:189:LEU:HA	1.98	0.44
2:K:206:LYS:HB2	2:K:223:LEU:HA	2.00	0.44
1:C:222:LYS:N	3:D:210:GLU:OE2	2.49	0.44
3:F:28:GLY:HA3	3:F:67:GLY:HA2	1.99	0.44
2:L:117:LEU:HD11	2:L:128:ILE:HG23	1.98	0.44
3:B:45:LEU:HD21	3:B:48:TYR:HB3	1.99	0.44
3:B:167:GLN:C	3:B:169:ASN:H	2.23	0.44
1:C:185:VAL:HG21	3:D:135:LEU:HD13	2.00	0.44
2:J:182:LYS:HD3	2:J:186:PHE:O	2.17	0.44
2:L:29:THR:OG1	2:L:30:ASN:N	2.51	0.44
1:A:204:HIS:CE1	1:A:206:PRO:HG2	2.52	0.44
2:K:16:VAL:HG11	2:K:258:TRP:HD1	1.83	0.44
3:D:53:ARG:HD3	3:D:61:PHE:O	2.18	0.44
3:F:53:ARG:HD3	3:F:61:PHE:O	2.17	0.44
2:I:278:LYS:HE2	2:I:287:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:LEU:HD11	2:L:140:PHE:CD1	2.53	0.44
1:A:11:VAL:HG22	1:A:114:THR:HB	1.99	0.44
2:L:57:PRO:O	2:L:60:SER:OG	2.29	0.44
3:F:108:GLN:N	3:F:108:GLN:OE1	2.50	0.44
2:L:29:THR:HG23	2:L:62:VAL:HG23	2.00	0.44
2:K:156:GLU:OE2	2:K:158:ARG:NH1	2.52	0.43
1:G:204:HIS:ND1	1:G:207:SER:OG	2.37	0.43
1:A:164:THR:HG22	1:A:164:THR:O	2.18	0.43
3:D:38:LYS:HG2	3:D:83:ALA:HB2	1.99	0.43
3:D:140:TYR:CG	3:D:141:PRO:HA	2.52	0.43
2:J:191:GLU:HB3	2:J:223:LEU:HD21	1.99	0.43
2:L:195:LYS:HE3	2:L:202:LYS:HE3	2.00	0.43
2:J:31:SER:HB3	2:J:60:SER:H	1.83	0.43
2:J:128:ILE:HG21	2:J:229:LEU:HD13	2.00	0.43
2:J:199:GLY:HA2	2:J:232:GLY:HA2	1.99	0.43
1:A:35:HIS:NE2	1:A:50:LEU:HD13	2.34	0.43
2:K:271:GLN:HE22	1:G:28:THR:HB	1.83	0.43
3:D:93:SER:HB2	2:I:296:LEU:HD13	2.00	0.43
3:F:149:LYS:HD3	3:F:154:PRO:HA	1.99	0.43
1:A:94:TYR:O	1:A:110:GLY:HA2	2.19	0.43
2:K:134:GLN:O	2:K:161:SER:N	2.52	0.43
1:G:36:TRP:NE1	1:G:81:LEU:HB2	2.34	0.43
2:I:120:VAL:HG23	2:I:127:VAL:HB	2.00	0.43
1:A:218:LYS:HD3	3:B:211:CYS:SG	2.59	0.43
2:K:118:LEU:HD11	2:K:120:VAL:HG13	2.01	0.43
3:F:50:ASP:OD1	3:F:50:ASP:N	2.50	0.43
2:K:254:SER:O	2:K:255:SER:C	2.61	0.43
1:G:83:MET:HE1	1:G:113:VAL:HG11	2.00	0.43
3:D:132:LEU:HD12	3:D:178:LEU:HD23	2.00	0.43
2:I:156:GLU:HG2	2:I:158:ARG:HD3	1.99	0.43
1:E:73:ASP:OD2	1:E:76:LYS:HE2	2.18	0.43
1:G:105:TYR:HA	1:G:106:PRO:HA	1.89	0.43
2:J:126:VAL:HB	2:J:174:PRO:HA	2.01	0.43
2:I:102:ARG:HD2	2:I:177:MET:HE1	2.00	0.43
2:L:135:PHE:CD1	2:L:160:TYR:HB3	2.53	0.43
2:K:140:PHE:CZ	2:K:158:ARG:HD3	2.54	0.43
1:G:153:PRO:HG2	1:G:206:PRO:HG3	2.00	0.43
2:J:128:ILE:HB	2:J:170:TYR:HB3	2.00	0.42
2:L:14:GLN:HG3	2:L:15:CYS:H	1.83	0.42
2:K:108:THR:HG22	2:K:236:THR:HG23	2.00	0.42
1:G:41:PRO:HD3	1:G:92:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD13	1:E:180:TYR:CD2	2.54	0.42
3:H:204:LYS:HD3	3:H:204:LYS:HA	1.87	0.42
2:L:89:GLY:HA3	2:L:270:LEU:HD12	2.00	0.42
1:E:41:PRO:HD3	1:E:92:ALA:HA	2.02	0.42
3:D:209:THR:HB	3:D:210:GLU:H	1.67	0.42
1:E:133:LYS:O	1:E:133:LYS:HG2	2.19	0.42
3:F:108:GLN:HB2	3:F:140:TYR:CE1	2.55	0.42
2:I:97:LYS:HA	2:I:179:LEU:HD23	2.01	0.42
2:L:177:MET:HE2	2:L:177:MET:HB3	1.94	0.42
2:L:189:LEU:HD13	2:L:191:GLU:OE2	2.19	0.42
1:G:22:CYS:HB3	1:G:79:LEU:HB3	2.02	0.42
1:G:37:VAL:HG22	1:G:47:TRP:HA	2.02	0.42
1:A:52:SER:O	1:A:72:ARG:NH1	2.53	0.42
2:J:102:ARG:CG	2:J:243:ALA:HB2	2.50	0.42
2:J:111:ASP:OD2	2:J:113:LYS:HG3	2.19	0.42
2:K:94:SER:O	2:K:190:ARG:HB2	2.20	0.42
2:K:118:LEU:O	2:K:128:ILE:HA	2.20	0.42
1:C:213:LYS:NZ	3:D:123:GLU:OE1	2.44	0.42
1:E:205:LYS:HD2	1:E:205:LYS:HA	1.79	0.42
2:I:118:LEU:HD11	2:I:120:VAL:HG13	2.01	0.42
2:J:117:LEU:HD22	2:J:231:ILE:HD13	2.02	0.42
1:E:47:TRP:CG	3:F:95:VAL:HB	2.55	0.42
1:G:100:LEU:HD11	1:G:105:TYR:HB3	2.02	0.42
2:K:246:ARG:HE	2:K:252:GLY:H	1.67	0.41
3:H:12:VAL:HG22	3:H:16:GLN:HB3	2.02	0.41
3:B:189:ARG:HH22	1:C:88:ALA:HB3	1.85	0.41
3:F:12:VAL:HG22	3:F:16:GLN:HB3	2.02	0.41
2:I:30:ASN:OD1	2:I:31:SER:N	2.53	0.41
1:G:94:TYR:O	1:G:110:GLY:HA2	2.20	0.41
2:L:110:LEU:HD12	2:L:237:ARG:HH21	1.86	0.41
1:C:108:GLY:O	3:D:42:SER:OG	2.38	0.41
1:E:167:VAL:HG22	1:E:186:VAL:HB	2.02	0.41
2:L:95:THR:HA	2:L:188:ASN:O	2.21	0.41
3:B:144:VAL:HG12	3:B:197:HIS:HB2	2.03	0.41
2:J:203:ILE:HB	2:J:227:VAL:HG12	2.03	0.41
1:C:188:VAL:HG11	1:C:198:TYR:CE1	2.56	0.41
1:G:61:ALA:O	1:G:65:LYS:HG3	2.20	0.41
1:G:128:LEU:HB3	3:H:118:PHE:CD1	2.56	0.41
2:I:120:VAL:HG21	2:I:157:PHE:HE2	1.85	0.41
2:L:68:ILE:CG2	2:L:260:ALA:HB1	2.51	0.41
2:K:122:ASN:CB	2:K:125:ASN:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:253:ASP:O	2:K:254:SER:C	2.61	0.41
3:F:35:TYR:CZ	3:F:45:LEU:HD13	2.56	0.41
1:G:150:PHE:HB3	1:G:151:PRO:HD3	2.03	0.41
2:I:231:ILE:HG13	2:I:232:GLY:N	2.35	0.41
2:L:28:TYR:HB3	2:L:61:ASN:OD1	2.20	0.41
1:A:24:ALA:HB1	1:A:27:PHE:CE1	2.56	0.41
2:K:247:SER:OG	2:K:257:GLY:HA2	2.21	0.41
3:B:189:ARG:HH22	1:C:88:ALA:H	1.68	0.41
1:C:34:MET:HB3	1:C:79:LEU:HD22	2.02	0.41
3:F:210:GLU:HG3	3:F:211:CYS:SG	2.61	0.41
2:J:25:PRO:HA	2:J:26:PRO:HD3	1.93	0.41
2:K:123:ALA:H	2:K:153:MET:HE2	1.86	0.41
2:I:52:GLN:HA	2:I:273:ARG:O	2.21	0.41
2:J:102:ARG:NH2	2:J:153:MET:SD	2.94	0.41
1:A:83:MET:HE1	1:A:113:VAL:HG21	2.02	0.40
3:H:110:LYS:HD2	3:H:141:PRO:HD3	2.03	0.40
2:I:128:ILE:HG21	2:I:229:LEU:HD13	2.03	0.40
2:L:68:ILE:O	2:L:262:ALA:HA	2.21	0.40
1:G:88:ALA:HA	1:G:115:VAL:HB	2.01	0.40
3:F:82:GLU:HG3	3:F:104:THR:HA	2.03	0.40
2:L:58:PHE:HB2	2:L:293:LEU:HD11	2.03	0.40
2:L:289:VAL:HG11	2:L:298:GLU:HG3	2.03	0.40
1:C:199:ILE:HA	1:C:214:ARG:HA	2.03	0.40
1:E:173:VAL:N	1:E:181:SER:O	2.55	0.40
3:F:45:LEU:HD11	3:F:48:TYR:HA	2.03	0.40
3:B:53:ARG:HD3	3:B:61:PHE:O	2.21	0.40
1:C:172:ALA:HB2	1:C:182:LEU:HD23	2.03	0.40
1:A:62:ASP:HA	1:A:65:LYS:HD2	2.04	0.40
1:C:83:MET:HB3	1:C:86:LEU:HD21	2.03	0.40
1:C:128:LEU:HB3	3:D:118:PHE:CD1	2.57	0.40
1:E:32:TYR:OH	2:L:271:GLN:HB3	2.22	0.40
2:J:56:LEU:HD22	2:J:91:TYR:CG	2.57	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	221/229 (96%)	209 (95%)	11 (5%)	1 (0%)	24	54
1	C	221/229 (96%)	214 (97%)	5 (2%)	2 (1%)	14	41
1	E	221/229 (96%)	215 (97%)	6 (3%)	0	100	100
1	G	219/229 (96%)	212 (97%)	6 (3%)	1 (0%)	24	54
2	I	268/298 (90%)	245 (91%)	23 (9%)	0	100	100
2	J	271/298 (91%)	252 (93%)	19 (7%)	0	100	100
2	K	271/298 (91%)	250 (92%)	21 (8%)	0	100	100
2	L	271/298 (91%)	248 (92%)	23 (8%)	0	100	100
3	B	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
3	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
3	F	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
3	H	209/212 (99%)	197 (94%)	12 (6%)	0	100	100
All	All	2800/2956 (95%)	2639 (94%)	157 (6%)	4 (0%)	48	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	C	165	SER
1	G	131	SER
1	C	130	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	187/193 (97%)	187 (100%)	0	100	100
1	C	187/193 (97%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	187/193 (97%)	187 (100%)	0	100	100
1	G	185/193 (96%)	185 (100%)	0	100	100
2	I	248/268 (92%)	248 (100%)	0	100	100
2	J	249/268 (93%)	249 (100%)	0	100	100
2	K	249/268 (93%)	249 (100%)	0	100	100
2	L	252/268 (94%)	252 (100%)	0	100	100
3	B	180/180 (100%)	180 (100%)	0	100	100
3	D	179/180 (99%)	178 (99%)	1 (1%)	78	80
3	F	179/180 (99%)	178 (99%)	1 (1%)	78	80
3	H	179/180 (99%)	178 (99%)	1 (1%)	78	80
All	All	2461/2564 (96%)	2458 (100%)	3 (0%)	88	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	211	CYS
3	F	211	CYS
3	H	211	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	208	ASN
2	K	52	GLN
2	K	125	ASN
3	B	184	GLN
1	C	46	GLN
1	C	82	GLN
1	C	84	ASN
1	C	168	HIS
1	E	82	GLN
1	E	84	ASN
1	G	13	GLN
1	G	208	ASN
3	D	16	GLN
3	F	128	ASN

