Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 12:21 PM GMT

PDB ID	:	6TM0
Title	:	N-Domain P40/P90 Mycoplasma pneumoniae complexed with 6'SL
Authors	:	Vizarraga, D.; Aparicio, D.; Illanes, R.; Fita, I.; Perez-Luque, R.; Martin, J.
Deposited on	:	2019-12-03
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

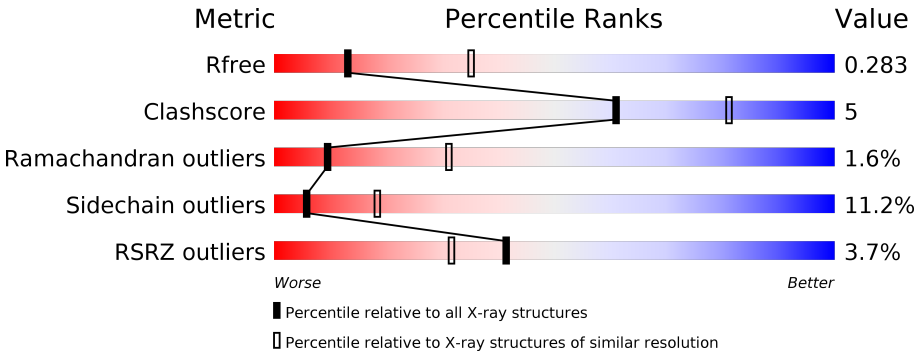
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	976	3% 65% 17% • 17%
1	B	976	3% 67% 14% • 17%
2	C	3	100%
2	D	3	67% 33%

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
