



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:34 PM UTC

PDB ID : 3F6K / pdb_00003f6k
Title : Crystal structure of the Vps10p domain of human sortilin/NTS3 in complex with neurotensin
Authors : Quistgaard, E.M.; Madsen, P.; Groftehauge, M.K.; Nissen, P.; Petersen, C.M.; Thirup, S.
Deposited on : 2008-11-06
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

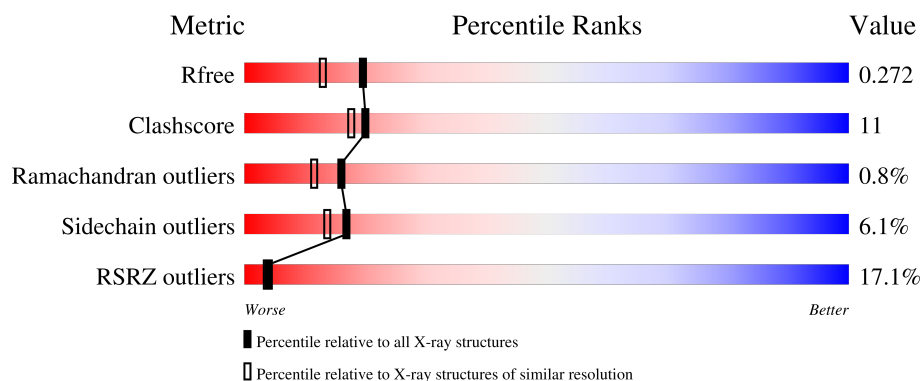
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	685	
2	N	13	
3	B	2	
4	C	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5600 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	0	0
			5176	3268	871	1009	28			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	MET	VAL	variant	UNP Q99523
A	724	HIS	-	expression tag	UNP Q99523
A	725	HIS	-	expression tag	UNP Q99523
A	726	HIS	-	expression tag	UNP Q99523
A	727	HIS	-	expression tag	UNP Q99523
A	728	HIS	-	expression tag	UNP Q99523
A	729	HIS	-	expression tag	UNP Q99523

- Molecule 2 is a protein called Neurotensin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	4	Total	C	N	O	0	0	0
			36	26	4	6			

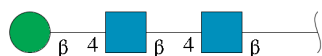
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

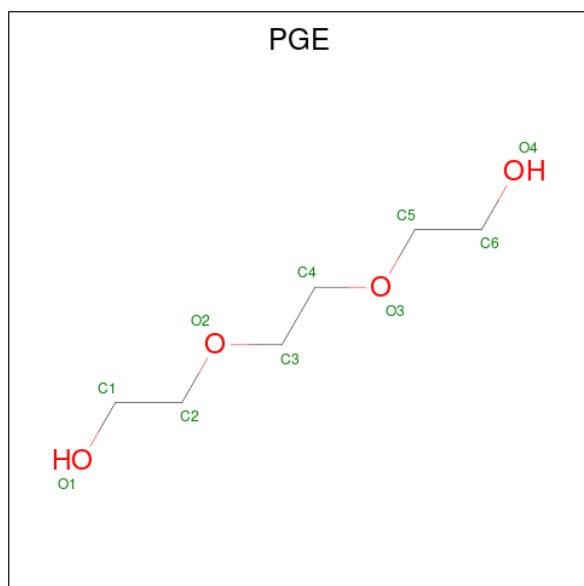
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	304	Total	O	0	0
			304	304		
7	N	1	Total	O	0	0
			1	1		