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Mol	Chain	Res	Type
3	H	108	GLN
2	I	115	GLN
2	I	164	ASN
2	J	121	ASN
2	L	17	ASN
2	L	49	HIS
2	L	99	ASN
2	L	121	ASN
2	L	164	ASN
2	L	207	HIS

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 ⓘ

26 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	M	1	4,2	14,14,15	0.69	0	17,19,21	1.15	2 (11%)
4	FUC	M	2	4	10,10,11	0.77	0	14,14,16	1.07	1 (7%)
5	NAG	N	1	2,5	14,14,15	0.80	0	17,19,21	1.79	4 (23%)
5	NAG	N	2	5	14,14,15	0.76	0	17,19,21	0.96	2 (11%)
5	BMA	N	3	5	11,11,12	0.81	0	15,15,17	2.36	5 (33%)
5	MAN	N	4	5	11,11,12	0.66	0	15,15,17	1.49	1 (6%)
5	FUC	N	5	5	10,10,11	0.79	0	14,14,16	2.18	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	1	4,2	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
4	FUC	O	2	4	10,10,11	0.84	0	14,14,16	0.92	0
4	NAG	P	1	4,2	14,14,15	0.72	0	17,19,21	0.90	0
4	FUC	P	2	4	10,10,11	0.83	0	14,14,16	0.94	0
6	NAG	Q	1	6,2	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
6	NAG	Q	2	6	14,14,15	0.75	0	17,19,21	0.97	0
6	BMA	Q	3	6	11,11,12	0.93	0	15,15,17	2.22	4 (26%)
6	MAN	Q	4	6	11,11,12	0.71	0	15,15,17	1.25	1 (6%)
6	FUC	Q	5	6	10,10,11	0.77	0	14,14,16	1.79	5 (35%)
7	NAG	R	1	2,7	14,14,15	0.68	0	17,19,21	1.04	1 (5%)
7	NAG	R	2	7	14,14,15	0.71	0	17,19,21	1.05	2 (11%)
7	BMA	R	3	7	11,11,12	0.88	0	15,15,17	2.08	3 (20%)
7	FUC	R	4	7	10,10,11	0.81	0	14,14,16	2.48	5 (35%)
8	NAG	S	1	8,2	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
8	NAG	S	2	8	14,14,15	0.71	0	17,19,21	0.85	0
7	NAG	T	1	2,7	14,14,15	0.78	0	17,19,21	1.52	4 (23%)
7	NAG	T	2	7	14,14,15	0.75	0	17,19,21	0.92	0
7	BMA	T	3	7	11,11,12	0.87	0	15,15,17	2.28	5 (33%)
7	FUC	T	4	7	10,10,11	0.70	0	14,14,16	2.35	6 (42%)

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	M	1	4,2	-	1/6/23/26	0/1/1/1
4	FUC	M	2	4	-	-	0/1/1/1
5	NAG	N	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	2/2/19/22	1/1/1/1
5	FUC	N	5	5	-	-	0/1/1/1
4	NAG	O	1	4,2	-	1/6/23/26	0/1/1/1
4	FUC	O	2	4	-	-	0/1/1/1
4	NAG	P	1	4,2	-	1/6/23/26	0/1/1/1
4	FUC	P	2	4	-	-	0/1/1/1
6	NAG	Q	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	FUC	Q	5	6	-	-	0/1/1/1
7	NAG	R	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	FUC	R	4	7	-	-	0/1/1/1
8	NAG	S	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	0/6/23/26	0/1/1/1
7	NAG	T	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	FUC	T	4	7	-	-	0/1/1/1

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	4	FUC	C1-C2-C3	6.76	117.97	109.67
7	T	3	BMA	C1-O5-C5	6.39	120.85	112.19
5	N	3	BMA	C1-O5-C5	6.39	120.84	112.19
5	N	5	FUC	C1-C2-C3	5.96	116.99	109.67
7	R	3	BMA	C1-O5-C5	5.75	119.98	112.19
6	Q	3	BMA	C1-O5-C5	5.73	119.96	112.19
5	N	4	MAN	C1-O5-C5	4.94	118.88	112.19
7	T	4	FUC	C1-O5-C5	4.82	123.69	112.78
7	T	4	FUC	C1-C2-C3	4.72	115.47	109.67
5	N	1	NAG	C3-C4-C5	4.53	118.33	110.24
7	R	4	FUC	C1-O5-C5	3.86	121.53	112.78
6	Q	4	MAN	C1-O5-C5	3.80	117.34	112.19
6	Q	5	FUC	C1-O5-C5	3.53	120.79	112.78
7	T	1	NAG	O5-C1-C2	-3.43	105.87	111.29
5	N	5	FUC	C1-O5-C5	3.36	120.39	112.78
6	Q	3	BMA	C3-C4-C5	3.33	116.18	110.24
5	N	3	BMA	C3-C4-C5	3.31	116.15	110.24
5	N	1	NAG	O5-C1-C2	-3.29	106.09	111.29
8	S	1	NAG	C2-N2-C7	3.25	127.53	122.90
6	Q	5	FUC	C1-C2-C3	3.25	113.66	109.67
7	R	4	FUC	C3-C4-C5	-3.15	104.86	109.77
7	T	3	BMA	C3-C4-C5	3.12	115.80	110.24
6	Q	3	BMA	C2-C3-C4	3.09	116.24	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	5	FUC	C3-C4-C5	-3.09	104.96	109.77
7	T	1	NAG	C3-C4-C5	3.02	115.63	110.24
7	R	1	NAG	O5-C1-C2	-2.93	106.66	111.29
7	T	4	FUC	C3-C4-C5	-2.83	105.36	109.77
4	O	1	NAG	O5-C1-C2	-2.80	106.87	111.29
4	M	1	NAG	O5-C1-C2	-2.78	106.90	111.29
7	T	3	BMA	C2-C3-C4	2.73	115.62	110.89
5	N	1	NAG	O4-C4-C3	-2.71	104.07	110.35
7	R	3	BMA	C3-C4-C5	2.63	114.93	110.24
7	T	4	FUC	O5-C1-C2	2.56	114.72	110.77
6	Q	1	NAG	O5-C1-C2	-2.54	107.28	111.29
6	Q	5	FUC	O5-C5-C4	2.52	114.04	109.52
7	T	1	NAG	O4-C4-C3	-2.48	104.61	110.35
7	T	4	FUC	O5-C5-C4	2.43	113.89	109.52
7	R	3	BMA	C2-C3-C4	2.43	115.10	110.89
5	N	3	BMA	O4-C4-C3	-2.41	104.78	110.35
5	N	2	NAG	O5-C1-C2	-2.39	107.52	111.29
8	S	1	NAG	C1-O5-C5	2.33	115.35	112.19
5	N	3	BMA	O3-C3-C4	2.31	115.68	110.35
6	Q	3	BMA	O4-C4-C3	-2.30	105.02	110.35
5	N	2	NAG	O4-C4-C3	-2.27	105.10	110.35
7	T	1	NAG	C1-O5-C5	-2.26	109.14	112.19
5	N	1	NAG	C1-O5-C5	-2.24	109.16	112.19
7	R	2	NAG	C1-O5-C5	2.24	115.22	112.19
7	R	4	FUC	O5-C1-C2	2.22	114.20	110.77
7	T	4	FUC	O4-C4-C5	2.22	114.59	109.67
6	Q	5	FUC	O4-C4-C5	2.22	114.58	109.67
5	N	3	BMA	C2-C3-C4	2.20	114.69	110.89
7	T	3	BMA	O4-C4-C3	-2.17	105.33	110.35
6	Q	5	FUC	C3-C4-C5	-2.15	106.42	109.77
4	M	1	NAG	C1-C2-N2	2.08	114.03	110.49
7	R	2	NAG	O5-C1-C2	-2.07	108.01	111.29
7	R	4	FUC	O4-C4-C5	2.06	114.24	109.67
7	T	3	BMA	O3-C3-C2	-2.03	106.11	109.99
4	M	2	FUC	C1-O5-C5	2.03	117.37	112.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Q	4	MAN	O5-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6