2	BGC	C	1	-	-	-	X
2	GAL	C	2	-	-	-	X
2	BGC	D	1	-	-	-	X
2	GAL	D	2	-	-	-	X

2 Entry composition

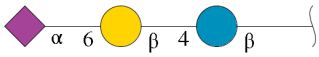
There are 2 unique types of molecules in this entry. The entry contains 12580 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6247	3931	1060	1251	5			
1	B	811	Total	C	N	O	S	0	0	0
			6247	3931	1060	1251	5			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.



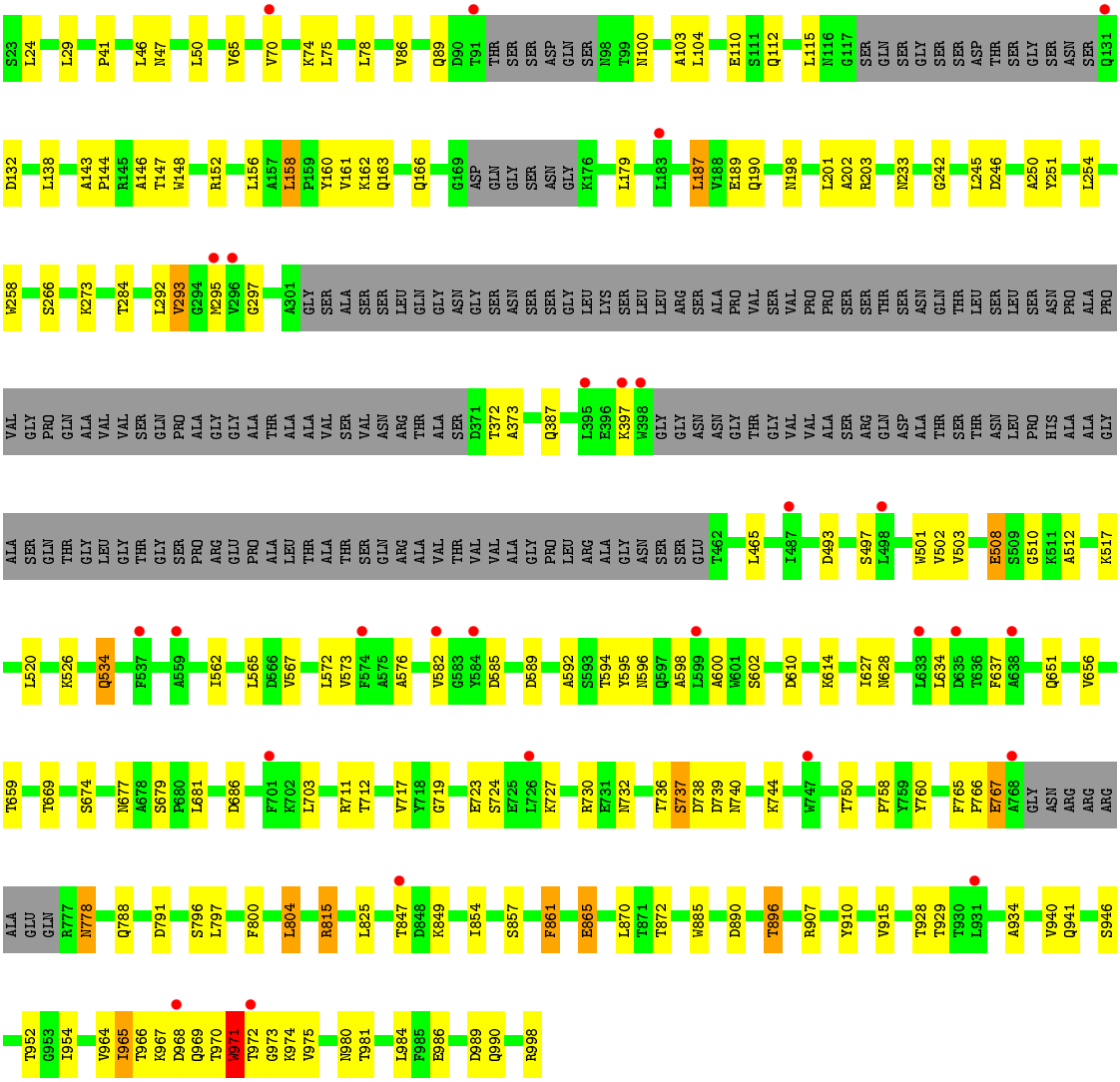
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	D	3	Total	C	N	O	0	0	0
			43	23	1	19			

