



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 AM UTC

PDB ID : 6GRT / pdb_00006grt
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 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

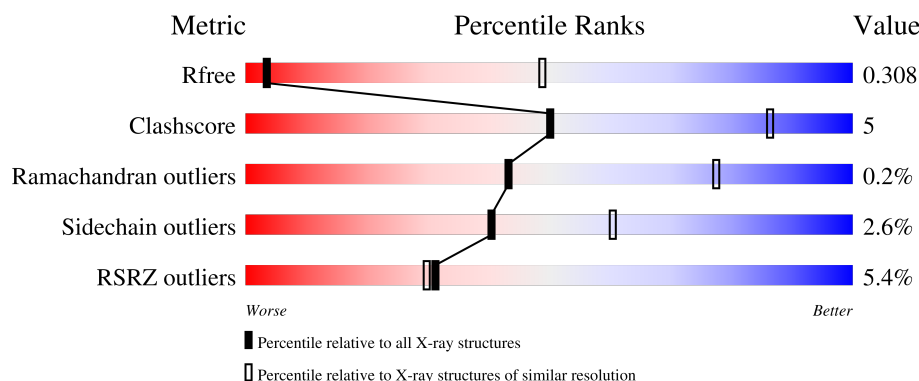
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	606	5% 83% 15% ..
1	B	606	6% 83% 14% ..
2	C	3	33% 33% 33%
3	D	5	40% 60%

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.

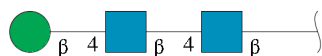
- Molecule 1 is a protein called Paired immunoglobulin-like receptor B.

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:

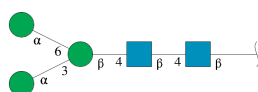
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q8K4V6
A	24	SER	-	expression tag	UNP Q8K4V6
A	620	ALA	-	expression tag	UNP Q8K4V6
A	621	ALA	-	expression tag	UNP Q8K4V6
A	622	ALA	-	expression tag	UNP Q8K4V6
A	623	HIS	-	expression tag	UNP Q8K4V6
A	624	HIS	-	expression tag	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.



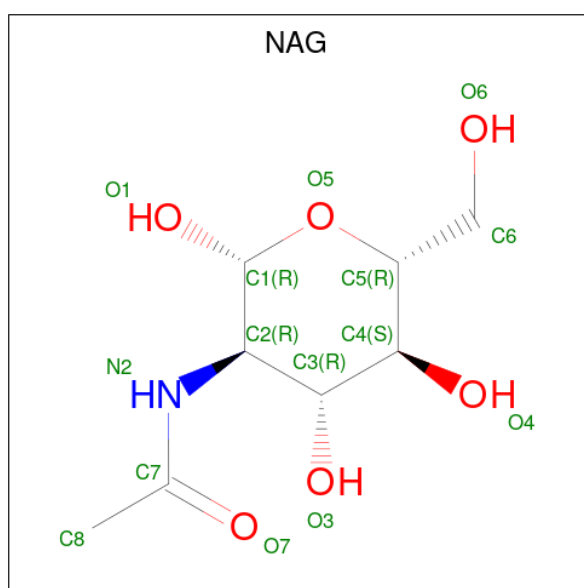
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