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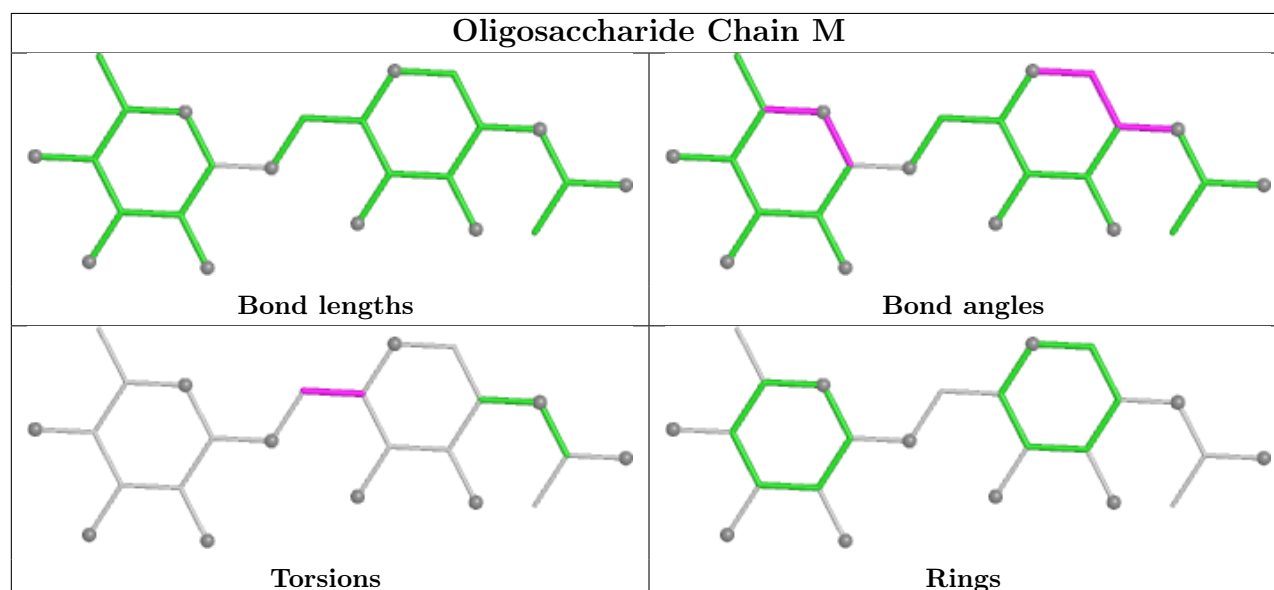
Mol	Chain	Res	Type	Atoms
5	N	1	NAG	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Q	4	MAN	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
5	N	4	MAN	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
8	S	1	NAG	C3-C2-N2-C7
7	R	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6

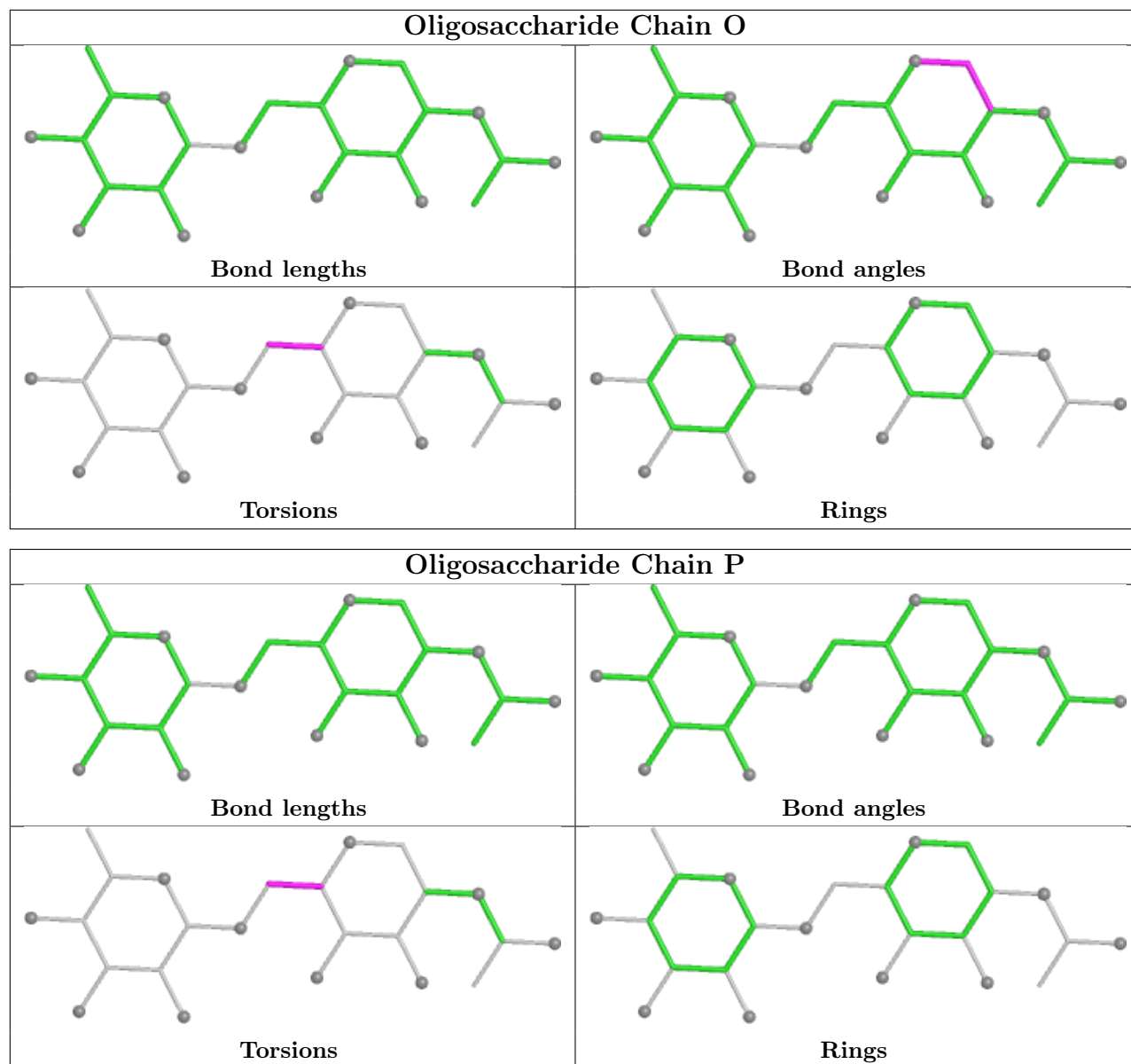
All (1) ring outliers are listed below:

