



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:31 PM BST

PDB ID : 6GRT
Title : Paired immunoglobulin-like receptor B (PirB) or Leukocyte immunoglobulin-like receptor subfamily B member 3 (LILRB3) full extracellular domain
Authors : Vlieg, H.C.; Huizinga, E.G.; Janssen, B.J.C.
Deposited on : 2018-06-12
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

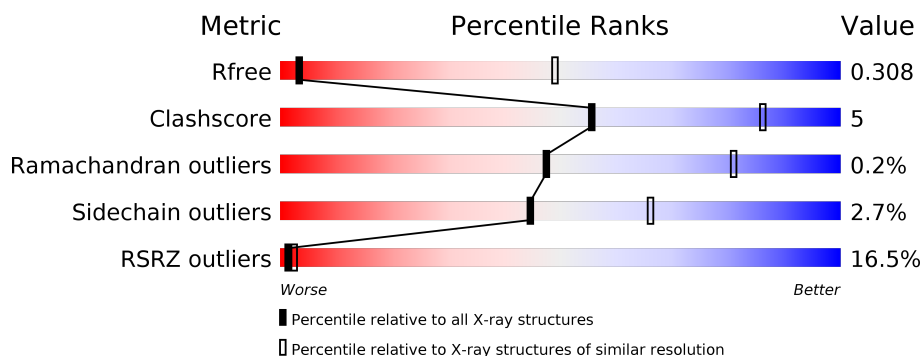
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	606	<div> <div>15%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	606	<div> <div>18%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	C	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	D	5	<div> <div>20%</div> <div>80%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	D	4	-	-	-	X
4	NAG	B	701	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9436 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 Paired immunoglobulin-like receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4652	2943	791	897	21			
1	B	594	Total	C	N	O	S	0	0	0
			4656	2945	792	898	21			

There are 22 discrepancies between the modelled and reference sequences:

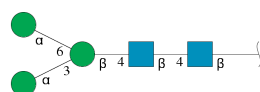
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q8K4V6
A	24	SER	-	expression tag	UNP Q8K4V6
A	620	ALA	-	expression tag	UNP Q8K4V6
A	621	ALA	-	expression tag	UNP Q8K4V6
A	622	ALA	-	expression tag	UNP Q8K4V6
A	623	HIS	-	expression tag	UNP Q8K4V6
A	624	HIS	-	expression tag	UNP Q8K4V6
A	625	HIS	-	expression tag	UNP Q8K4V6
A	626	HIS	-	expression tag	UNP Q8K4V6
A	627	HIS	-	expression tag	UNP Q8K4V6
A	628	HIS	-	expression tag	UNP Q8K4V6
B	23	GLY	-	expression tag	UNP Q8K4V6
B	24	SER	-	expression tag	UNP Q8K4V6
B	620	ALA	-	expression tag	UNP Q8K4V6
B	621	ALA	-	expression tag	UNP Q8K4V6
B	622	ALA	-	expression tag	UNP Q8K4V6
B	623	HIS	-	expression tag	UNP Q8K4V6
B	624	HIS	-	expression tag	UNP Q8K4V6
B	625	HIS	-	expression tag	UNP Q8K4V6
B	626	HIS	-	expression tag	UNP Q8K4V6
B	627	HIS	-	expression tag	UNP Q8K4V6
B	628	HIS	-	expression tag	UNP Q8K4V6

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



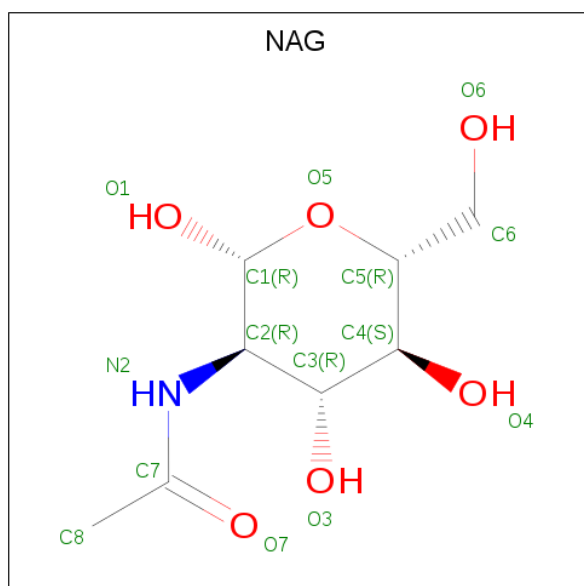
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