Chain B:  100%

MAG1
MAG2

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

Chain C:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.76 Å 74.53 Å 108.33 Å 90.00° 131.87° 90.00°	Depositor
Resolution (Å)	40.32 – 2.00 40.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.32-2.00) 97.4 (40.32-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.229 (Not available) , 0.272	Depositor DCC
R_{free} test set	3381 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5600	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, PGE, GOL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	14/5298 (0.3%)	1.12	16/7176 (0.2%)
2	N	0.68	0/37	1.40	1/48 (2.1%)
All	All	1.17	14/5335 (0.3%)	1.12	17/7224 (0.2%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	LEU	N-CA	6.96	1.54	1.45
1	A	372	THR	CA-C	5.91	1.59	1.52
1	A	550	ILE	CA-CB	5.90	1.62	1.54
1	A	698	ARG	CZ-NH1	5.81	1.40	1.32
1	A	606	LYS	CA-C	-5.69	1.46	1.52
1	A	472	VAL	CA-CB	5.49	1.60	1.54
1	A	323	ALA	C-O	5.34	1.30	1.23
1	A	700	VAL	CA-CB	5.24	1.59	1.54
1	A	454	ILE	C-O	-5.22	1.18	1.24
1	A	372	THR	C-O	-5.16	1.18	1.23
1	A	352	VAL	C-O	-5.13	1.18	1.24
1	A	341	GLY	C-O	5.12	1.27	1.23
1	A	456	ILE	CA-CB	5.08	1.61	1.54
1	A	487	GLU	C-O	-5.04	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	ILE	N-CA-C	-8.50	103.55	111.45
1	A	651	ASN	N-CA-C	6.38	118.29	109.29
1	A	441	VAL	CA-C-N	6.26	126.00	119.05
1	A	441	VAL	C-N-CA	6.26	126.00	119.05
1	A	293	ARG	CB-CA-C	-6.20	96.43	110.07
1	A	243	SER	N-CA-C	5.83	123.21	110.80
1	A	448	GLU	CA-C-N	5.72	125.85	119.32
1	A	448	GLU	C-N-CA	5.72	125.85	119.32
1	A	90	VAL	N-CA-C	5.45	116.61	108.54
2	N	11	TYR	CB-CA-C	-5.41	102.73	110.62
1	A	679	THR	N-CA-C	5.23	116.80	108.79
1	A	606	LYS	CB-CA-C	-5.22	100.31	109.71
1	A	379	GLY	CA-C-N	-5.13	116.46	122.93
1	A	379	GLY	C-N-CA	-5.13	116.46	122.93
1	A	289	ASP	N-CA-C	5.13	116.64	108.79
1	A	687	GLY	N-CA-C	-5.07	108.33	115.32
1	A	376	SER	CA-CB-OG	-5.06	100.98	111.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	652	ASP	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	5176	0	4965	117	0
2	N	36	0	38	2	0
3	B	28	0	25	0	0
4	C	39	0	34	0	0
5	A	10	0	14	1	0
6	A	6	0	8	2	0
7	A	304	0	0	10	0
7	N	1	0	0	0	0
All	All	5600	0	5084	117	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 11.