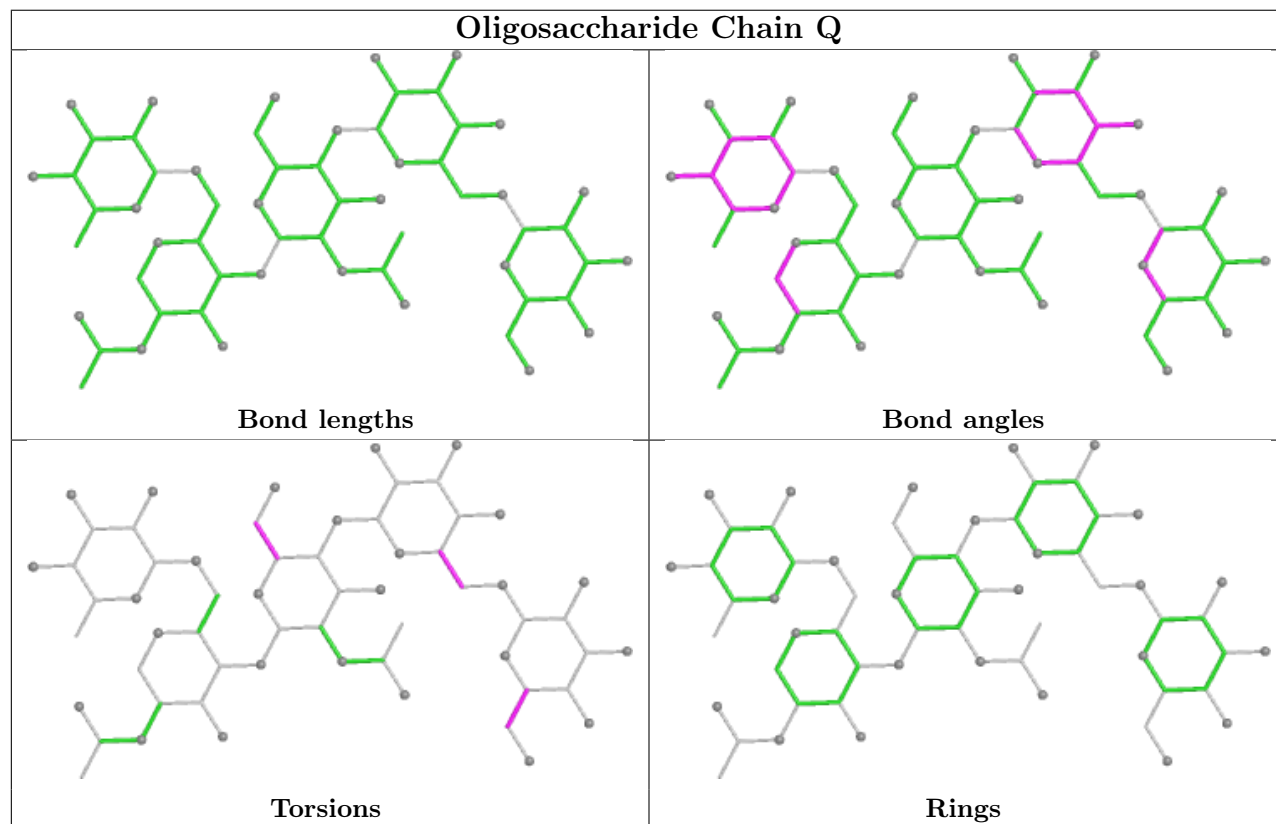
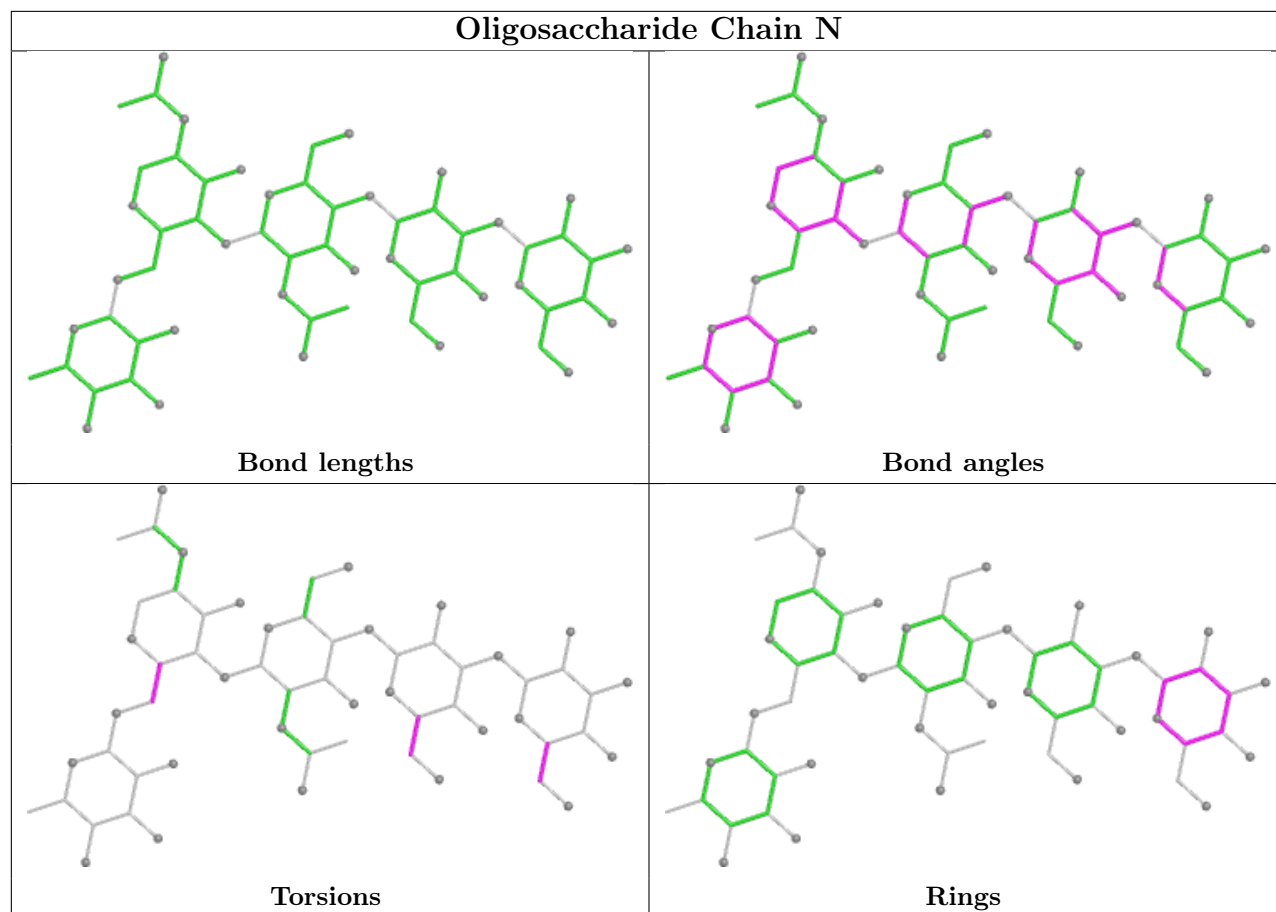
Mol	Chain	Res	Type	Atoms
5	N	4	MAN	C1-C2-C3-C4-C5-O5

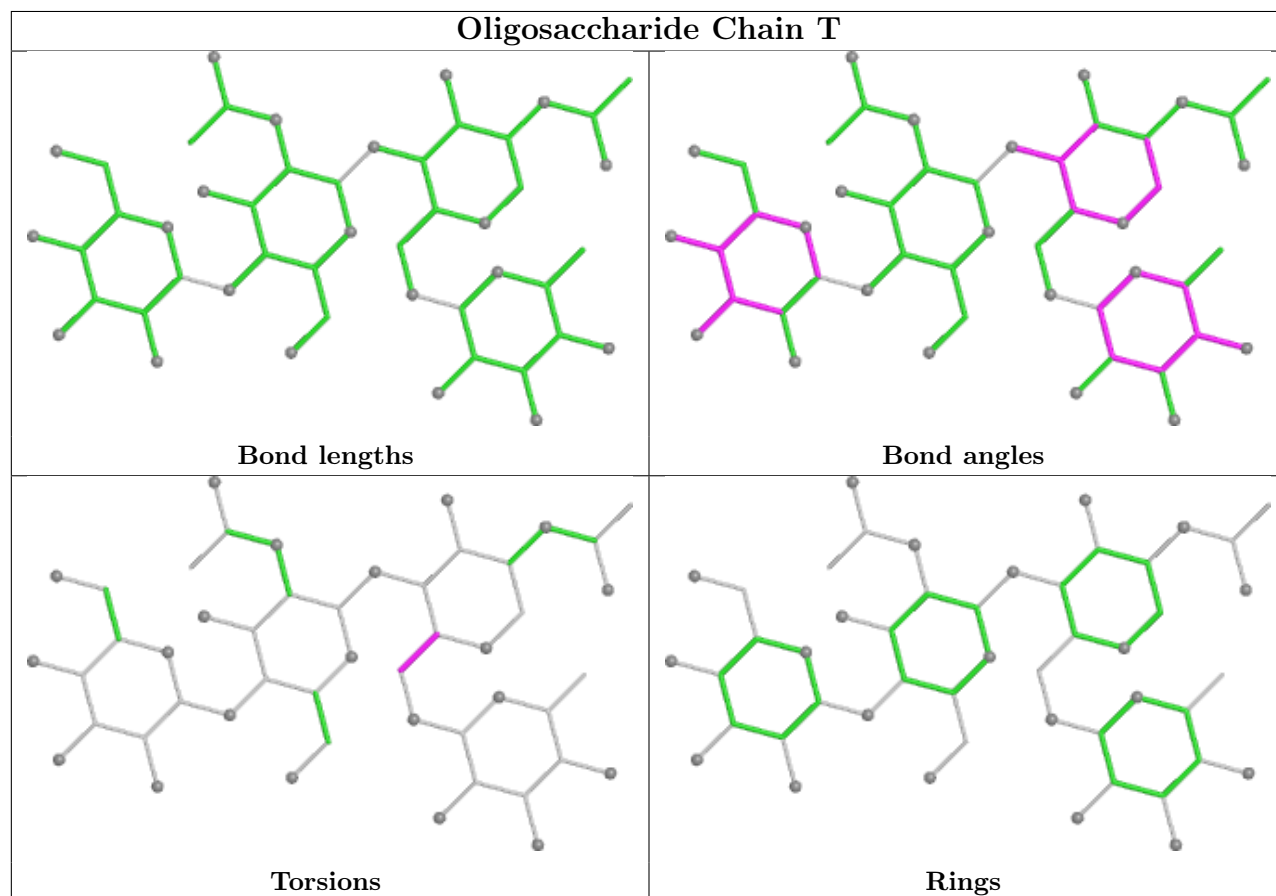
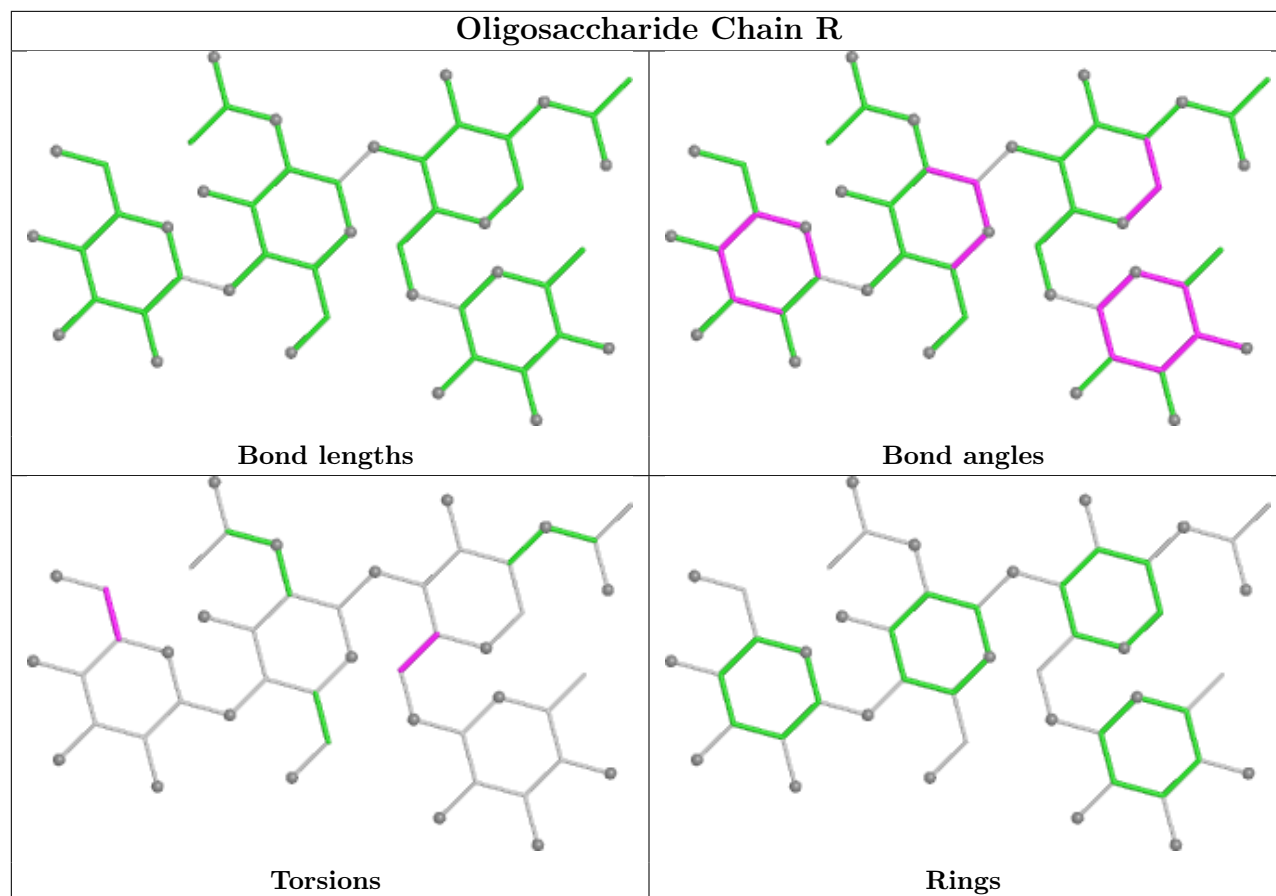
No monomer is involved in short contacts.