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.

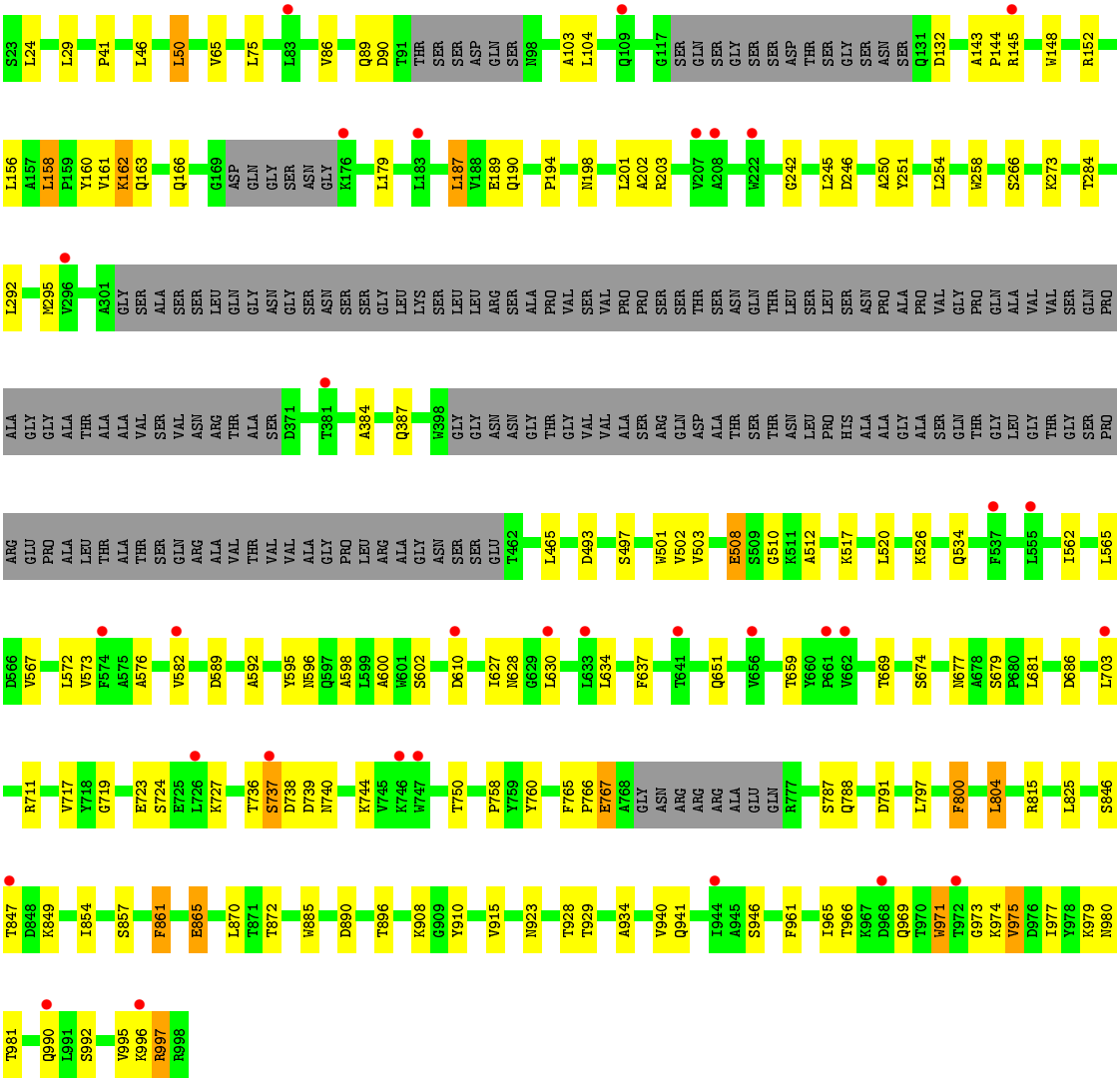
- Molecule 1: Mgp-operon protein 3

Chain A:



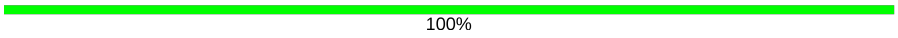
- Molecule 1: Mgp-operon protein 3

Chain B:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.33Å 107.38Å 160.45Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	80.22 – 2.80 80.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.22-2.80) 96.5 (80.23-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.208 , 0.265 0.228 , 0.283	Depositor DCC
R_{free} test set	2396 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12580	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SIA, BGC, GAL

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	0.49	0/6375	0.71	0/8668
1	B	0.48	0/6375	0.71	0/8668
All	All	0.49	0/12750	0.71	0/17336