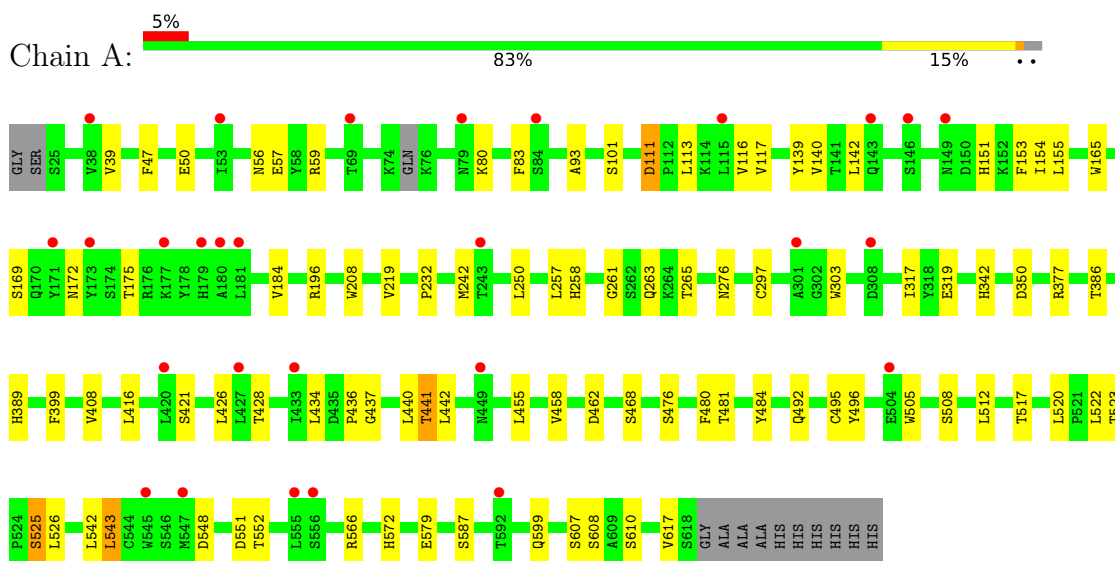


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

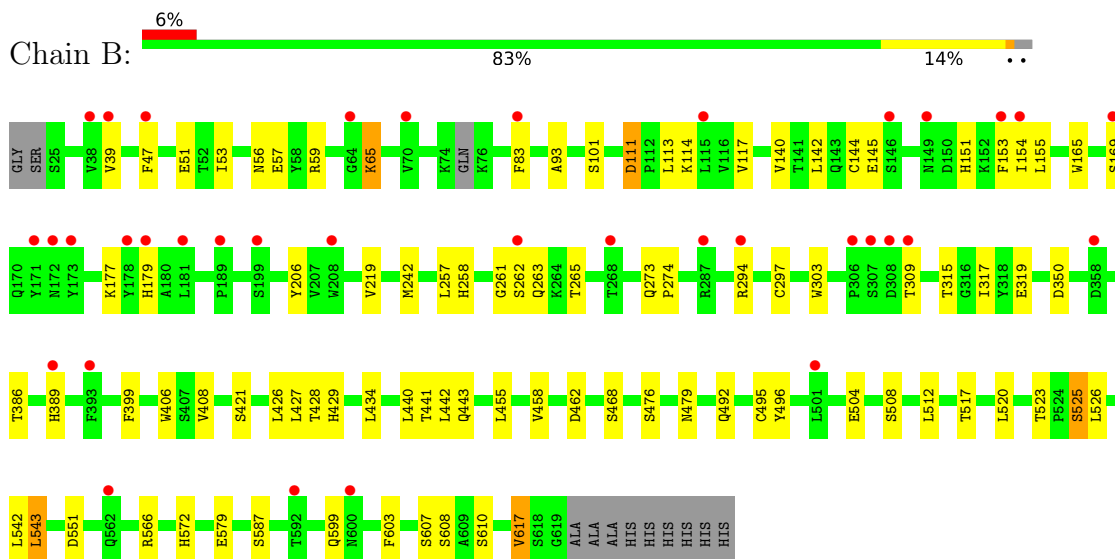
3 Residue-property plots [i](#)

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: 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

Chain C:  33% 33% 33%



● Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain D:  40% 60%



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) 98.5 (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 0.261 , 0.308	Depositor DCC
R_{free} test set	691 reflections (4.91%)	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 , 336.0	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

5.1 Standard geometry

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

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	0.11	0/4778	0.34	0/6498
1	B	0.12	0/4782	0.35	0/6503
All	All	0.11	0/9560	0.34	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

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	47	0
1	B	4656	0	4501	49	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	98	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 (98) 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:OD1	1:B:111:ASP:N	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:56:ASN:HB3	1:A:101:SER:O	2.06	0.55
1:A:552:THR:HG21	1:A:566:ARG:HH11	1.72	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:525:SER:HA	1:B:610:SER:HB2	1.93	0.51
1:B:543:LEU:HG	1:B:579:GLU:HG2	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:57:GLU:HG2	1:A:101:SER:HB2	2.01	0.43
1:A:428:THR:HG22	1:A:512:LEU:HD22	2.00	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:B:242:MET:HE3	1:B:242:MET:HB2	1.95	0.42
1:A:93:ALA:HB2	1:A:117:VAL:HG23	2.00	0.42
1:A:442:LEU:HD12	1:A:455:LEU:HD21	2.01	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:242:MET:HE3	1:A:242:MET:HB2	1.96	0.42
1:A:517:THR:OG1	1:A:607:SER:O	2.37	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: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:B:443:GLN:HG3	1:B:479:ASN:OD1	2.20	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 ⓘ