All (117) 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:A:648:ARG:HD2	1:A:653:SER:HA	1.30	1.06
1:A:96:THR:HG21	1:A:135:THR:OG1	1.58	1.02
1:A:502:VAL:HG11	1:A:514:ILE:HD11	1.44	0.96
1:A:502:VAL:CG1	1:A:514:ILE:HD11	1.98	0.93
1:A:293:ARG:HH22	1:A:667:GLU:CD	1.82	0.87
1:A:661:LEU:CD2	1:A:707:CYS:SG	2.67	0.81
1:A:81:LEU:HD11	1:A:91:ILE:HG21	1.62	0.80
1:A:81:LEU:HD13	1:A:93:VAL:HG22	1.64	0.78
1:A:519:ASP:OD2	1:A:522:GLN:HB2	1.84	0.77
1:A:648:ARG:HD2	1:A:653:SER:CA	2.12	0.76
1:A:487:GLU:H	1:A:487:GLU:CD	1.95	0.75
1:A:75:LEU:HD23	1:A:79:VAL:HG21	1.69	0.74
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.53	0.74
1:A:96:THR:CG2	1:A:135:THR:OG1	2.37	0.73
1:A:560:LEU:H	1:A:560:LEU:HD12	1.54	0.72
1:A:81:LEU:HD11	1:A:91:ILE:CG2	2.21	0.71
1:A:548:MET:HE1	1:A:575:LEU:HB2	1.73	0.71
1:A:648:ARG:CD	1:A:653:SER:HA	2.18	0.69
1:A:320:ILE:HD13	1:A:330:MET:SD	2.33	0.69
1:A:669:CYS:HG	1:A:707:CYS:HG	0.74	0.68
1:A:513:VAL:CG1	1:A:526:THR:HG23	2.23	0.68
1:A:81:LEU:CD1	1:A:91:ILE:CG2	2.72	0.68
1:A:513:VAL:HG13	1:A:526:THR:HG23	1.75	0.67
1:A:661:LEU:HD22	1:A:707:CYS:SG	2.34	0.66
1:A:506:HIS:CE1	5:A:951:PGE:H1	2.32	0.65
1:A:334:GLU:HG3	1:A:335:PRO:HD2	1.79	0.65
1:A:546:ARG:NH1	1:A:624:TYR:O	2.23	0.65
1:A:320:ILE:CD1	1:A:330:MET:HE1	2.27	0.65
1:A:684:LYS:HE2	1:A:690:CYS:SG	2.38	0.64
1:A:409:LYS:HD3	1:A:425:CYS:SG	2.37	0.64
1:A:320:ILE:HD11	1:A:330:MET:HE1	1.80	0.63
1:A:192:GLN:OE1	1:A:231:ASP:HA	1.99	0.62
1:A:75:LEU:HD21	1:A:79:VAL:HG11	1.81	0.62
1:A:699:GLU:HA	1:A:699:GLU:OE1	1.99	0.62
1:A:238:THR:OG1	1:A:252:GLU:HG3	1.99	0.61
1:A:395:MET:HE1	1:A:406:HIS:ND1	2.15	0.61
1:A:395:MET:HE1	1:A:406:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:MET:CE	1:A:575:LEU:HD12	2.31	0.60
1:A:548:MET:HE3	1:A:575:LEU:HD12	1.81	0.60
1:A:241:ASN:HB2	1:A:247:ASP:OD2	2.01	0.60
1:A:444:ALA:HB1	1:A:445:PRO:CD	2.33	0.59
1:A:293:ARG:NH2	1:A:667:GLU:CD	2.57	0.59
1:A:81:LEU:CD1	1:A:93:VAL:HG22	2.33	0.58
1:A:312:VAL:HB	1:A:316:GLN:HB2	1.87	0.57
1:A:355:LYS:HD3	1:A:358:ASP:OD2	2.04	0.57
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.70	0.56
1:A:520:GLU:OE1	1:A:614:LYS:HE2	2.04	0.56
1:A:454:ILE:HD13	1:A:476:ASP:HA	1.86	0.56
1:A:363:THR:O	1:A:367:GLY:HA2	2.06	0.56
1:A:395:MET:HA	1:A:395:MET:HE2	1.86	0.55
1:A:342:THR:HG22	7:A:1275:HOH:O	2.05	0.55
1:A:661:LEU:HD23	1:A:707:CYS:SG	2.47	0.55
1:A:607:GLU:OE1	7:A:1270:HOH:O	2.18	0.54
1:A:78:SER:HB2	1:A:96:THR:HG23	1.90	0.54
1:A:337:ASP:HA	7:A:1269:HOH:O	2.08	0.54
1:A:548:MET:SD	7:A:1277:HOH:O	2.59	0.54
1:A:645:GLY:HA3	1:A:703:LEU:HD13	1.89	0.53
1:A:556:THR:O	1:A:562:SER:HB2	2.08	0.53
1:A:576:GLU:OE1	6:A:952:GOL:C1	2.56	0.53
1:A:77:GLY:HA3	1:A:96:THR:O	2.09	0.52
1:A:185:THR:HB	7:A:1240:HOH:O	2.09	0.52
1:A:387:SER:HB2	1:A:393:GLN:OE1	2.08	0.52
1:A:706:LYS:HG2	1:A:707:CYS:SG	2.50	0.51
1:A:81:LEU:HD12	1:A:91:ILE:CG2	2.41	0.51
1:A:198:LEU:HD12	1:A:198:LEU:C	2.36	0.50
1:A:264:LYS:HD3	1:A:266:ILE:CG2	2.41	0.50
1:A:705:LYS:O	1:A:709:SER:HB2	2.13	0.49
1:A:75:LEU:HB3	1:A:564:TRP:CD1	2.47	0.49
1:A:520:GLU:OE1	1:A:614:LYS:CE	2.61	0.49
1:A:320:ILE:CD1	1:A:330:MET:CE	2.91	0.49
1:A:337:ASP:HA	7:A:1237:HOH:O	2.12	0.49
1:A:207:TRP:CE2	1:A:218:GLU:HB3	2.48	0.48
1:A:380:VAL:HA	1:A:397:THR:O	2.14	0.47
1:A:716:LYS:HB3	1:A:716:LYS:HE2	1.58	0.47
1:A:242:GLY:O	1:A:243:SER:O	2.33	0.47
1:A:502:VAL:CG1	1:A:514:ILE:CD1	2.84	0.47
1:A:271:TYR:CD1	1:A:285:MET:SD	3.08	0.47
1:A:704:LYS:HE3	1:A:708:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:NZ	2:N:11:TYR:HE1	2.14	0.46
1:A:502:VAL:HG13	1:A:514:ILE:HD11	1.92	0.46
1:A:264:LYS:HE3	1:A:302:ASP:OD1	2.16	0.46
1:A:281:PHE:HZ	1:A:328:VAL:HG11	1.81	0.46
1:A:617:MET:HE1	7:A:1287:HOH:O	2.14	0.45
1:A:641:LEU:HG	1:A:683:ARG:O	2.16	0.45
1:A:338:THR:HB	1:A:340:PHE:CE2	2.52	0.45
1:A:160:ARG:HG3	1:A:160:ARG:NH1	2.32	0.45
1:A:210:LYS:NZ	1:A:217:GLU:OE2	2.50	0.45
1:A:411:GLU:HG2	7:A:1133:HOH:O	2.17	0.44
1:A:513:VAL:HG11	1:A:526:THR:HG23	1.98	0.44
1:A:139:MET:HG2	1:A:151:LEU:CD2	2.47	0.44
1:A:227:LYS:NZ	2:N:11:TYR:CE1	2.86	0.44
1:A:556:THR:CG2	1:A:563:GLN:HG2	2.48	0.43
1:A:81:LEU:HD13	1:A:93:VAL:CG2	2.42	0.43
1:A:249:GLY:HA2	1:A:285:MET:HG3	2.00	0.43
1:A:264:LYS:HD3	1:A:266:ILE:HG22	2.00	0.43
1:A:266:ILE:HA	7:A:1261:HOH:O	2.18	0.43
1:A:271:TYR:HD1	1:A:285:MET:SD	2.41	0.43
1:A:116:ASP:O	1:A:117:TYR:HB2	2.19	0.42
1:A:425:CYS:HB2	1:A:462:GLY:O	2.19	0.42
1:A:69:GLN:HG3	1:A:567:TYR:CE1	2.55	0.42
1:A:590:HIS:CG	1:A:602:ILE:HG13	2.55	0.42
1:A:444:ALA:HB1	1:A:445:PRO:HD2	2.01	0.42
1:A:76:ARG:HA	1:A:76:ARG:HD3	1.62	0.42
1:A:407:LEU:N	1:A:407:LEU:HD12	2.34	0.42
1:A:560:LEU:H	1:A:560:LEU:CD1	2.26	0.42
1:A:395:MET:CE	1:A:406:HIS:ND1	2.83	0.41
1:A:403:ARG:HG3	1:A:403:ARG:NH1	2.28	0.41
1:A:674:GLU:HG2	1:A:675:GLU:N	2.35	0.41
1:A:256:THR:O	1:A:256:THR:HG23	2.19	0.41
1:A:576:GLU:OE1	6:A:952:GOL:H11	2.19	0.41
1:A:68:HIS:HE1	7:A:1135:HOH:O	2.04	0.41
1:A:98:HIS:O	1:A:100:PRO:HD3	2.21	0.41
1:A:254:TRP:CE3	1:A:263:PHE:HB3	2.56	0.41
1:A:556:THR:HG22	1:A:563:GLN:HG2	2.02	0.41
1:A:536:PHE:HE1	1:A:552:ILE:HG23	1.87	0.40
1:A:548:MET:HE1	1:A:575:LEU:CB	2.47	0.40
1:A:349:ARG:HB3	1:A:351:ILE:HD12	2.02	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	653/685 (95%)	621 (95%)	27 (4%)	5 (1%)	16	11
2	N	2/13 (15%)	2 (100%)	0	0	100	100
All	All	655/698 (94%)	623 (95%)	27 (4%)	5 (1%)	16	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	243	SER
1	A	653	SER
1	A	650	GLU
1	A	337	ASP