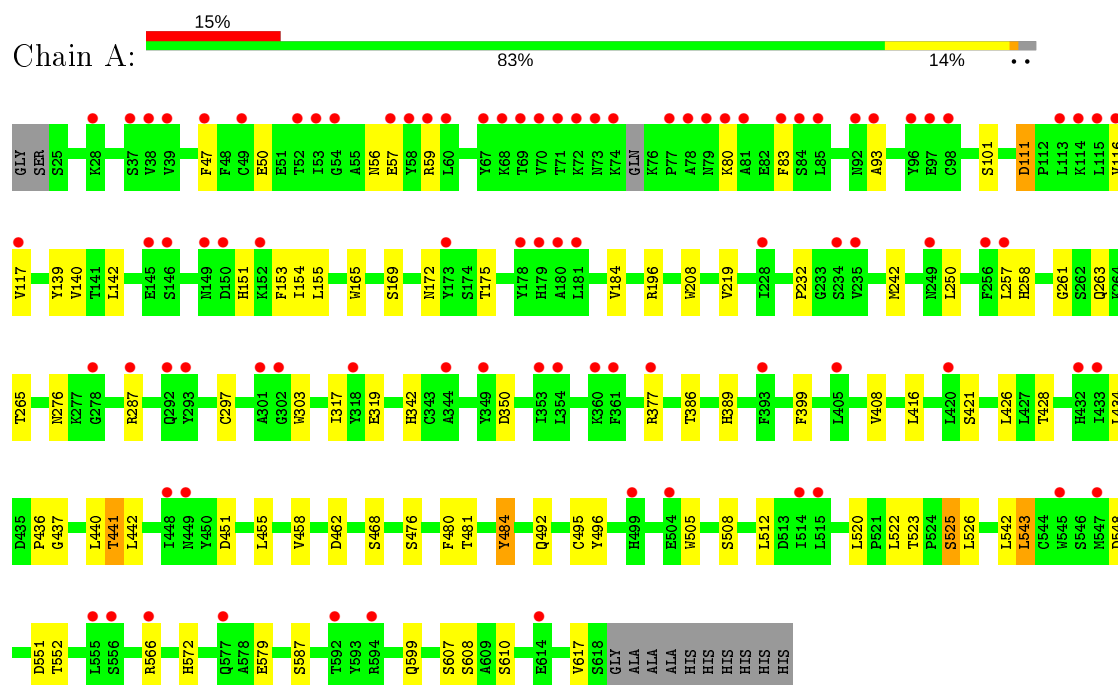


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

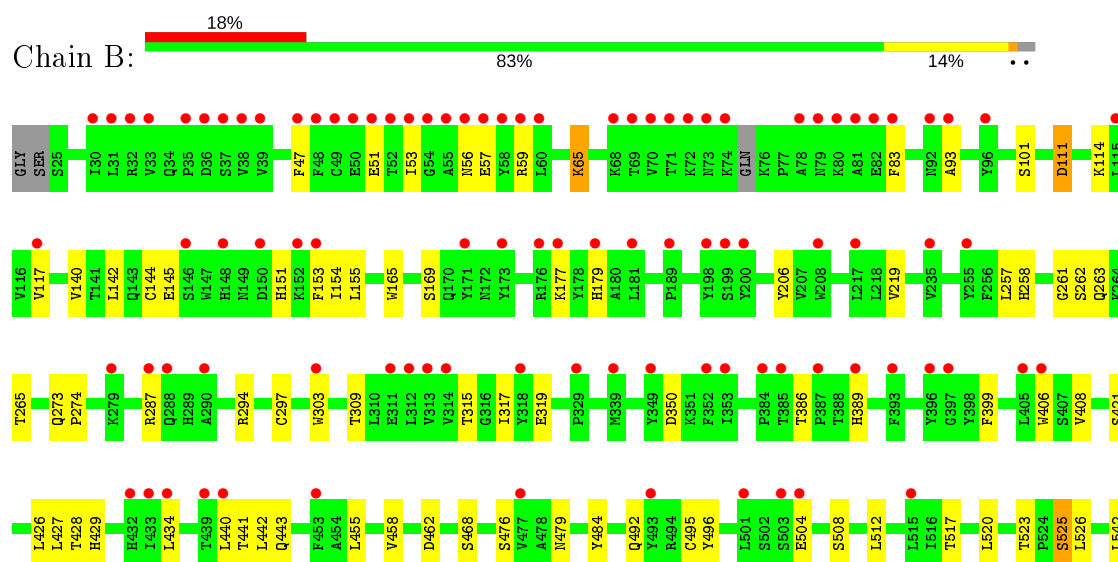
3 Residue-property plots

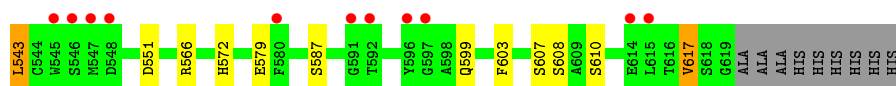
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Paired immunoglobulin-like receptor B



• Molecule 1: Paired immunoglobulin-like receptor B





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.25Å 127.10Å 144.08Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	70.07 – 4.50 70.07 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (70.07-4.50) 98.2 (70.07-4.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 4.46Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.259 , 0.307 0.259 , 0.308	Depositor DCC
R_{free} test set	690 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	162.5	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 329.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9436	wwPDB-VP
Average B, all atoms (Å ²)	224.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.24	0/4778	0.46	0/6498
1	B	0.24	0/4782	0.46	0/6503
All	All	0.24	0/9560	0.46	0/13001