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	6247	0	6077	58	0
1	B	6247	0	6077	54	0
2	C	43	0	37	0	0
2	D	43	0	37	0	0
All	All	12580	0	12228	112	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 (112) 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:861:PHE:HB2	1:A:865:GLU:HG3	1.54	0.90
1:B:143:ALA:HB1	1:B:144:PRO:HD2	1.55	0.87
1:B:861:PHE:HB2	1:B:865:GLU:HG3	1.57	0.84
1:A:143:ALA:HB1	1:A:144:PRO:HD2	1.61	0.82
1:B:160:TYR:OH	1:B:162:LYS:HG2	1.88	0.74
1:A:47:ASN:HD21	1:A:146:ALA:HB3	1.51	0.73
1:A:861:PHE:HB2	1:A:865:GLU:CG	2.24	0.66
1:B:103:ALA:HB3	1:B:161:VAL:HG13	1.76	0.66
1:A:103:ALA:HB3	1:A:161:VAL:HG13	1.79	0.64
1:A:187:LEU:HD21	1:A:273:LYS:HB2	1.82	0.62
1:B:187:LEU:HD21	1:B:273:LYS:HB2	1.82	0.62
1:B:974:LYS:HG3	1:B:996:LYS:HE2	1.82	0.61
1:A:967:LYS:HB3	1:A:972:THR:HG23	1.86	0.57
1:B:800:PHE:HE2	1:B:870:LEU:HB3	1.69	0.57
1:B:103:ALA:HB2	1:B:163:GLN:HB3	1.89	0.54
1:A:47:ASN:ND2	1:A:146:ALA:HB3	2.22	0.53
1:A:800:PHE:HE1	1:A:870:LEU:HB3	1.73	0.53
1:A:65:VAL:HB	1:A:78:LEU:HD23	1.90	0.53
1:B:143:ALA:HB1	1:B:144:PRO:CD	2.35	0.53
1:B:965:ILE:HD12	1:B:975:VAL:HG22	1.91	0.52
1:A:766:PRO:HB3	1:A:788:GLN:HE22	1.76	0.51
1:A:582:VAL:HG11	1:A:600:ALA:HB2	1.94	0.50
1:B:974:LYS:O	1:B:996:LYS:HG2	2.12	0.50
1:B:50:LEU:HD13	1:B:148:TRP:HB2	1.94	0.50
1:B:582:VAL:HG11	1:B:600:ALA:HB2	1.95	0.49
1:B:961:PHE:CE1	1:B:979:LYS:HB2	2.48	0.49
1:A:50:LEU:HD13	1:A:148:TRP:HB2	1.93	0.49
1:A:501:TRP:CE2	1:A:512:ALA:HB2	2.48	0.49
1:B:198:ASN:HD21	1:B:787:SER:HB2	1.77	0.49
1:B:501:TRP:CE2	1:B:512:ALA:HB2	2.48	0.49
1:A:24:LEU:HA	1:A:41:PRO:HG2	1.94	0.48
1:B:24:LEU:HA	1:B:41:PRO:HG2	1.94	0.48
1:A:758:PRO:HB3	1:A:760:TYR:CZ	2.48	0.48
1:A:872:THR:HB	1:A:890:ASP:O	2.12	0.48
1:B:872:THR:HB	1:B:890:ASP:O	2.12	0.48
1:A:242:GLY:HA3	1:A:598:ALA:O	2.14	0.48
1:B:758:PRO:HB3	1:B:760:TYR:CZ	2.49	0.48
1:B:977:ILE:CD1	1:B:995:VAL:HG11	2.43	0.48
1:A:156:LEU:HB3	1:A:501:TRP:CE2	2.49	0.47
1:A:585:ASP:HB3	1:A:594:THR:O	2.15	0.47
1:B:198:ASN:ND2	1:B:787:SER:HB2	2.29	0.47
1:B:242:GLY:HA3	1:B:598:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HB	1:A:74:LYS:HB3	1.96	0.47
1:A:896:THR:HA	1:A:907:ARG:NH1	2.30	0.47
1:B:156:LEU:HB3	1:B:501:TRP:CE2	2.50	0.47
1:B:861:PHE:HB2	1:B:865:GLU:CG	2.38	0.46
1:B:766:PRO:HB3	1:B:788:GLN:HE22	1.80	0.46
1:B:997:ARG:HE	1:B:997:ARG:HA	1.80	0.46
1:A:112:GLN:HA	1:A:115:LEU:HD12	1.97	0.45
1:B:719:GLY:HA3	1:B:750:THR:HG22	1.99	0.45
1:A:592:ALA:HB3	1:A:595:TYR:HB2	1.99	0.45
1:A:760:TYR:HB3	1:A:767:GLU:H	1.82	0.44
1:B:592:ALA:HB3	1:B:595:TYR:HB2	1.99	0.44
1:A:189:GLU:HB2	1:A:677:ASN:HA	1.99	0.44
1:B:190:GLN:HB3	1:B:250:ALA:HB3	1.98	0.44