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	574/599 (96%)	539 (94%)	35 (6%)	17	14
2	N	4/12 (33%)	4 (100%)	0	100	100
All	All	578/611 (95%)	543 (94%)	35 (6%)	17	14

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	73	ASP
1	A	75	LEU
1	A	76	ARG
1	A	96	THR
1	A	126	ASP
1	A	160	ARG
1	A	175	VAL
1	A	198	LEU
1	A	227	LYS
1	A	252	GLU
1	A	261	LYS
1	A	262	SER
1	A	275	LEU
1	A	278	ARG
1	A	285	MET
1	A	306	MET
1	A	364	THR
1	A	395	MET
1	A	470	PRO
1	A	487	GLU
1	A	531	ARG
1	A	532	ASP
1	A	560	LEU
1	A	576	GLU
1	A	647	TYR
1	A	661	LEU
1	A	675	GLU
1	A	684	LYS
1	A	697	VAL
1	A	699	GLU
1	A	700	VAL
1	A	705	LYS
1	A	707	CYS
1	A	716	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	525	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	B	1	3,1	14,14,15	1.42	3 (21%)	17,19,21	2.12	6 (35%)
3	NAG	B	2	3	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
4	NAG	C	1	4,1	14,14,15	1.19	2 (14%)	17,19,21	1.41	3 (17%)
4	NAG	C	2	4	14,14,15	1.00	1 (7%)	17,19,21	1.48	2 (11%)
4	BMA	C	3	4	11,11,12	0.65	0	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
4	NAG	C	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	C1-C2	3.15	1.56	1.52
4	C	1	NAG	C2-N2	-2.77	1.41	1.46
4	C	1	NAG	C1-C2	2.58	1.55	1.52
3	B	1	NAG	C2-N2	2.53	1.50	1.46
3	B	1	NAG	C3-C2	2.37	1.57	1.52
4	C	2	NAG	C1-C2	2.31	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C2-N2-C7	-4.10	117.40	122.90
4	C	2	NAG	C4-C3-C2	3.84	116.64	111.02
3	B	1	NAG	O5-C5-C4	-3.26	102.88	110.83
4	C	1	NAG	C1-O5-C5	3.22	116.51	112.19
3	B	1	NAG	C4-C3-C2	3.20	115.71	111.02
3	B	1	NAG	O5-C1-C2	-3.01	106.63	111.29
3	B	1	NAG	C1-C2-N2	2.98	115.13	110.43
4	C	2	NAG	C1-C2-N2	2.92	115.03	110.43
4	C	1	NAG	O5-C1-C2	-2.55	107.35	111.29
3	B	2	NAG	C1-O5-C5	2.45	115.47	112.19
4	C	3	BMA	C1-O5-C5	2.37	115.36	112.19
4	C	1	NAG	C6-C5-C4	-2.27	107.45	113.02
3	B	1	NAG	C8-C7-N2	2.26	119.86	116.12

There are no chirality outliers.