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	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	4652	0	4498	45	0
1	B	4656	0	4501	48	0
2	C	39	0	34	2	0
3	D	61	0	52	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
All	All	9436	0	9111	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG22	1:B:608:SER:HB2	1.76	0.67
1:A:523:THR:HG22	1:A:608:SER:HB2	1.76	0.66
1:B:294:ARG:HE	1:B:309:THR:HG22	1.61	0.64
1:B:111:ASP:N	1:B:111:ASP:OD1	2.30	0.64
1:A:434:LEU:HD11	1:A:440:LEU:HD13	1.81	0.63
1:B:350:ASP:HB2	1:B:399:PHE:HA	1.81	0.63
1:B:434:LEU:HD11	1:B:440:LEU:HD13	1.82	0.62
1:B:566:ARG:NH2	1:B:603:PHE:O	2.33	0.61
1:A:350:ASP:HB2	1:A:399:PHE:HA	1.82	0.61
1:B:257:LEU:HG	1:B:265:THR:HB	1.83	0.61
1:A:257:LEU:HG	1:A:265:THR:HB	1.85	0.59
1:A:111:ASP:N	1:A:111:ASP:OD1	2.31	0.58
1:A:551:ASP:HB2	1:A:599:GLN:HA	1.88	0.56
1:B:59:ARG:NH1	1:B:101:SER:OG	2.30	0.56
1:A:552:THR:HG21	1:A:566:ARG:HH11	1.72	0.55
1:A:56:ASN:HB3	1:A:101:SER:O	2.06	0.55
1:B:51:GLU:HG3	1:B:53:ILE:H	1.72	0.54
1:B:258:HIS:ND1	1:B:263:GLN:O	2.39	0.54
1:A:496:TYR:CE2	1:A:508:SER:HB3	2.43	0.54
1:B:551:ASP:HB2	1:B:599:GLN:HA	1.91	0.53
1:A:587:SER:HA	1:A:617:VAL:HB	1.90	0.53
1:B:56:ASN:HB3	1:B:101:SER:O	2.08	0.53
1:A:154:ILE:HA	1:A:165:TRP:O	2.08	0.53
1:B:587:SER:HA	1:B:617:VAL:HB	1.91	0.53
1:A:59:ARG:NH1	1:A:101:SER:OG	2.33	0.52
1:A:543:LEU:HG	1:A:579:GLU:HG2	1.92	0.52
1:B:543:LEU:HG	1:B:579:GLU:HG2	1.93	0.51
1:B:525:SER:HA	1:B:610:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:VAL:HB	1:B:492:GLN:HB3	1.93	0.51
1:A:142:LEU:HD12	1:A:155:LEU:HD21	1.93	0.51
1:B:154:ILE:HA	1:B:165:TRP:O	2.09	0.50
1:B:496:TYR:CE2	1:B:508:SER:HB3	2.46	0.50
1:A:520:LEU:HB2	1:A:607:SER:HA	1.94	0.49
1:B:144:CYS:HB3	1:B:179:HIS:CE1	2.47	0.49
1:A:232:PRO:HG2	1:A:242:MET:HA	1.93	0.49
1:B:427:LEU:HB2	1:B:443:GLN:HB3	1.94	0.49
1:A:458:VAL:HB	1:A:492:GLN:HB3	1.94	0.48
1:B:144:CYS:HB3	1:B:179:HIS:NE2	2.28	0.48
1:A:525:SER:HA	1:A:610:SER:HB2	1.95	0.48
1:B:145:GLU:OE2	1:B:177:LYS:HD3	2.14	0.48
1:B:520:LEU:HB2	1:B:607:SER:HA	1.96	0.47
1:B:526:LEU:HD11	1:B:542:LEU:HD13	1.96	0.47
1:A:552:THR:HG21	1:A:566:ARG:NH1	2.30	0.47
2:C:1:NAG:H4	2:C:2:NAG:C7	2.45	0.47
1:A:441:THR:HG22	1:A:481:THR:HA	1.96	0.46
1:A:526:LEU:HD11	1:A:542:LEU:HD13	1.98	0.46
1:A:47:PHE:HB2	1:A:83:PHE:HB2	1.98	0.46
1:B:261:GLY:HA2	1:B:262:SER:HB2	1.97	0.45
1:B:429:HIS:CE1	3:D:1:NAG:H62	2.52	0.45
1:B:386:THR:H	1:B:389:HIS:CE1	2.35	0.45
1:B:47:PHE:HB2	1:B:83:PHE:HB2	1.99	0.45
1:B:93:ALA:HB2	1:B:117:VAL:HG23	1.99	0.45
1:B:468:SER:HB2	1:B:476:SER:HB3	1.99	0.45
1:B:428:THR:HG22	1:B:512:LEU:HD22	1.99	0.45
1:A:468:SER:HB2	1:A:476:SER:HB3	1.98	0.44
1:A:116:VAL:HG11	1:A:208:TRP:CD2	2.53	0.44
2:C:1:NAG:H4	2:C:2:NAG:N2	2.33	0.44
1:A:436:PRO:HA	1:A:437:GLY:HA2	1.59	0.44
1:B:273:GLN:HA	1:B:274:PRO:HA	1.79	0.44
1:A:139:TYR:HA	1:A:184:VAL:O	2.18	0.43
1:A:437:GLY:HA3	1:A:484:TYR:CE2	2.52	0.43
1:B:442:LEU:HD12	1:B:455:LEU:HD21	2.00	0.43
1:A:153:PHE:HE2	1:A:169:SER:HB3	1.83	0.43
1:A:416:LEU:HD11	1:A:505:TRP:CE2	2.54	0.43
1:B:65:LYS:HE2	1:B:65:LYS:HB3	1.86	0.43
1:A:428:THR:HG22	1:A:512:LEU:HD22	2.00	0.43
1:A:57:GLU:HG2	1:A:101:SER:HB2	2.01	0.43
1:B:219:VAL:HB	1:B:303:TRP:CG	2.54	0.43
1:A:386:THR:H	1:A:389:HIS:CE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:HE2	1:B:169:SER:HB3	1.83	0.42
1:B:142:LEU:HD12	1:B:155:LEU:HD21	2.01	0.42
1:A:442:LEU:HD12	1:A:455:LEU:HD21	2.01	0.42
1:A:93:ALA:HB2	1:A:117:VAL:HG23	2.00	0.42
1:B:319:GLU:HA	1:B:408:VAL:CG2	2.49	0.42
1:B:426:LEU:HD21	1:B:495:CYS:HB2	2.01	0.42
1:A:426:LEU:HD21	1:A:495:CYS:HB2	2.01	0.42
1:B:114:LYS:HG2	1:B:206:TYR:HE1	1.84	0.42
1:A:258:HIS:ND1	1:A:263:GLN:O	2.51	0.42
1:A:219:VAL:HB	1:A:303:TRP:CG	2.55	0.42
1:A:250:LEU:HD22	1:A:276:ASN:H	1.84	0.42
1:B:315:THR:HG22	1:B:406:TRP:HB2	2.01	0.42
1:B:443:GLN:HG3	1:B:479:ASN:OD1	2.20	0.41
1:B:51:GLU:OE2	1:B:53:ILE:HG12	2.19	0.41
1:B:93:ALA:HB1	1:B:206:TYR:HB3	2.01	0.41
1:A:342:HIS:NE2	1:A:377:ARG:HG3	2.36	0.41
1:B:59:ARG:HH12	1:B:101:SER:CB	2.31	0.41
1:A:522:LEU:HD22	1:A:548:ASP:OD2	2.21	0.41
1:B:434:LEU:O	1:B:517:THR:HG22	2.21	0.41
1:A:172:ASN:HB2	1:A:175:THR:OG1	2.21	0.40
1:B:57:GLU:HG2	1:B:101:SER:HB2	2.03	0.40
1:A:50:GLU:HG2	1:A:80:LYS:HD3	2.02	0.40
1:A:319:GLU:HA	1:A:408:VAL:CG2	2.52	0.40
1:A:442:LEU:O	1:A:480:PHE:HB2	2.21	0.40
1:B:294:ARG:NE	1:B:309:THR:HG22	2.32	0.40
1:A:155:LEU:HD12	1:A:196:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	589/606 (97%)	544 (92%)	44 (8%)	1 (0%)	47	81
1	B	590/606 (97%)	545 (92%)	44 (8%)	1 (0%)	47	81
All	All	1179/1212 (97%)	1089 (92%)	88 (8%)	2 (0%)	47	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	SER
1	B	421	SER