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	589/606 (97%)	544 (92%)	44 (8%)	1 (0%)	43 77
1	B	590/606 (97%)	545 (92%)	44 (8%)	1 (0%)	43 77
All	All	1179/1212 (97%)	1089 (92%)	88 (8%)	2 (0%)	43 77

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%)	514 (98%)	12 (2%)	44 63
1	B	526/534 (98%)	511 (97%)	15 (3%)	37 58
All	All	1052/1068 (98%)	1025 (97%)	27 (3%)	40 60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	111	ASP
1	A	113	LEU
1	A	140	VAL
1	A	151	HIS
1	A	297	CYS
1	A	317	ILE
1	A	441	THR
1	A	462	ASP
1	A	525	SER
1	A	543	LEU
1	A	572	HIS
1	B	39	VAL
1	B	65	LYS

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Mol	Chain	Res	Type
1	B	111	ASP
1	B	113	LEU
1	B	140	VAL
1	B	151	HIS
1	B	297	CYS
1	B	317	ILE
1	B	441	THR
1	B	462	ASP
1	B	504	GLU
1	B	525	SER
1	B	543	LEU
1	B	572	HIS
1	B	617	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	143	GLN
1	A	149	ASN
1	A	369	HIS
1	A	456	HIS
1	A	469	GLN
1	A	492	GLN
1	B	120	HIS
1	B	149	ASN
1	B	369	HIS
1	B	456	HIS
1	B	492	GLN

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	0.42	0	17,19,21	0.79	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	0.87	1 (5%)
2	BMA	C	3	2	11,11,12	0.60	0	15,15,17	0.68	0
3	NAG	D	1	3,1	14,14,15	0.34	0	17,19,21	0.63	0
3	NAG	D	2	3	14,14,15	0.78	1 (7%)	17,19,21	0.86	0
3	BMA	D	3	3	11,11,12	0.57	0	15,15,17	0.64	0
3	MAN	D	4	3	11,11,12	0.86	0	15,15,17	0.89	0
3	MAN	D	5	3	11,11,12	0.60	0	15,15,17	1.01	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	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	3/6/23/26	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	2.37	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	2.62	115.70	112.19
2	C	2	NAG	C1-O5-C5	2.28	115.24	112.19
3	D	5	MAN	O2-C2-C3	-2.14	105.73	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