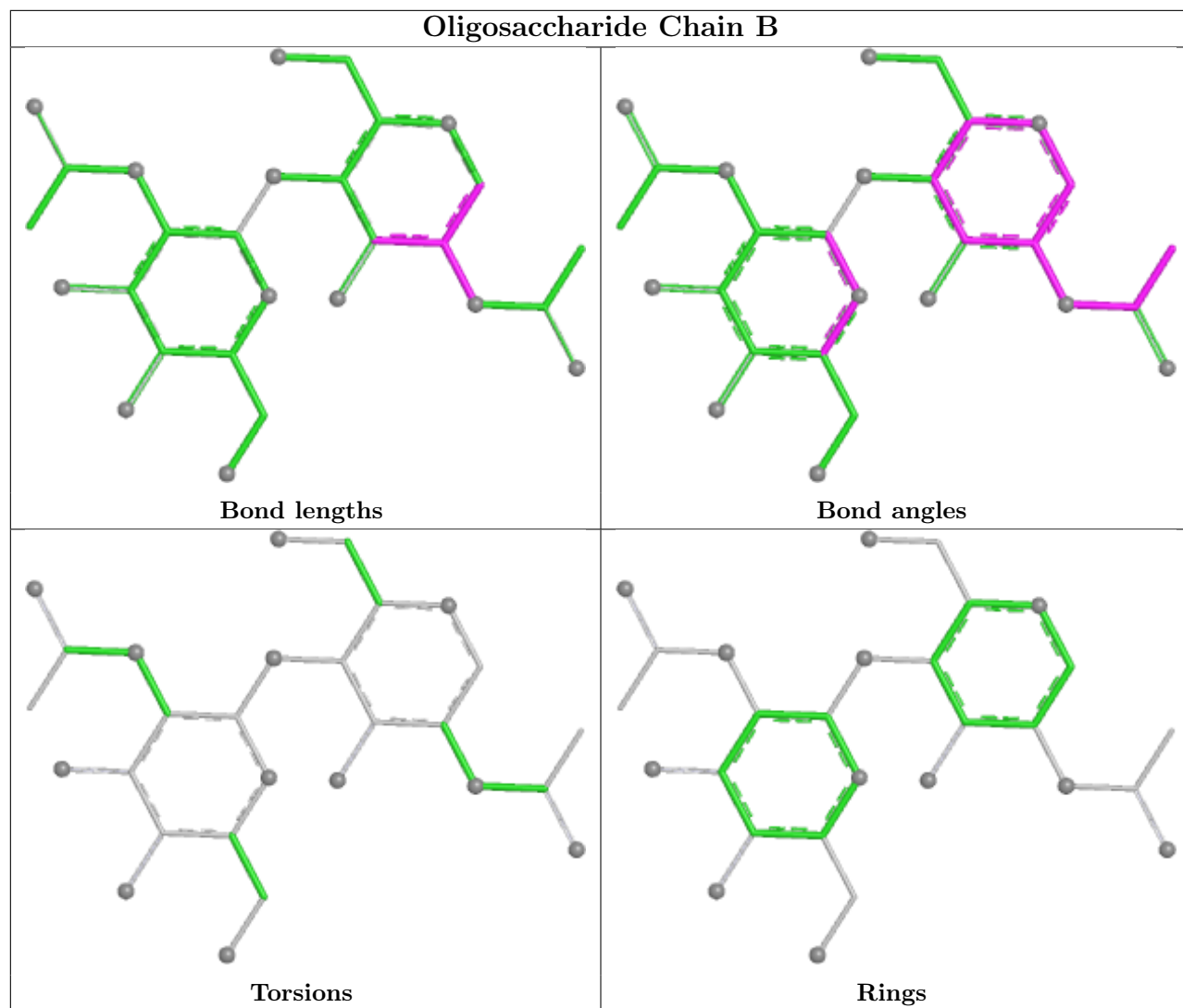
All (4) torsion outliers are listed below:

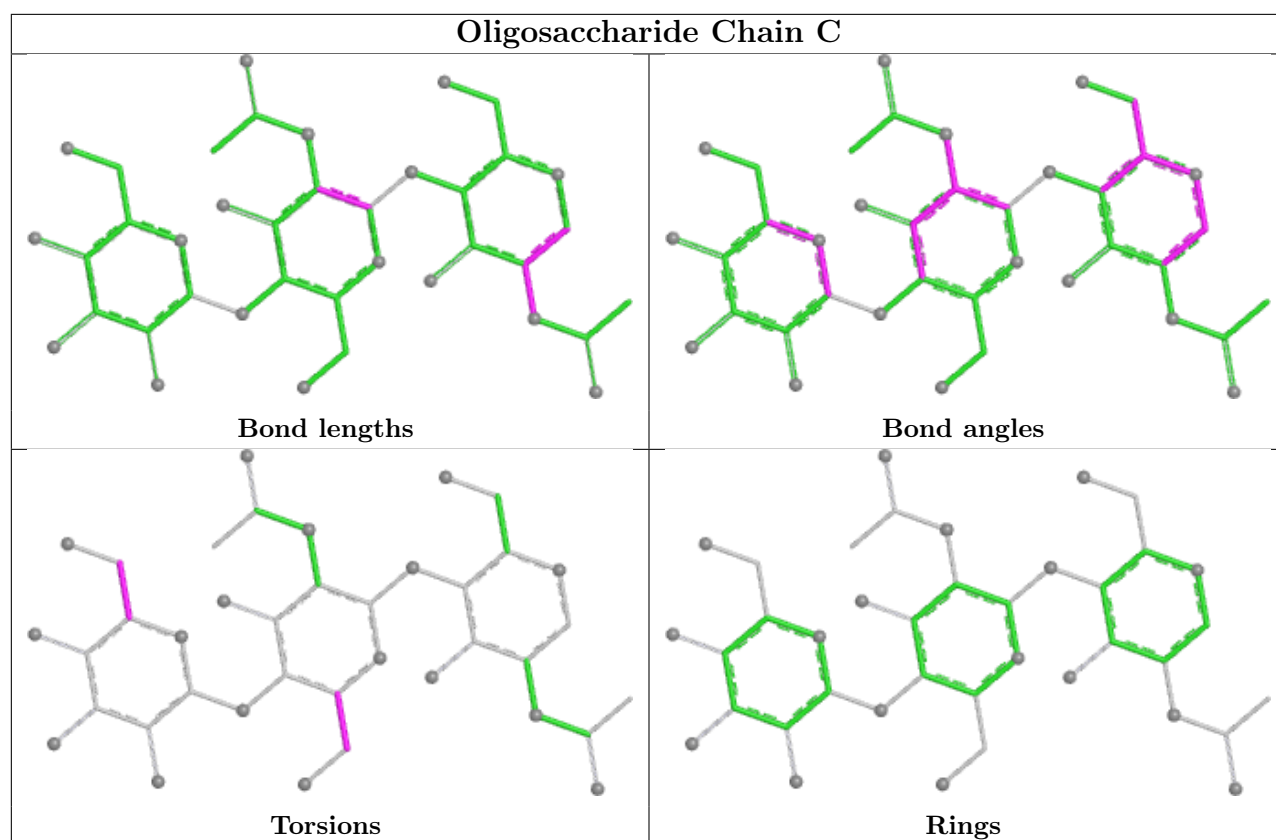
Mol	Chain	Res	Type	Atoms
4	C	3	BMA	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