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	526/534 (98%)	513 (98%)	13 (2%)	47	68
1	B	526/534 (98%)	511 (97%)	15 (3%)	42	64
All	All	1052/1068 (98%)	1024 (97%)	28 (3%)	44	66

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASP
1	A	140	VAL
1	A	151	HIS
1	A	287	ARG
1	A	297	CYS
1	A	317	ILE
1	A	441	THR
1	A	451	ASP
1	A	462	ASP
1	A	484	TYR
1	A	525	SER
1	A	543	LEU
1	A	572	HIS
1	B	65	LYS

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Mol	Chain	Res	Type
1	B	111	ASP
1	B	140	VAL
1	B	151	HIS
1	B	287	ARG
1	B	297	CYS
1	B	317	ILE
1	B	441	THR
1	B	462	ASP
1	B	484	TYR
1	B	504	GLU
1	B	525	SER
1	B	543	LEU
1	B	572	HIS
1	B	617	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.44	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
2	BMA	C	3	2	11,11,12	0.62	0	15,15,17	0.71	0
3	NAG	D	1	1,3	14,14,15	0.36	0	17,19,21	0.61	0
3	NAG	D	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.84	0
3	BMA	D	3	3	11,11,12	0.58	0	15,15,17	0.68	0
3	MAN	D	4	3	11,11,12	0.87	0	15,15,17	0.92	1 (6%)
3	MAN	D	5	3	11,11,12	0.61	0	15,15,17	1.04	2 (13%)

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
2	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

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

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	2.59	115.70	112.19
2	C	2	NAG	C1-O5-C5	2.25	115.24	112.19
3	D	5	MAN	O2-C2-C3	-2.20	105.73	110.14
3	D	4	MAN	O2-C2-C3	-2.06	106.01	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