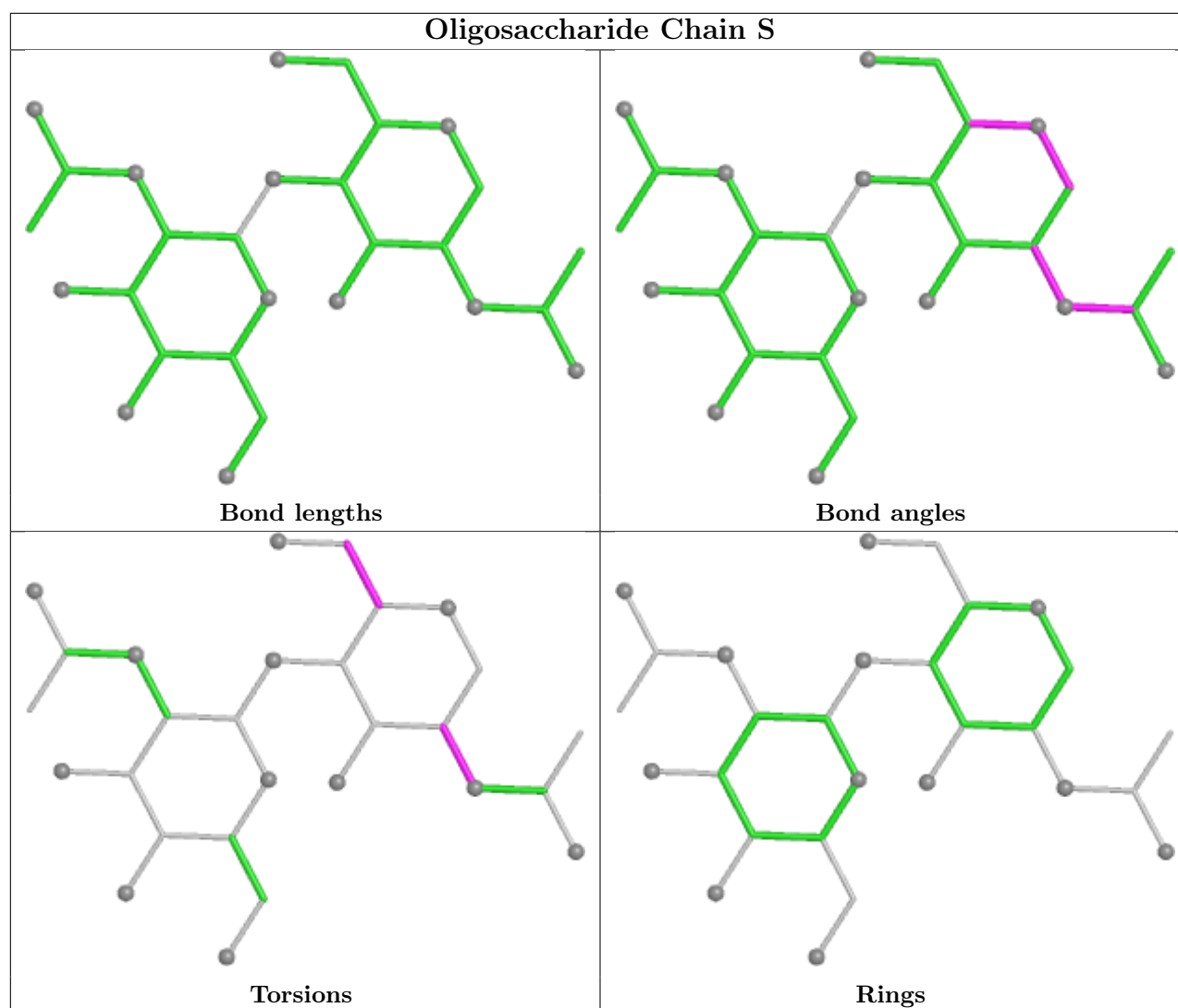
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
9	NAG	J	401	2	14,14,15	0.76	0	17,19,21	0.96	0
9	NAG	I	401	2	14,14,15	0.72	0	17,19,21	0.87	0
9	NAG	L	403	2	14,14,15	0.71	0	17,19,21	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	K	402	2	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
9	NAG	J	404	2	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
9	NAG	K	401	2	14,14,15	0.71	0	17,19,21	0.79	0
9	NAG	J	402	2	14,14,15	0.72	0	17,19,21	0.84	0
9	NAG	I	402	2	14,14,15	0.73	0	17,19,21	0.86	0
9	NAG	J	403	2	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
9	NAG	L	401	2	14,14,15	0.74	0	17,19,21	0.87	0
9	NAG	L	402	2	14,14,15	0.67	0	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	J	401	2	-	2/6/23/26	0/1/1/1
9	NAG	I	401	2	-	0/6/23/26	0/1/1/1
9	NAG	L	403	2	-	1/6/23/26	0/1/1/1
9	NAG	K	402	2	-	2/6/23/26	0/1/1/1
9	NAG	J	404	2	-	2/6/23/26	0/1/1/1
9	NAG	K	401	2	-	0/6/23/26	0/1/1/1
9	NAG	J	402	2	-	0/6/23/26	0/1/1/1
9	NAG	I	402	2	-	0/6/23/26	0/1/1/1
9	NAG	J	403	2	-	0/6/23/26	0/1/1/1
9	NAG	L	401	2	-	0/6/23/26	0/1/1/1
9	NAG	L	402	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	403	NAG	C2-N2-C7	3.11	127.34	122.90
9	L	402	NAG	O5-C1-C2	-2.71	107.01	111.29
9	J	404	NAG	O5-C1-C2	-2.58	107.22	111.29
9	K	402	NAG	C1-O5-C5	2.42	115.47	112.19
9	J	403	NAG	C1-O5-C5	2.31	115.33	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	402	NAG	C4-C5-C6-O6
9	J	401	NAG	O5-C5-C6-O6
9	K	402	NAG	O5-C5-C6-O6
9	J	401	NAG	C4-C5-C6-O6
9	J	404	NAG	C8-C7-N2-C2
9	J	404	NAG	O7-C7-N2-C2
9	L	402	NAG	C8-C7-N2-C2
9	L	402	NAG	O7-C7-N2-C2
9	L	402	NAG	O5-C5-C6-O6
9	L	403	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	402	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	223/229 (97%)	0.67	16 (7%) 21 11	17, 33, 71, 116	0
1	C	223/229 (97%)	0.71	16 (7%) 21 11	16, 36, 80, 141	0
1	E	223/229 (97%)	0.89	16 (7%) 21 11	17, 40, 83, 123	0
1	G	221/229 (96%)	0.85	22 (9%) 12 6	17, 40, 69, 111	0
2	I	276/298 (92%)	1.00	40 (14%) 6 3	13, 40, 88, 108	0
2	J	277/298 (92%)	1.12	57 (20%) 2 1	12, 41, 104, 117	0
2	K	277/298 (92%)	1.15	54 (19%) 3 1	16, 43, 97, 120	0
2	L	279/298 (93%)	1.14	52 (18%) 3 1	16, 40, 91, 116	0
3	B	212/212 (100%)	0.72	10 (4%) 36 19	17, 40, 61, 122	0
3	D	211/212 (99%)	0.82	15 (7%) 22 11	16, 43, 65, 114	0
3	F	211/212 (99%)	0.92	17 (8%) 18 9	21, 48, 72, 109	0
3	H	211/212 (99%)	0.89	12 (5%) 29 15	23, 46, 67, 112	0
All	All	2844/2956 (96%)	0.92	327 (11%) 9 5	12, 41, 89, 141	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	185	ASN	5.1
2	K	262	ALA	5.0
2	K	249	LEU	4.9
2	K	252	GLY	4.8
2	K	251	PRO	4.7
1	E	132	SER	4.6
2	K	144	TYR	4.4
2	J	67	ALA	4.4
2	I	70	VAL	4.4
2	K	250	THR	4.3
3	F	141	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
2	L	177	MET	4.3
3	B	211	CYS	4.3
1	C	137	GLY	4.3
2	L	145	TYR	4.3
2	I	123	ALA	4.3
2	L	79	PHE	4.2
2	J	259	THR	4.2
2	I	67	ALA	4.2
2	J	263	ALA	4.1
2	J	15	CYS	4.1
2	J	177	MET	4.0
2	K	258	TRP	4.0
2	J	24	LEU	4.0
2	L	19	THR	3.9
3	B	93	SER	3.9
1	E	137	GLY	3.9
2	L	262	ALA	3.9
2	L	153	MET	3.8
1	C	134	SER	3.8
3	D	209	THR	3.7
3	H	51	SER	3.7
1	G	130	PRO	3.7
2	I	145	TYR	3.7
2	L	69	HIS	3.7
2	J	144	TYR	3.6
2	K	24	LEU	3.6
2	L	178	ASP	3.6
2	L	125	ASN	3.6
3	F	48	TYR	3.6
1	E	131	SER	3.6
1	G	221	ASP	3.6
2	I	69	HIS	3.6
2	J	245	HIS	3.6
2	L	214	ARG	3.6
3	D	211	CYS	3.6
2	I	19	THR	3.6
2	K	179	LEU	3.5
1	E	134	SER	3.5
2	K	260	ALA	3.5
2	J	145	TYR	3.5
1	G	151	PRO	3.5
1	E	221	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	144	TYR	3.4
2	I	261	GLY	3.4
3	H	77	THR	3.4
1	G	135	THR	3.4
1	A	102	SER	3.4
2	I	254	SER	3.4
2	K	79	PHE	3.4
2	I	71	SER	3.4
2	J	251	PRO	3.4
2	L	66	HIS	3.4
1	C	131	SER	3.3
1	G	134	SER	3.3
1	C	135	THR	3.3
2	I	154	GLU	3.3
1	E	133	LYS	3.3
2	J	248	TYR	3.3
2	J	262	ALA	3.3
2	J	260	ALA	3.3
1	A	136	SER	3.3
3	F	211	CYS	3.3
3	H	209	THR	3.3
3	B	212	SER	3.2
2	K	80	ASP	3.2
2	K	215	ASP	3.2
2	J	19	THR	3.2
2	I	185	ASN	3.2
1	A	131	SER	3.2
2	L	24	LEU	3.2
3	D	49	GLN	3.2
1	A	134	SER	3.2
2	K	31	SER	3.2
2	K	263	ALA	3.2
2	K	68	ILE	3.2
2	I	179	LEU	3.1
2	L	70	VAL	3.1
2	L	123	ALA	3.1
1	E	165	SER	3.1
2	J	157	PHE	3.1
2	K	153	MET	3.1
3	F	140	TYR	3.1
3	F	93	SER	3.1
2	K	32	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	152	TRP	3.1
2	I	20	THR	3.0
2	I	153	MET	3.0
2	L	80	ASP	3.0
2	J	22	THR	3.0
3	F	2	PHE	3.0
1	C	7	SER	3.0
2	K	16	VAL	3.0
2	K	20	THR	3.0
2	K	22	THR	3.0
1	A	160	SER	3.0
2	K	261	GLY	3.0
1	C	132	SER	2.9
2	K	247	SER	2.9
3	D	48	TYR	2.9
2	K	253	ASP	2.9
1	A	116	SER	2.9
2	J	98	SER	2.9
1	G	137	GLY	2.9
2	L	261	GLY	2.9
1	E	136	SER	2.9
2	J	179	LEU	2.9
3	F	209	THR	2.9
2	K	157	PHE	2.9
2	K	18	LEU	2.9
2	K	155	SER	2.8
2	I	25	PRO	2.8
2	L	124	THR	2.8
3	H	48	TYR	2.8
2	J	211	ASN	2.8
2	L	306	HIS	2.8
2	J	255	SER	2.8
3	F	210	GLU	2.8
2	L	176	LEU	2.8
2	J	20	THR	2.8
2	L	180	GLU	2.8
1	G	150	PHE	2.8
2	L	68	ILE	2.8
1	A	198	TYR	2.8
1	E	222	LYS	2.8
1	E	102	SER	2.8
2	J	247	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	H	93	SER	2.8
2	I	68	ILE	2.8
2	J	95	THR	2.8
2	I	144	TYR	2.7
2	I	15	CYS	2.7
2	K	110	LEU	2.7
1	A	135	THR	2.7
1	A	139	THR	2.7
3	F	50	ASP	2.7
1	G	102	SER	2.7
3	B	21	THR	2.7
2	K	145	TYR	2.7
2	K	154	GLU	2.7
2	I	180	GLU	2.7
1	E	139	THR	2.7
3	H	138	ASP	2.7
2	I	186	PHE	2.7
1	C	133	LYS	2.7
2	K	259	THR	2.7
3	B	163	THR	2.7
2	J	152	TRP	2.7
2	K	100	ILE	2.6
1	G	139	THR	2.6
2	L	179	LEU	2.6
1	A	195	THR	2.6
1	A	133	LYS	2.6
2	L	25	PRO	2.6
2	I	80	ASP	2.6
1	A	223	THR	2.6
2	I	178	ASP	2.6
2	I	188	ASN	2.6
2	J	181	GLY	2.6
2	J	249	LEU	2.6
2	L	98	SER	2.6
2	L	14	GLN	2.6
2	I	184	GLY	2.6
2	K	137	ASN	2.6
2	L	150	LYS	2.6
1	A	197	THR	2.6
2	L	22	THR	2.6
2	J	25	PRO	2.5
1	E	56	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	131	SER	2.5
2	K	255	SER	2.5
2	L	18	LEU	2.5
1	G	61	ALA	2.5
2	J	153	MET	2.5
2	J	207	HIS	2.5
2	J	189	LEU	2.5
2	L	257	GLY	2.5
2	L	305	SER	2.5
3	F	146	VAL	2.5
1	C	129	ALA	2.5
1	C	194	GLY	2.5
2	J	246	ARG	2.5
3	F	3	MET	2.5
2	J	250	THR	2.5
1	A	217	PRO	2.5
2	K	257	GLY	2.5
1	G	56	SER	2.5
2	L	254	SER	2.5
2	K	178	ASP	2.5
3	H	151	ASP	2.5
1	G	129	ALA	2.4
2	K	98	SER	2.4
2	K	166	CYS	2.4
2	L	155	SER	2.4
2	J	79	PHE	2.4
2	K	81	ASN	2.4
2	L	263	ALA	2.4
1	G	136	SER	2.4
1	G	192	SER	2.4
2	L	166	CYS	2.4
3	F	200	SER	2.4
3	H	187	SER	2.4
2	K	109	THR	2.4
3	D	21	THR	2.4
2	J	252	GLY	2.4
2	K	123	ALA	2.4
2	J	182	LYS	2.4
1	G	160	SER	2.4
3	H	23	SER	2.4
2	K	26	PRO	2.4
2	L	26	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	139	THR	2.4
2	I	72	GLY	2.4
3	D	1	ASN	2.4
2	I	262	ALA	2.4
2	K	177	MET	2.4
3	F	23	SER	2.4
2	J	26	PRO	2.4
2	J	139	PRO	2.4
1	E	122	GLY	2.3
2	K	181	GLY	2.3
1	E	35	HIS	2.3
2	L	246	ARG	2.3
2	L	260	ALA	2.3
3	B	150	ALA	2.3
2	I	249	LEU	2.3
2	J	96	GLU	2.3
2	J	132	GLU	2.3
3	D	93	SER	2.3
1	C	197	THR	2.3
2	L	99	ASN	2.3
2	J	257	GLY	2.3
2	K	185	ASN	2.3
2	J	186	PHE	2.3
3	F	105	VAL	2.3
2	I	102	ARG	2.3
2	J	258	TRP	2.3
2	L	256	SER	2.3
1	G	62	ASP	2.3
2	K	23	GLN	2.3
2	I	264	ALA	2.3
2	J	14	GLN	2.3
3	H	211	CYS	2.3
3	H	50	ASP	2.3
1	A	103	GLY	2.2
2	J	133	PHE	2.2
2	I	99	ASN	2.2
3	D	84	ASP	2.2
3	D	151	ASP	2.2
2	I	21	ARG	2.2
2	L	215	ASP	2.2
2	I	133	PHE	2.2
1	C	223	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	66	HIS	2.2
1	E	63	SER	2.2
2	J	121	ASN	2.2
2	L	156	GLU	2.2
1	G	15	GLY	2.2
2	K	147	LYS	2.2
1	E	198	TYR	2.2
2	L	231	ILE	2.2
3	B	152	SER	2.2
3	B	200	SER	2.2
3	D	3	MET	2.2
1	C	140	ALA	2.2
2	J	99	ASN	2.2
3	D	102	GLU	2.2
2	J	80	ASP	2.2
2	J	138	ASP	2.2
3	D	146	VAL	2.1
1	A	163	LEU	2.1
1	G	183	SER	2.1
2	I	256	SER	2.1
2	J	31	SER	2.1
2	J	256	SER	2.1
2	J	154	GLU	2.1
3	D	198	GLU	2.1
2	K	139	PRO	2.1
2	L	135	PHE	2.1
2	K	245	HIS	2.1
2	I	259	THR	2.1
3	H	129	LYS	2.1
2	K	305	SER	2.1
2	I	155	SER	2.1
3	F	92	SER	2.1
1	C	164	THR	2.1
3	F	172	TYR	2.1
2	I	163	ALA	2.1
2	L	218	GLN	2.1
1	C	161	GLY	2.1
1	G	152	GLU	2.1
2	L	188	ASN	2.1
2	L	23	GLN	2.1
2	K	272	PRO	2.1
3	B	2	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	125	ASN	2.1
3	B	169	ASN	2.1
2	J	253	ASP	2.1
2	I	260	ALA	2.1
2	J	163	ALA	2.1
1	G	138	GLY	2.1
2	K	304	LYS	2.0
3	D	122	SER	2.0
2	I	141	LEU	2.0
2	J	17	ASN	2.0
2	L	210	ILE	2.0
3	D	83	ALA	2.0
2	K	42	VAL	2.0
1	C	192	SER	2.0
2	J	197	ILE	2.0
2	L	161	SER	2.0
2	L	258	TRP	2.0
1	G	198	TYR	2.0
2	I	166	CYS	2.0
2	J	150	LYS	2.0
3	F	108	GLN	2.0
2	L	154	GLU	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
6	BMA	Q	3	11/12	0.20	0.22	82,102,114,116	0
4	FUC	P	2	10/11	0.21	0.22	62,85,93,103	0
7	BMA	T	3	11/12	0.22	0.24	69,99,110,119	0
6	MAN	Q	4	11/12	0.44	0.19	68,92,113,119	0
6	NAG	Q	2	14/15	0.46	0.21	57,99,102,103	0
7	BMA	R	3	11/12	0.50	0.19	90,104,125,128	0