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	$\# Z > 2$
6	GOL	A	952	-	5,5,5	0.28	0	5,5,5	0.64	0
5	PGE	A	951	-	9,9,9	1.03	0	8,8,8	0.29	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
6	GOL	A	952	-	-	2/4/4/4	-
5	PGE	A	951	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	952	GOL	O1-C1-C2-O2
6	A	952	GOL	O1-C1-C2-C3
5	A	951	PGE	O1-C1-C2-O2
5	A	951	PGE	O3-C5-C6-O4
5	A	951	PGE	C4-C3-O2-C2
5	A	951	PGE	C1-C2-O2-C3
5	A	951	PGE	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	952	GOL	2	0
5	A	951	PGE	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	657/685 (95%)	1.10	110 (16%) 4 4	12, 28, 46, 58	0
2	N	4/13 (30%)	2.66	3 (75%) 0 0	52, 53, 61, 62	0
All	All	661/698 (94%)	1.11	113 (17%) 4 4	12, 28, 47, 62	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	PHE	6.4
1	A	366	GLY	5.1
1	A	243	SER	4.4
1	A	242	GLY	4.4
1	A	99	VAL	4.4
1	A	697	VAL	4.3
1	A	287	ASP	4.0
1	A	672	GLY	4.0
1	A	101	LEU	3.9
2	N	11	TYR	3.8
1	A	56	VAL	3.8
1	A	77	GLY	3.7
1	A	74	ASP	3.7
1	A	289	ASP	3.6
1	A	248	LEU	3.5
1	A	630	PRO	3.5
1	A	707	CYS	3.5
1	A	154	GLU	3.5
1	A	78	SER	3.5
1	A	89	GLY	3.4
1	A	601	CYS	3.4
1	A	671	TYR	3.4
1	A	290	THR	3.4
1	A	90	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	286	ALA	3.4
1	A	192	GLN	3.4
1	A	424	GLU	3.3
1	A	700	VAL	3.3
1	A	687	GLY	3.2
1	A	247	ASP	3.2
1	A	98	HIS	3.2
1	A	337	ASP	3.2
1	A	59	PHE	3.2
1	A	158	GLY	3.2
1	A	669	CYS	3.2
1	A	647	TYR	3.2
1	A	224	CYS	3.2
1	A	532	ASP	3.1
1	A	96	THR	3.1
1	A	468	MET	3.1
1	A	365	THR	3.0
1	A	299	ASP	3.0
1	A	594	PRO	3.0
1	A	135	THR	3.0
1	A	246	ALA	2.9
1	A	132	PHE	2.9
1	A	129	ASN	2.9
1	A	169	ASP	2.8
1	A	673	ARG	2.8
1	A	159	SER	2.8
2	N	13	LEU	2.8
1	A	364	THR	2.8
1	A	288	LYS	2.8
1	A	689	LYS	2.8
1	A	561	THR	2.8
1	A	653	SER	2.7
1	A	285	MET	2.7
1	A	679	THR	2.7
2	N	10	PRO	2.7
1	A	130	ASN	2.7
1	A	108	GLN	2.6
1	A	678	THR	2.6
1	A	313	GLY	2.6
1	A	573	ASP	2.5
1	A	63	LEU	2.5
1	A	57	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	649	PRO	2.5
1	A	623	ASP	2.4
1	A	659	PRO	2.4
1	A	165	PHE	2.4
1	A	155	VAL	2.4
1	A	144	GLU	2.4
1	A	79	VAL	2.4
1	A	244	CYS	2.4
1	A	579	CYS	2.4
1	A	411	GLU	2.4
1	A	715	GLU	2.3
1	A	67	THR	2.3
1	A	556	THR	2.3
1	A	179	LEU	2.3
1	A	641	LEU	2.3
1	A	209	SER	2.3
1	A	85	GLY	2.3
1	A	201	SER	2.2
1	A	60	VAL	2.2
1	A	265	THR	2.2
1	A	222	ALA	2.2
1	A	229	GLY	2.2
1	A	252	GLU	2.2
1	A	388	GLU	2.2
1	A	674	GLU	2.2
1	A	564	TRP	2.2
1	A	654	LYS	2.2
1	A	688	ASP	2.2
1	A	138	GLY	2.2
1	A	58	ASP	2.2
1	A	589	ALA	2.1
1	A	560	LEU	2.1
1	A	587	TRP	2.1
1	A	161	GLY	2.1
1	A	631	SER	2.1
1	A	66	ASN	2.1
1	A	100	PRO	2.1
1	A	202	THR	2.1
1	A	686	PRO	2.1
1	A	419	ALA	2.1
1	A	241	ASN	2.0
1	A	86	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	592	THR	2.0
1	A	656	VAL	2.0
1	A	591	SER	2.0
1	A	648	ARG	2.0
1	A	690	CYS	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](#)

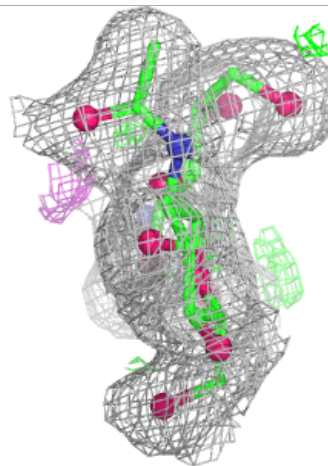
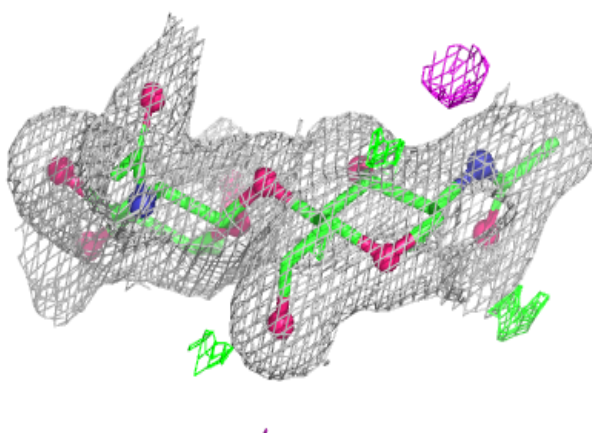
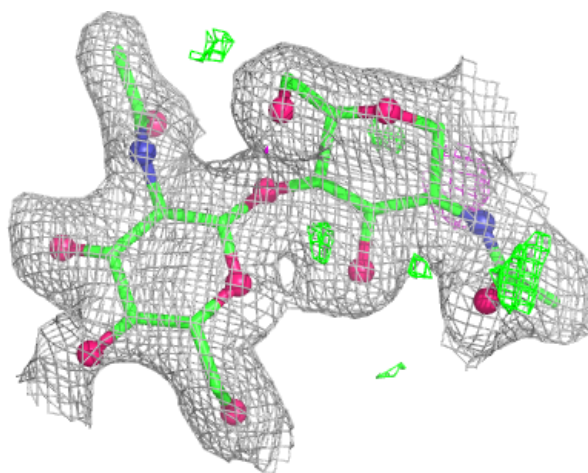
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