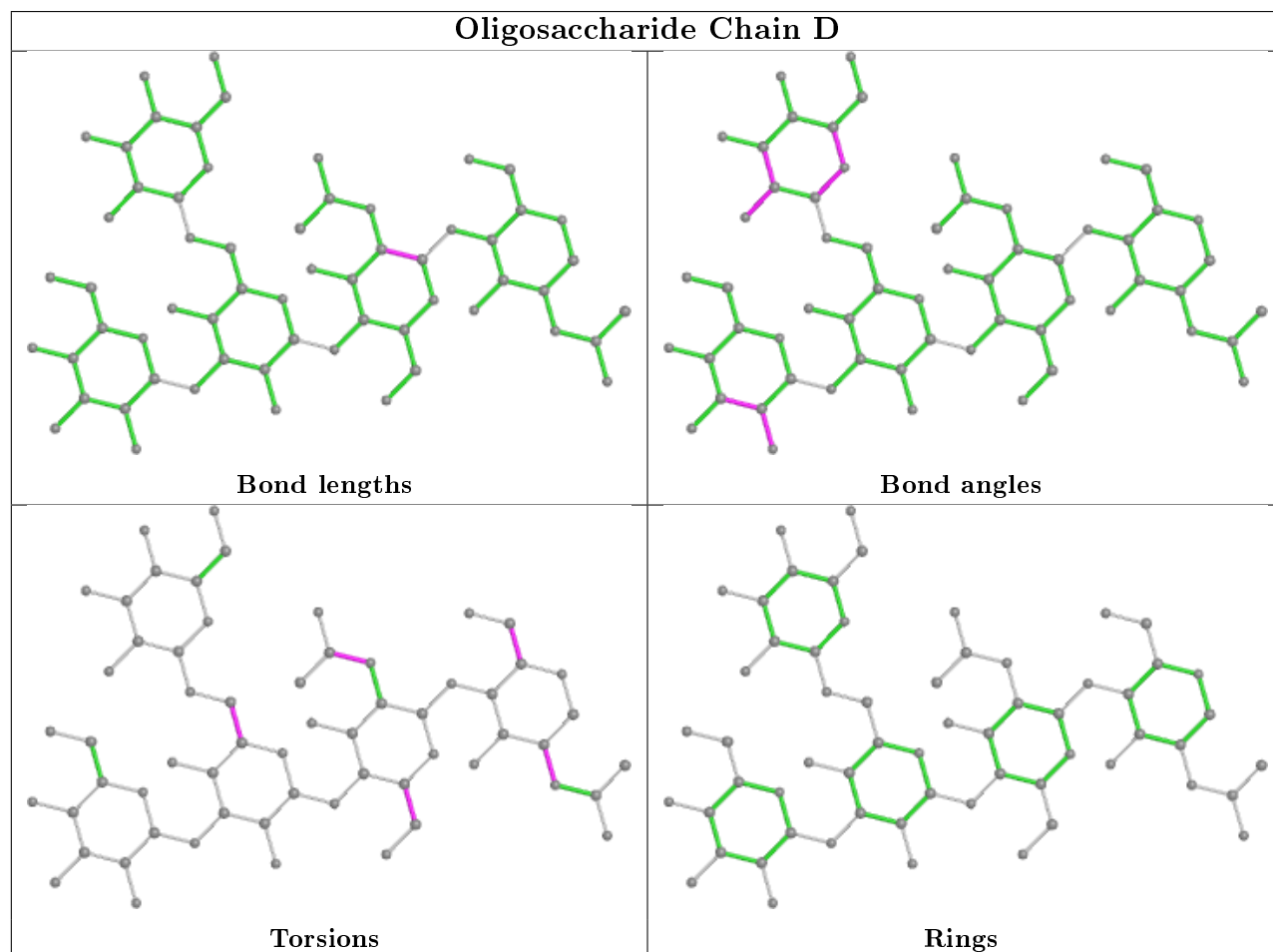
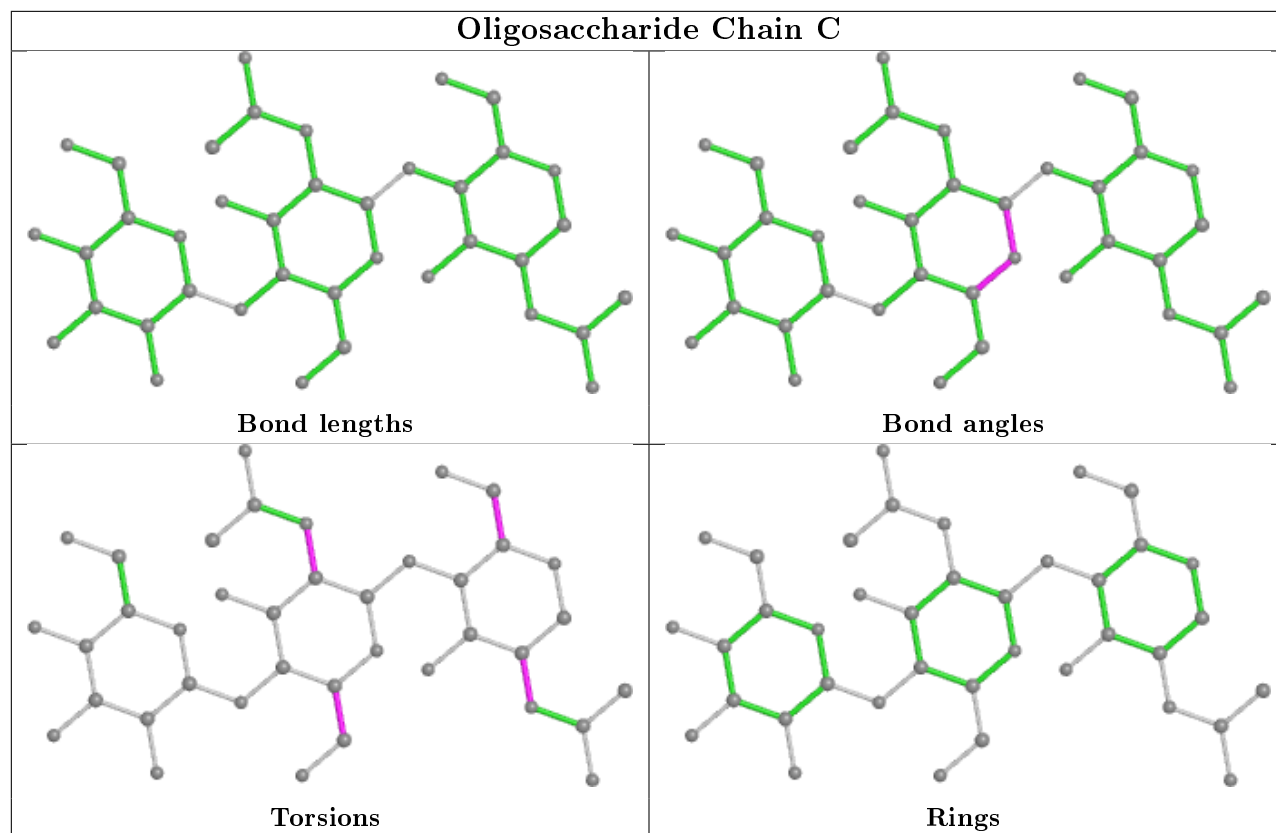
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
3	D	1	NAG	1	0
2	C	2	NAG	2	0