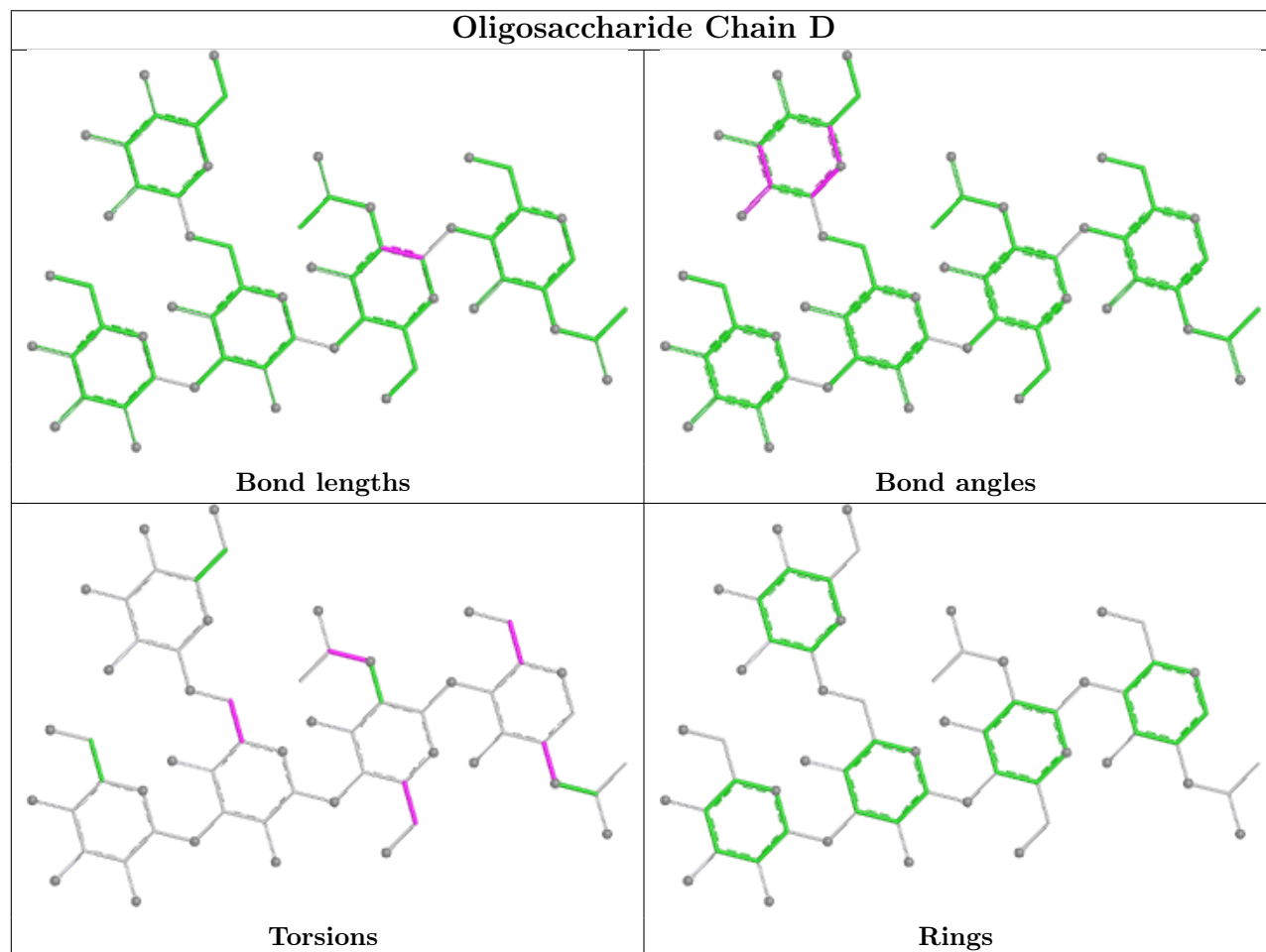
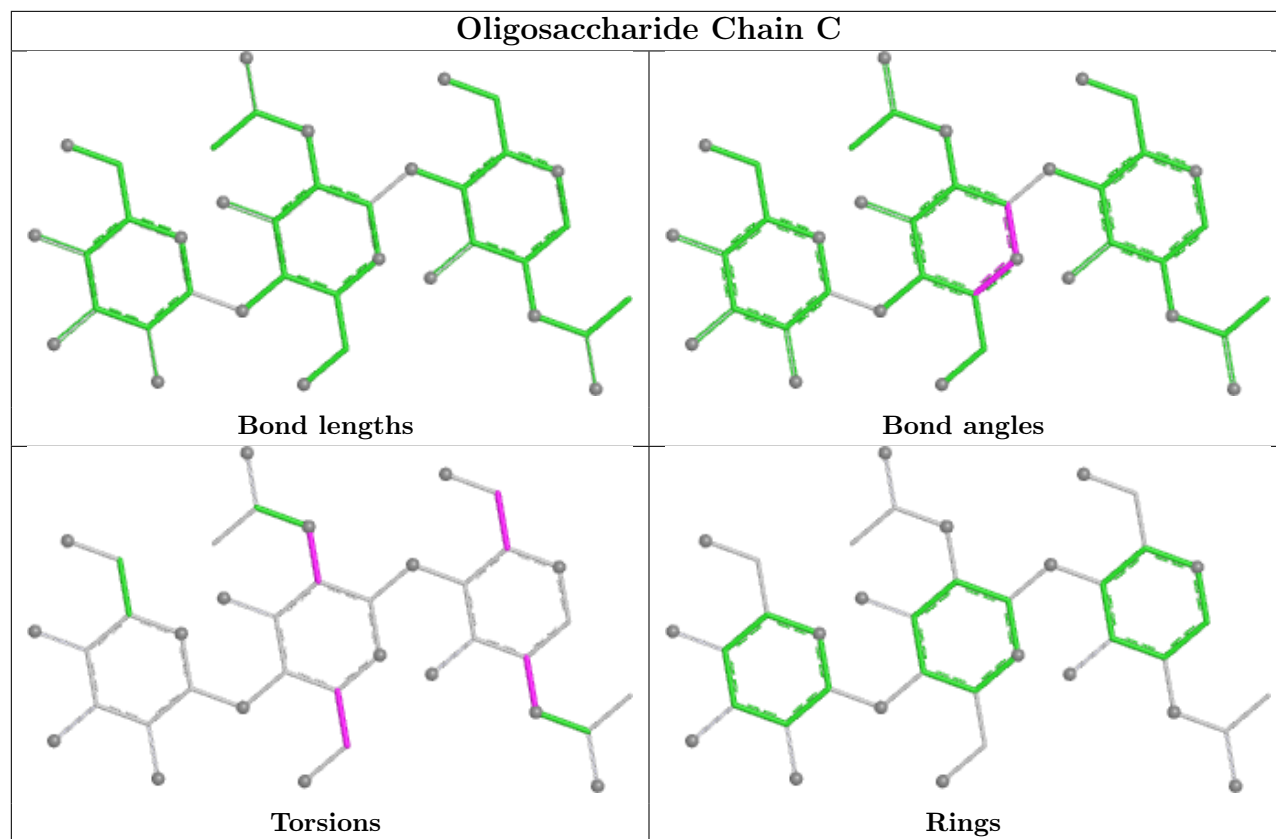
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
3	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
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	1.23	2 (11%)
4	NAG	B	701	1	14,14,15	0.36	0	17,19,21	0.44	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	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C2-N2-C7	3.59	127.71	122.90
4	A	704	NAG	C1-C2-N2	2.05	113.67	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	NAG	C3-C2-N2-C7
4	A	704	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	593/606 (97%)	0.40	28 (4%) 36 33	150, 216, 285, 312	0
1	B	594/606 (98%)	0.56	36 (6%) 27 28	155, 220, 276, 310	0
All	All	1187/1212 (97%)	0.48	64 (5%) 31 30	150, 218, 281, 312	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	TYR	7.6
1	A	173	TYR	5.5
1	A	547	MET	5.5
1	B	592	THR	5.5
1	A	79	ASN	5.2
1	A	592	THR	4.8
1	B	47	PHE	4.8