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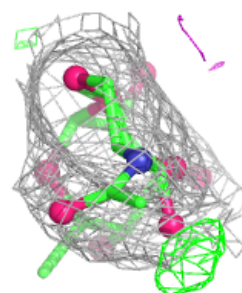
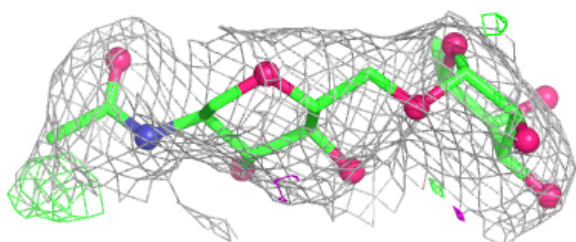
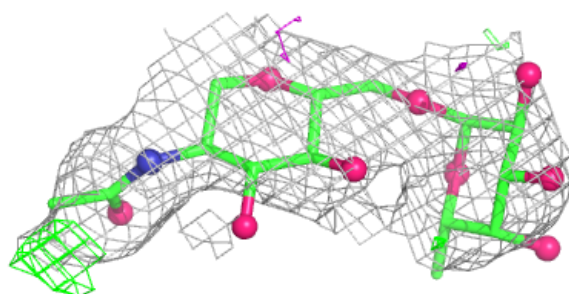
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	N	3	11/12	0.50	0.17	72,112,118,124	0
7	NAG	T	2	14/15	0.56	0.16	44,79,88,96	0
4	FUC	O	2	10/11	0.57	0.23	70,81,91,99	0
8	NAG	S	1	14/15	0.59	0.23	44,73,88,89	0
4	FUC	M	2	10/11	0.61	0.18	52,75,80,87	0
8	NAG	S	2	14/15	0.62	0.16	53,82,92,96	0
7	FUC	R	4	10/11	0.65	0.27	61,83,101,114	0
5	FUC	N	5	10/11	0.68	0.28	75,89,105,105	0
7	FUC	T	4	10/11	0.68	0.23	58,71,90,96	0
7	NAG	R	2	14/15	0.70	0.16	66,97,115,123	0
6	FUC	Q	5	10/11	0.70	0.26	61,90,113,114	0
5	MAN	N	4	11/12	0.72	0.16	69,94,115,118	0
5	NAG	N	2	14/15	0.72	0.17	60,91,105,115	0
4	NAG	P	1	14/15	0.74	0.15	42,57,86,90	0
5	NAG	N	1	14/15	0.77	0.20	66,78,89,97	0
4	NAG	M	1	14/15	0.78	0.14	35,52,77,87	0
4	NAG	O	1	14/15	0.82	0.12	31,50,60,72	0
7	NAG	R	1	14/15	0.82	0.16	63,79,93,93	0
6	NAG	Q	1	14/15	0.83	0.16	57,67,94,97	0
7	NAG	T	1	14/15	0.86	0.14	61,80,86,87	0