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



5.6 Ligand geometry

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	$\# Z > 2$
4	NAG	A	704	1	14,14,15	0.34	0	17,19,21	1.17	1 (5%)
4	NAG	B	701	1	14,14,15	0.34	0	17,19,21	0.43	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	A	704	1	-	1/6/23/26	0/1/1/1
4	NAG	B	701	1	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
4	A	704	NAG	C2-N2-C7	3.38	127.71	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	593/606 (97%)	0.85	89 (15%) 2 3	150, 216, 285, 312	0
1	B	594/606 (98%)	1.06	107 (18%) 1 2	155, 220, 276, 310	0
All	All	1187/1212 (97%)	0.96	196 (16%) 1 2	150, 218, 281, 312	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	VAL	11.2
1	B	72	LYS	10.5
1	B	71	THR	9.7
1	B	58	TYR	9.2
1	B	50	GLU	8.9
1	B	81	ALA	8.9
1	A	69	THR	8.6
1	B	74	LYS	7.7
1	B	80	LYS	7.3
1	B	49	CYS	7.3
1	B	78	ALA	7.1
1	B	57	GLU	6.9
1	B	69	THR	6.8
1	A	96	TYR	6.8
1	A	84	SER	6.8
1	B	79	ASN	6.6
1	A	59	ARG	6.6
1	B	592	THR	6.3
1	A	114	LYS	6.2
1	B	54	GLY	5.6
1	A	78	ALA	5.6
1	B	504	GLU	5.4
1	B	73	ASN	5.4
1	A	74	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLU	5.3
1	A	146	SER	5.3
1	B	83	PHE	5.0
1	A	115	LEU	4.8
1	B	47	PHE	4.8
1	A	592	THR	4.6
1	A	79	ASN	4.5
1	A	256	PHE	4.5
1	B	55	ALA	4.5
1	A	179	HIS	4.4
1	B	199	SER	4.4
1	A	432	HIS	4.3
1	B	397	GLY	4.3
1	B	53	ILE	4.2
1	B	591	GLY	4.2
1	A	83	PHE	4.1
1	B	48	PHE	3.9
1	B	51	GLU	3.8
1	A	504	GLU	3.8
1	A	180	ALA	3.8
1	A	116	VAL	3.8
1	A	449	ASN	3.7
1	A	54	GLY	3.7
1	B	208	TRP	3.7
1	A	360	LYS	3.7
1	A	555	LEU	3.7
1	B	32	ARG	3.6
1	A	318	TYR	3.6
1	A	70	VAL	3.6
1	A	68	LYS	3.6
1	A	556	SER	3.6
1	B	59	ARG	3.5
1	B	318	TYR	3.5
1	B	287	ARG	3.5
1	B	146	SER	3.5
1	B	82	GLU	3.4
1	A	80	LYS	3.3
1	A	433	ILE	3.3
1	A	145	GLU	3.2
1	B	153	PHE	3.2
1	B	176	ARG	3.2
1	B	181	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	53	ILE	3.2
1	B	432	HIS	3.1
1	B	56	ASN	3.1
1	A	545	TRP	3.1
1	A	85	LEU	3.1
1	B	352	PHE	3.1
1	A	58	TYR	3.1
1	A	57	GLU	3.1
1	A	98	CYS	3.1
1	B	36	ASP	3.0
1	A	354	LEU	3.0
1	B	547	MET	3.0
1	B	198	TYR	3.0
1	B	503	SER	2.9
1	B	179	HIS	2.9
1	A	393	PHE	2.9
1	B	115	LEU	2.9
1	B	329	PRO	2.9
1	B	393	PHE	2.9