1	B	308	ASP	4.3
1	B	181	LEU	4.2
1	A	179	HIS	4.2
1	B	208	TRP	3.9
1	A	545	TRP	3.9
1	A	301	ALA	3.6
1	A	433	ILE	3.6
1	B	179	HIS	3.6
1	B	153	PHE	3.5
1	B	199	SER	3.5
1	B	189	PRO	3.3
1	B	178	TYR	3.3
1	B	389	HIS	3.3
1	B	307	SER	3.2
1	B	294	ARG	3.2
1	A	146	SER	3.2
1	A	115	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	501	LEU	3.1
1	B	83	PHE	3.0
1	A	555	LEU	3.0
1	A	504	GLU	2.9
1	A	53	ILE	2.9
1	A	181	LEU	2.9
1	B	146	SER	2.8
1	B	562	GLN	2.8
1	A	449	ASN	2.7
1	B	149	ASN	2.7
1	B	154	ILE	2.6
1	B	169	SER	2.6
1	A	84	SER	2.5
1	B	306	PRO	2.5
1	B	393	PHE	2.5
1	B	64	GLY	2.5
1	A	243	THR	2.4
1	A	38	VAL	2.4
1	A	556	SER	2.4
1	B	600	ASN	2.4
1	B	262	SER	2.4
1	B	287	ARG	2.3
1	A	177	LYS	2.3
1	B	171	TYR	2.3
1	B	309	THR	2.2
1	B	39	VAL	2.2
1	A	143	GLN	2.2
1	B	70	VAL	2.2
1	B	115	LEU	2.2
1	A	427	LEU	2.2
1	A	149	ASN	2.1
1	A	420	LEU	2.1
1	A	69	THR	2.1
1	A	180	ALA	2.1
1	A	308	ASP	2.1
1	B	172	ASN	2.1
1	A	171	TYR	2.1
1	B	38	VAL	2.1
1	B	358	ASP	2.1
1	B	268	THR	2.0