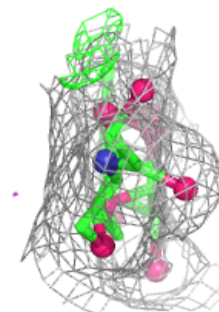
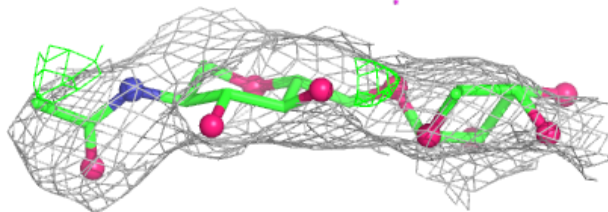
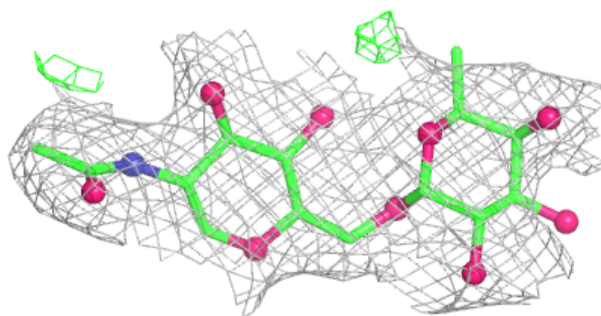
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

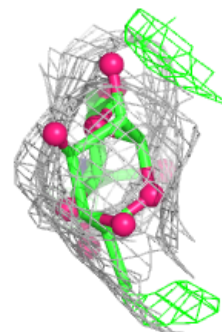
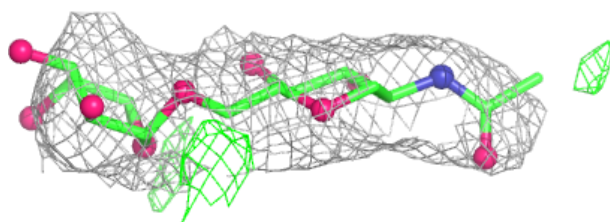
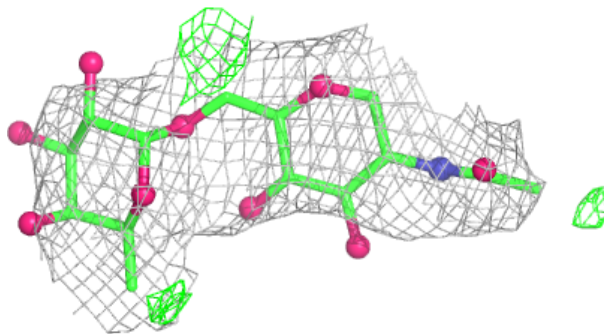
**Electron density around Chain O:**

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



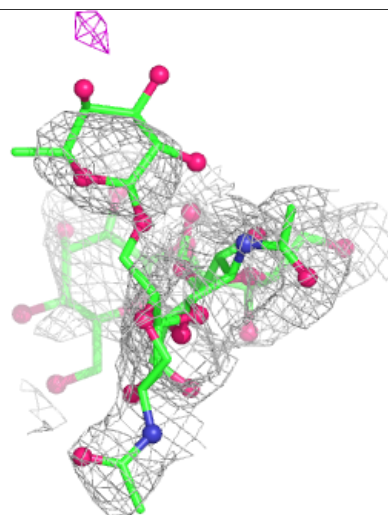
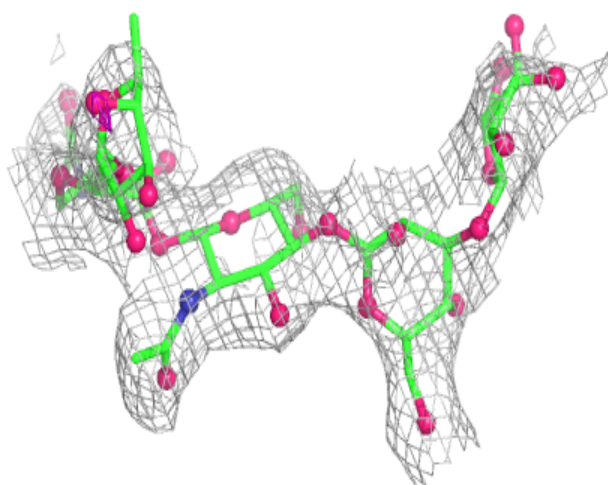
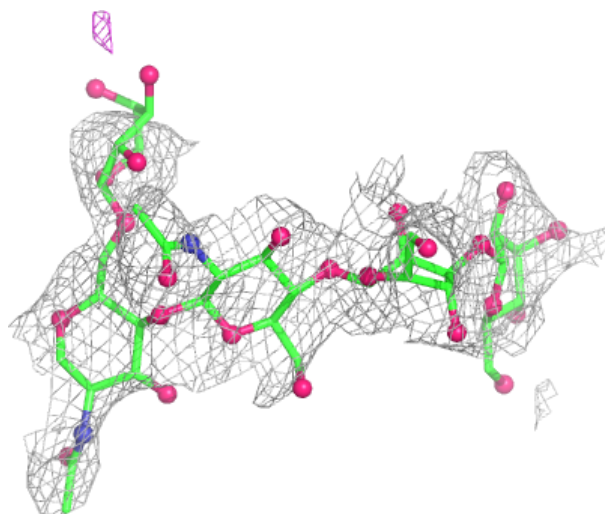
Electron density around Chain P:

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



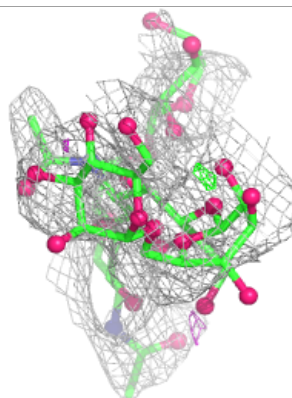
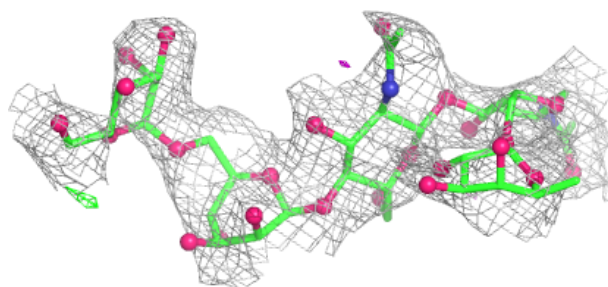
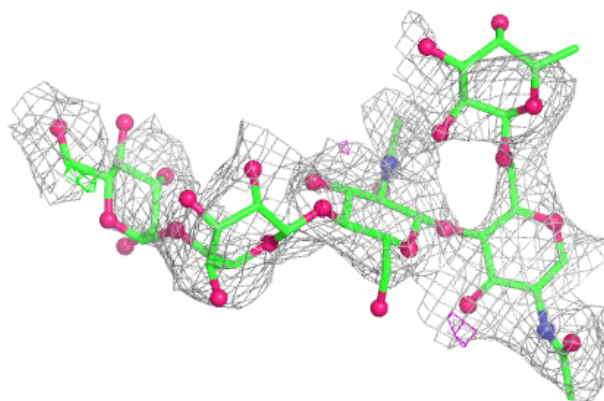
Electron density around Chain N:

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



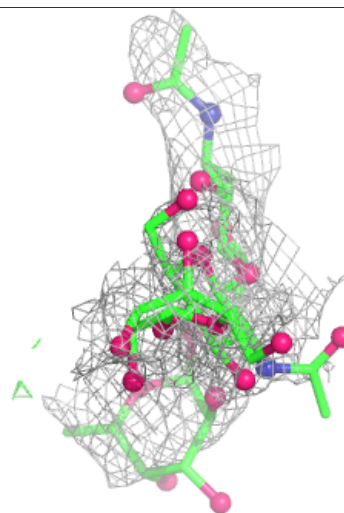
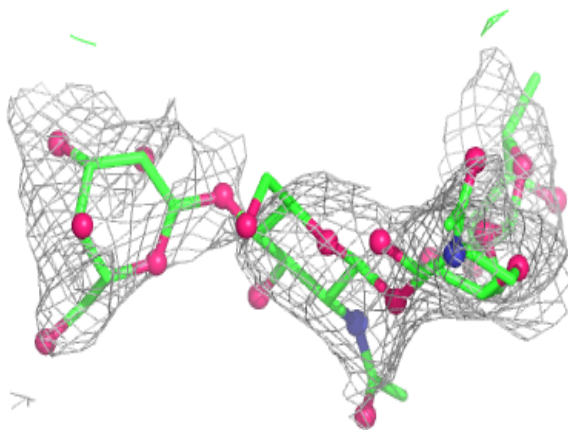
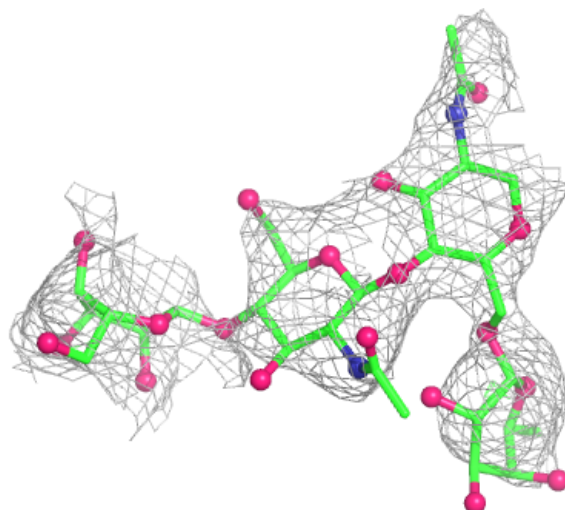
Electron density around Chain Q:

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



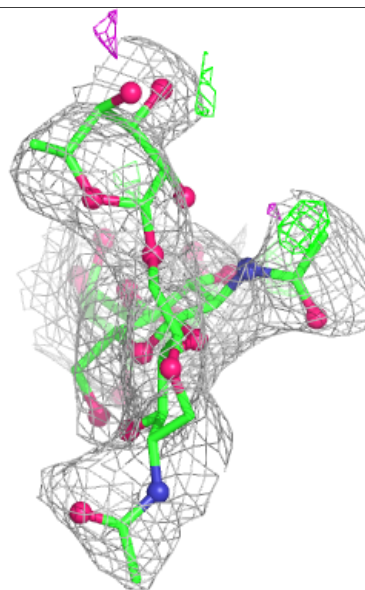
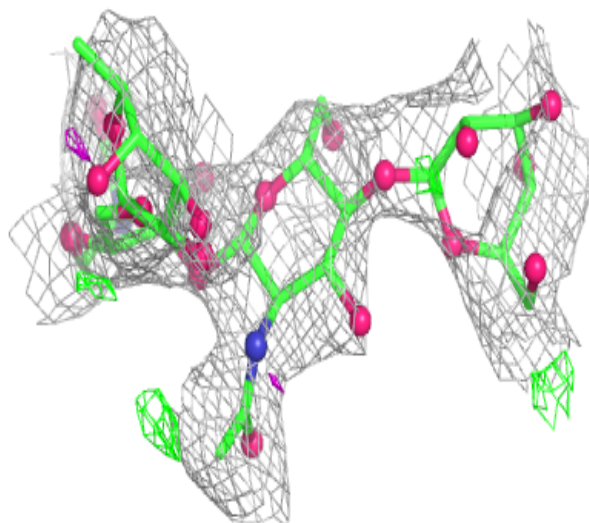
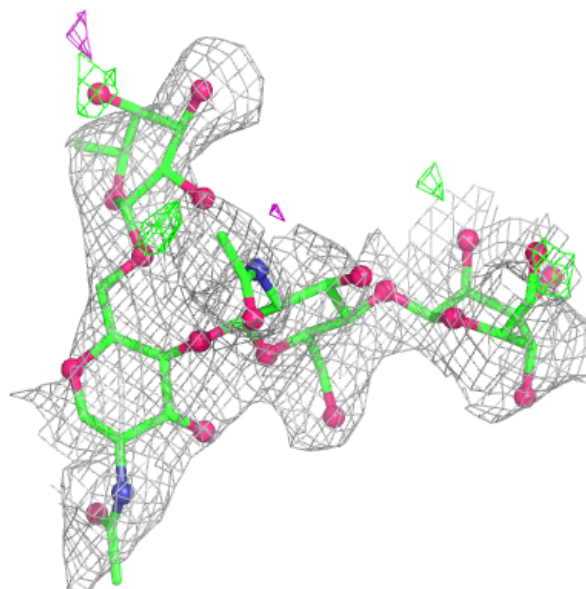
Electron density around Chain R:

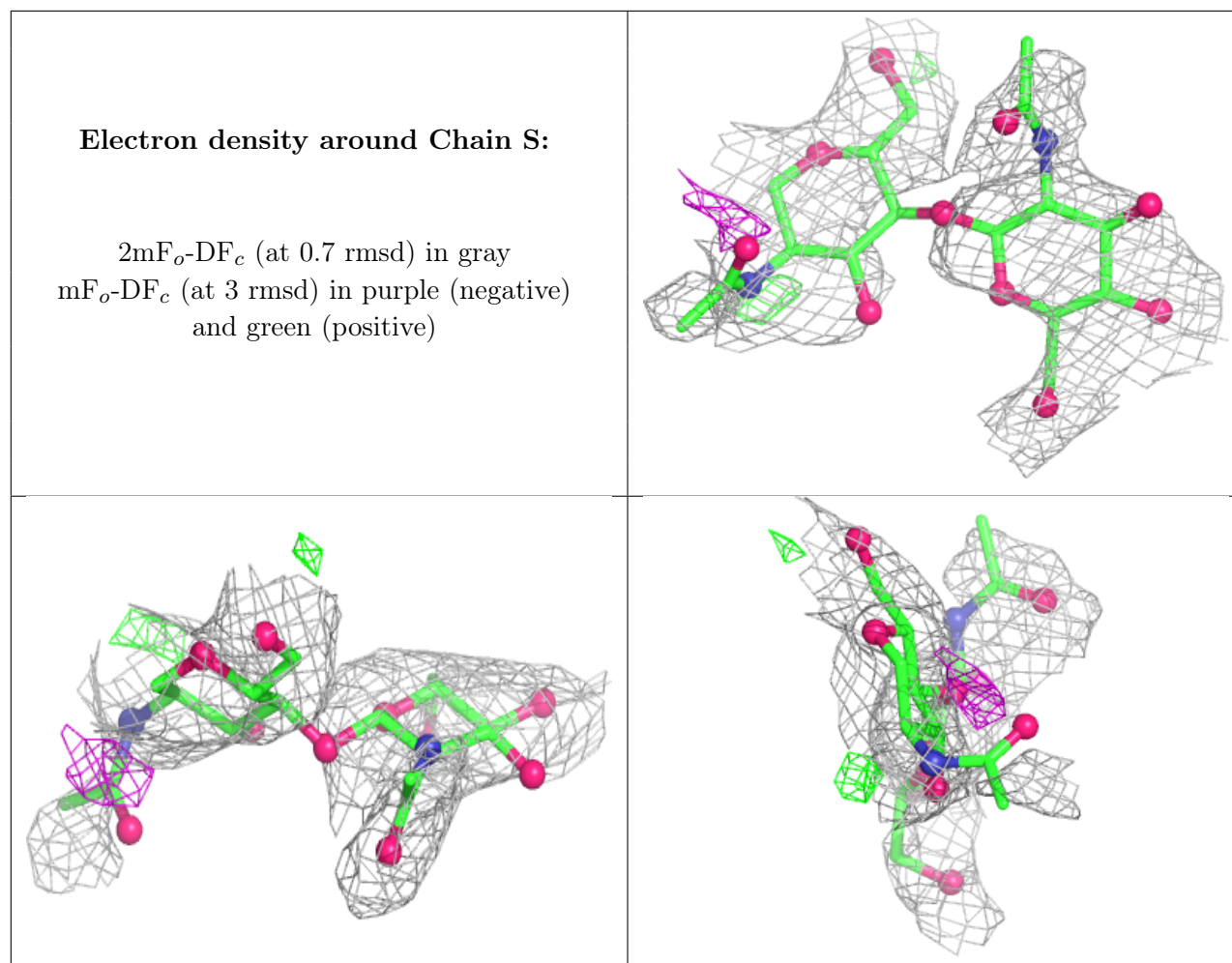
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	L	403	14/15	0.47	0.21	79,90,101,112	0
9	NAG	K	402	14/15	0.60	0.20	51,65,81,88	0
9	NAG	J	401	14/15	0.64	0.16	58,73,80,80	0
9	NAG	I	401	14/15	0.66	0.19	61,82,105,108	0
9	NAG	J	404	14/15	0.66	0.19	69,87,108,110	0
9	NAG	I	402	14/15	0.66	0.19	75,90,103,104	0
9	NAG	J	402	14/15	0.71	0.18	36,67,82,96	0
9	NAG	J	403	14/15	0.75	0.15	48,62,73,74	0
9	NAG	L	401	14/15	0.79	0.14	44,72,89,90	0
9	NAG	K	401	14/15	0.81	0.11	30,43,61,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	L	402	14/15	0.84	0.14	30,48,58,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.