1	A	249	ASN	2.9
1	A	235	VAL	2.9
1	A	292	GLN	2.9
1	B	596	TYR	2.9
1	A	73	ASN	2.9
1	A	117	VAL	2.8
1	A	113	LEU	2.8
1	B	433	ILE	2.8
1	B	177	LYS	2.8
1	B	396	TYR	2.8
1	A	149	ASN	2.8
1	A	594	ARG	2.7
1	A	405	LEU	2.7
1	A	566	ARG	2.7
1	B	312	LEU	2.7
1	A	178	TYR	2.7
1	B	339	MET	2.7
1	B	615	LEU	2.7
1	A	28	LYS	2.7
1	A	515	LEU	2.7
1	A	234	SER	2.7
1	B	96	TYR	2.7
1	A	420	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	448	ILE	2.6
1	A	228	ILE	2.6
1	B	548	ASP	2.6
1	B	68	LYS	2.6
1	B	60	LEU	2.6
1	B	313	VAL	2.6
1	B	39	VAL	2.6
1	B	152	LYS	2.6
1	A	361	PHE	2.5
1	B	37	SER	2.5
1	A	181	LEU	2.5
1	A	47	PHE	2.5
1	A	37	SER	2.5
1	A	301	ALA	2.5
1	B	614	GLU	2.5
1	B	173	TYR	2.5
1	B	171	TYR	2.5
1	B	453	PHE	2.5
1	B	288	GLN	2.5
1	B	52	THR	2.5
1	A	499	HIS	2.4
1	B	477	VAL	2.4
1	B	493	TYR	2.4
1	A	38	VAL	2.4
1	A	349	TYR	2.4
1	A	150	ASP	2.4
1	B	92	ASN	2.4
1	A	52	THR	2.4
1	A	614	GLU	2.4
1	B	314	VAL	2.4
1	B	434	LEU	2.4
1	A	547	MET	2.4
1	A	92	ASN	2.4
1	B	545	TRP	2.4
1	A	377	ARG	2.4
1	B	38	VAL	2.4
1	B	385	THR	2.4
1	B	580	PHE	2.3
1	B	349	TYR	2.3
1	B	389	HIS	2.3
1	B	501	LEU	2.3
1	B	303	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	439	THR	2.3
1	A	293	TYR	2.3
1	B	515	LEU	2.3
1	A	67	TYR	2.3
1	A	77	PRO	2.3
1	B	387	PRO	2.3
1	B	31	LEU	2.3
1	B	93	ALA	2.3
1	B	189	PRO	2.3
1	A	577	GLN	2.3
1	A	60	LEU	2.3
1	B	353	ILE	2.3
1	B	311	GLU	2.2
1	A	278	GLY	2.2
1	B	597	GLY	2.2
1	A	257	LEU	2.2
1	A	353	ILE	2.2
1	A	72	LYS	2.2
1	B	546	SER	2.2
1	B	405	LEU	2.2
1	B	35	PRO	2.2
1	A	152	LYS	2.2
1	A	93	ALA	2.1
1	A	302	GLY	2.1
1	A	39	VAL	2.1
1	A	71	THR	2.1
1	A	81	ALA	2.1
1	B	406	TRP	2.1
1	A	49	CYS	2.1
1	B	235	VAL	2.1
1	B	279	LYS	2.1
1	B	217	LEU	2.1
1	A	514	ILE	2.1
1	B	30	ILE	2.1
1	B	150	ASP	2.1
1	B	255	TYR	2.1
1	B	117	VAL	2.1
1	B	33	VAL	2.0
1	B	290	ALA	2.0
1	B	440	LEU	2.0
1	A	287	ARG	2.0
1	B	384	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	173	TYR	2.0
1	B	148	HIS	2.0
1	A	344	ALA	2.0
1	B	200	TYR	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](#)

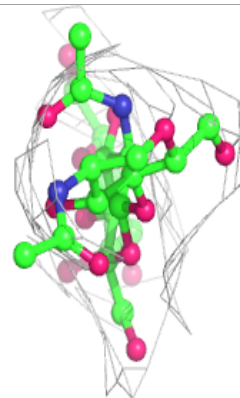
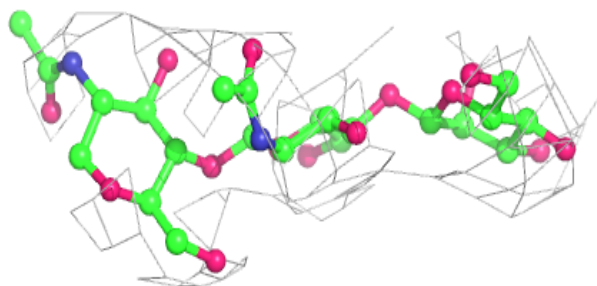
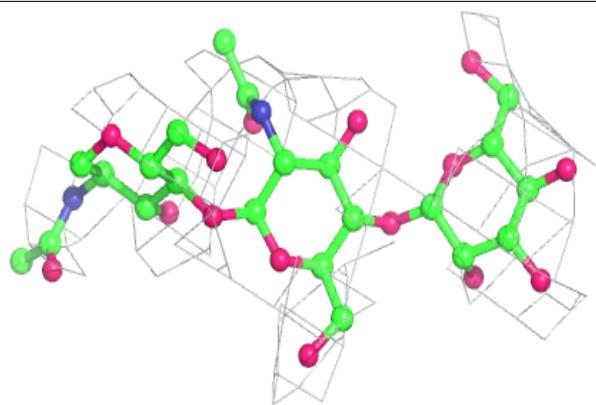
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