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

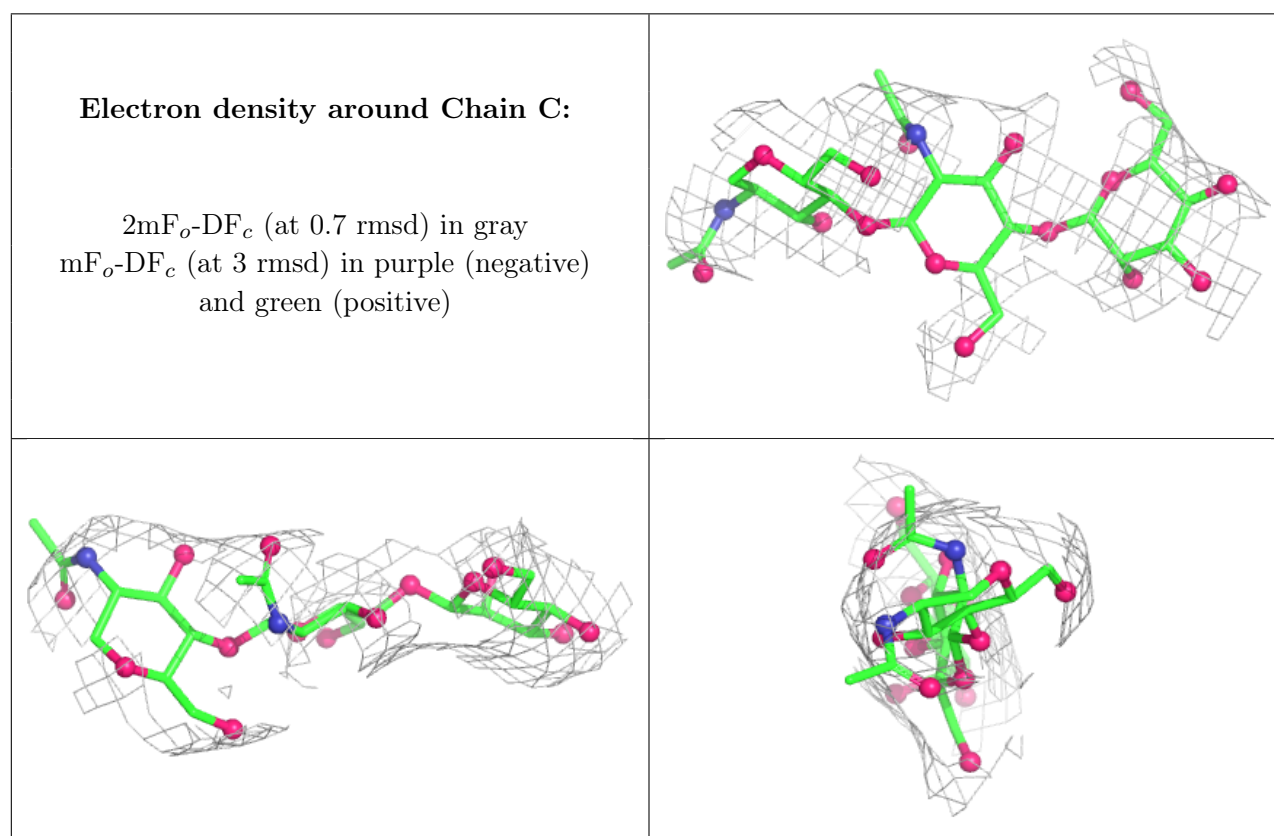
There are no non-standard protein/DNA/RNA residues in this entry.