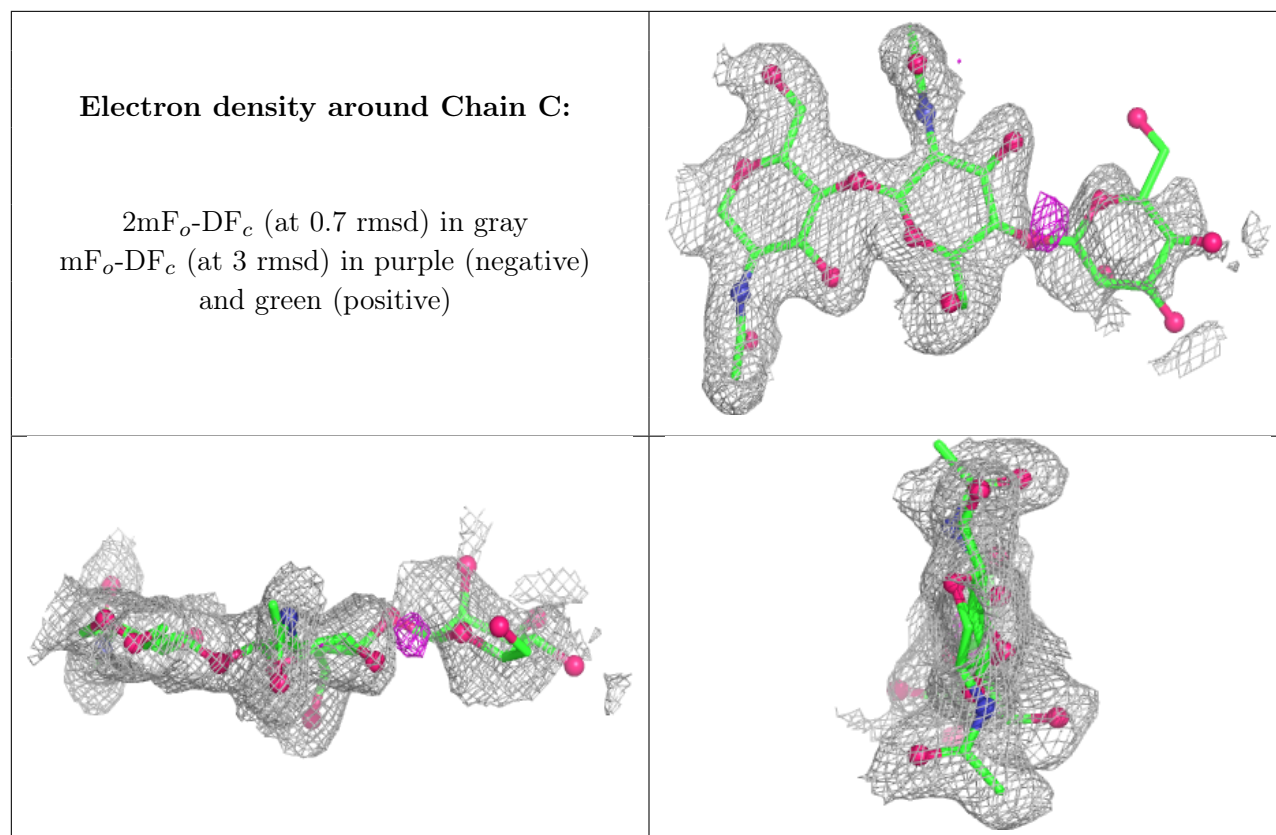
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	24,28,30,32	0
3	NAG	B	2	14/15	-	-	41,47,59,60	0
4	NAG	C	2	14/15	0.83	0.15	52,58,64,72	0
4	NAG	C	1	14/15	0.93	0.09	25,30,38,46	0
4	BMA	C	3	11/12	-	-	79,83,84,86	0

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 B:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	952	6/6	0.80	0.14	60,64,65,66	0
5	PGE	A	951	10/10	0.87	0.14	66,69,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.