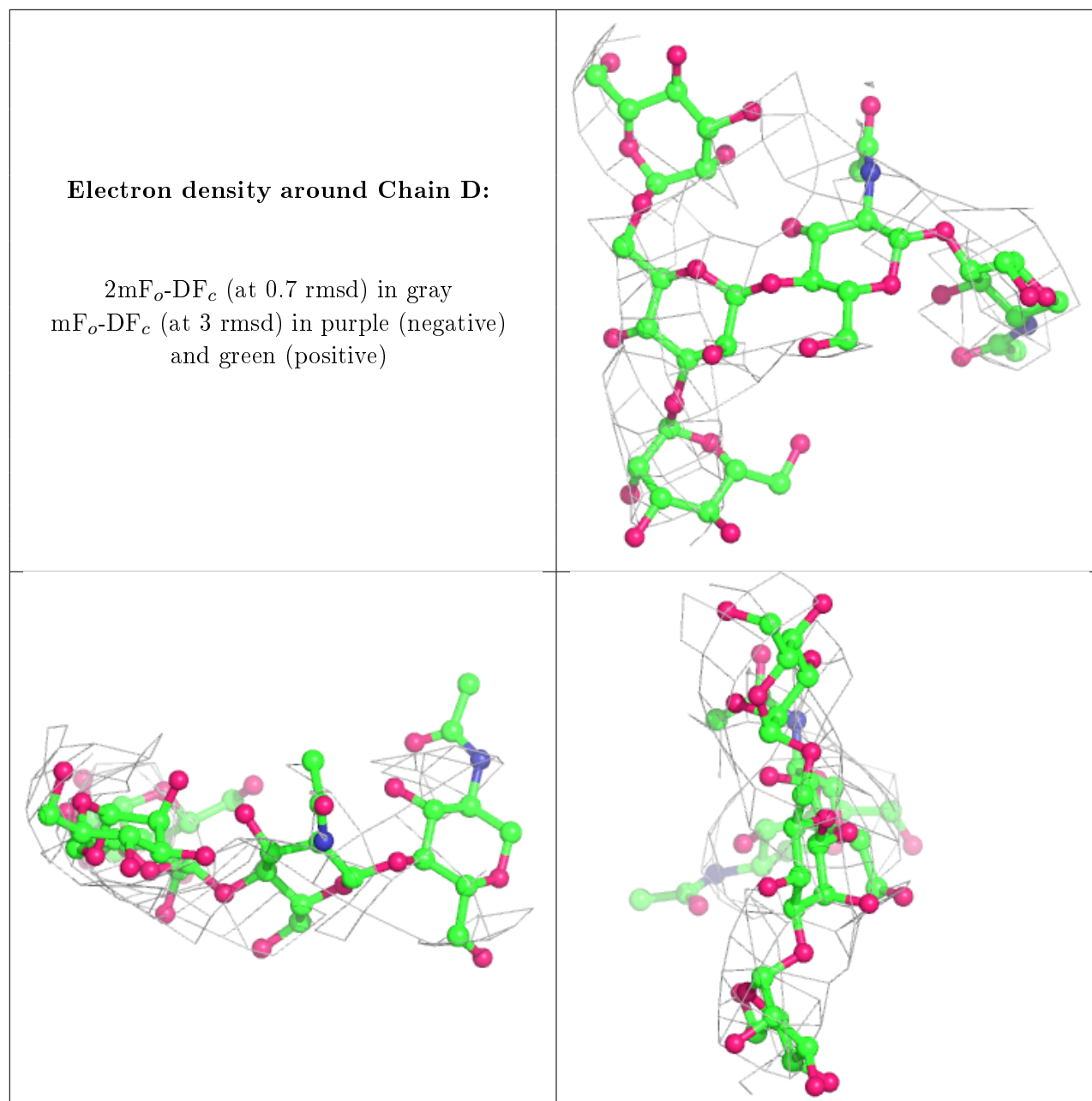
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	D	5	11/12	0.62	0.24	246,273,287,289	0
2	BMA	C	3	11/12	0.67	0.26	199,265,280,280	0
3	MAN	D	4	11/12	0.75	0.66	241,281,293,303	0
3	NAG	D	2	14/15	0.82	0.33	229,268,284,284	0
3	BMA	D	3	11/12	0.82	0.33	263,276,292,379	0
3	NAG	D	1	14/15	0.83	0.42	234,251,281,298	0
2	NAG	C	2	14/15	0.84	0.18	222,260,271,274	0
2	NAG	C	1	14/15	0.89	0.27	241,259,264,269	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 C:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
4	NAG	B	701	14/15	0.68	1.53	229,256,266,271	0
4	NAG	A	704	14/15	0.72	0.29	175,243,256,258	0

6.5 Other polymers

There are no such residues in this entry.