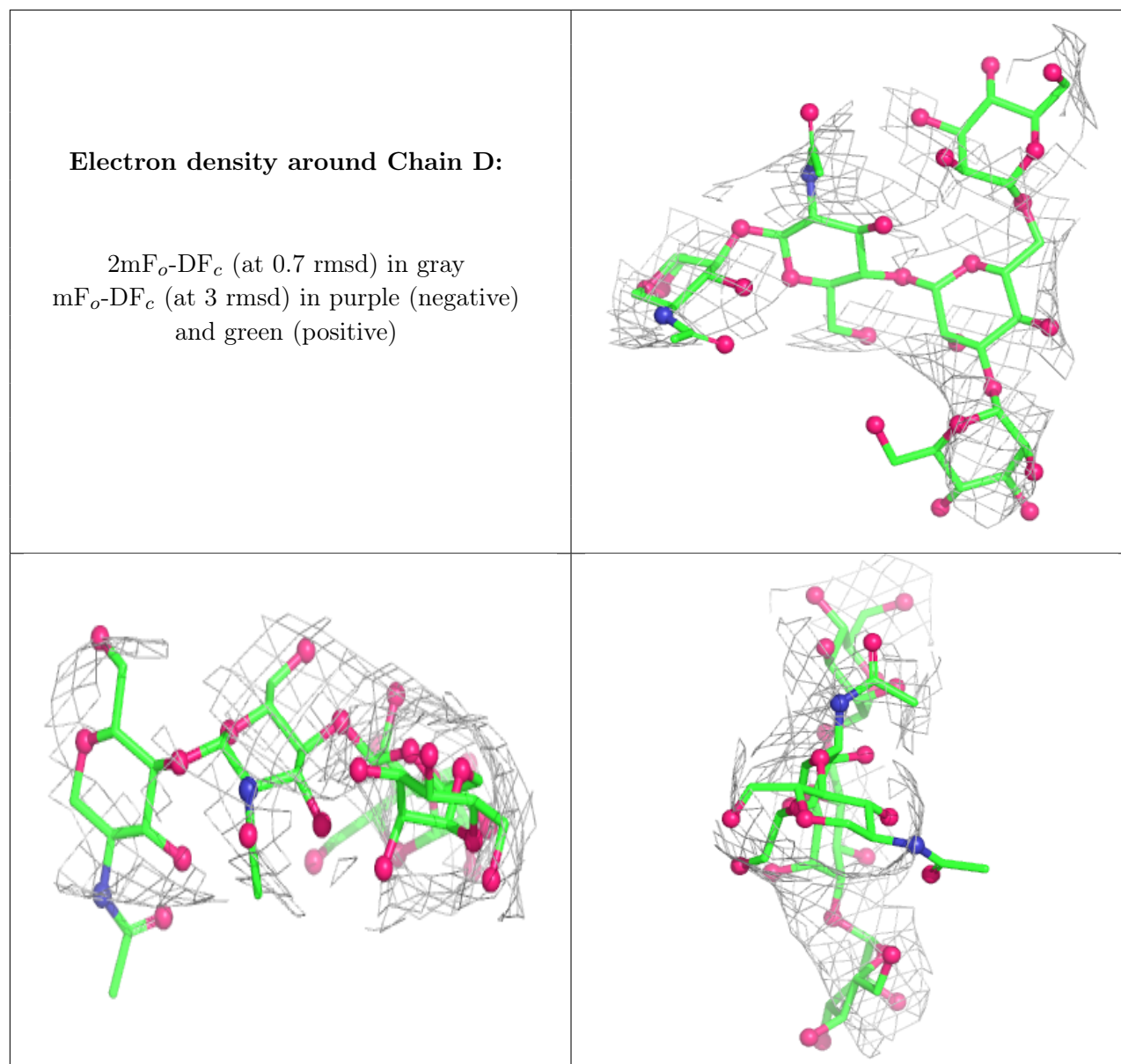
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	MAN	D	5	11/12	0.35	0.13	246,273,287,289	0
2	NAG	C	2	14/15	0.61	0.13	222,260,271,274	0
2	BMA	C	3	11/12	0.68	0.11	199,265,280,280	0
3	NAG	D	2	14/15	0.85	0.11	229,268,284,284	0
3	NAG	D	1	14/15	0.87	0.12	234,251,281,298	0
3	MAN	D	4	11/12	0.88	0.12	241,281,293,303	0
3	BMA	D	3	11/12	0.89	0.08	263,276,292,379	0
2	NAG	C	1	14/15	0.91	0.08	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.





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
4	NAG	B	701	14/15	0.70	0.17	229,256,266,271	0
4	NAG	A	704	14/15	0.79	0.11	175,243,256,258	0

6.5 Other polymers [i](#)

There are no such residues in this entry.