1:A:233:ASN:O	1:A:656:VAL:HG13	2.17	0.44
1:A:952:THR:HB	1:A:965:ILE:HG23	1.99	0.44
1:B:245:LEU:HD21	1:B:598:ALA:HB2	1.98	0.44
1:A:190:GLN:HB3	1:A:250:ALA:HB3	1.98	0.44
1:B:189:GLU:HB2	1:B:677:ASN:HA	2.00	0.44
1:B:202:ALA:O	1:B:266:SER:HB2	2.18	0.44
1:B:681:LEU:HD11	1:B:797:LEU:HD13	2.00	0.44
1:B:681:LEU:HD11	1:B:797:LEU:CD1	2.48	0.44
1:A:202:ALA:O	1:A:266:SER:HB2	2.18	0.44
1:A:719:GLY:HA3	1:A:750:THR:HG22	2.00	0.44
1:A:681:LEU:HD11	1:A:797:LEU:HD13	2.00	0.44
1:A:520:LEU:HD13	1:A:717:VAL:HG11	2.00	0.43
1:B:520:LEU:HD13	1:B:717:VAL:HG11	2.00	0.43
1:A:187:LEU:HG	1:A:251:TYR:HB3	1.99	0.43
1:A:245:LEU:HD21	1:A:598:ALA:HB2	1.99	0.43
1:A:152:ARG:NH1	1:A:508:GLU:HA	2.34	0.43
1:A:198:ASN:HD21	1:A:796:SER:H	1.66	0.43
1:B:187:LEU:HG	1:B:251:TYR:HB3	1.99	0.43
1:B:760:TYR:HB3	1:B:767:GLU:H	1.84	0.43
1:A:681:LEU:HD11	1:A:797:LEU:CD1	2.48	0.43
1:B:152:ARG:NH1	1:B:508:GLU:HA	2.34	0.43
1:A:258:TRP:O	1:A:465:LEU:HD12	2.19	0.43
1:B:160:TYR:HE2	1:B:737:SER:HB2	1.82	0.43
1:A:160:TYR:HE2	1:A:737:SER:HB2	1.82	0.43
1:B:854:ILE:HA	1:B:934:ALA:HB2	1.99	0.43
1:A:854:ILE:HA	1:A:934:ALA:HB2	1.99	0.42
1:B:573:VAL:HG23	1:B:804:LEU:HD21	2.01	0.42
1:A:573:VAL:HG23	1:A:804:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HD13	1:B:517:LYS:HE3	2.01	0.42
1:A:179:LEU:HD13	1:A:517:LYS:HE3	2.01	0.42
1:B:503:VAL:HG12	1:B:510:GLY:HA3	2.01	0.42
1:B:258:TRP:O	1:B:465:LEU:HD12	2.20	0.42
1:B:86:VAL:HG13	1:B:158:LEU:HD21	2.02	0.42
1:A:534:GLN:NE2	1:A:712:THR:HG21	2.34	0.41
1:A:954:ILE:HG12	1:A:964:VAL:HG22	2.01	0.41
1:B:992:SER:O	1:B:996:LYS:HB2	2.20	0.41
1:A:562:ILE:HA	1:A:576:ALA:HB2	2.01	0.41
1:A:86:VAL:HG13	1:A:158:LEU:HD21	2.02	0.41
1:B:562:ILE:HA	1:B:576:ALA:HB2	2.02	0.41
1:A:103:ALA:HA	1:A:163:GLN:HE21	1.86	0.41
1:B:602:SER:HB3	1:B:628:ASN:HB2	2.03	0.41
1:B:885:TRP:HB2	1:B:915:VAL:HB	2.03	0.41
1:A:143:ALA:HB1	1:A:144:PRO:CD	2.40	0.41
1:A:970:THR:O	1:A:971:TRP:HB3	2.21	0.41
1:A:503:VAL:HG12	1:A:510:GLY:HA3	2.02	0.41
1:A:602:SER:HB3	1:A:628:ASN:HB2	2.03	0.41
1:A:885:TRP:HB2	1:A:915:VAL:HB	2.03	0.41
1:A:502:VAL:O	1:A:502:VAL:HG12	2.21	0.41
1:A:614:LYS:HB2	1:A:849:LYS:HB2	2.03	0.41
1:B:194:PRO:HD2	1:B:384:ALA:HB1	2.03	0.41
1:B:254:LEU:HA	1:B:254:LEU:HD12	1.96	0.41
1:B:910:TYR:CE2	1:B:946:SER:HB3	2.56	0.41
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.96	0.40
1:A:758:PRO:HB3	1:A:760:TYR:CE2	2.55	0.40
1:A:910:TYR:CE2	1:A:946:SER:HB3	2.56	0.40
1:B:502:VAL:HG12	1:B:502:VAL:O	2.21	0.40
1:B:758:PRO:HB3	1:B:760:TYR:CE2	2.55	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	797/976 (82%)	724 (91%)	57 (7%)	16 (2%)	7 24
1	B	797/976 (82%)	732 (92%)	55 (7%)	10 (1%)	12 36
All	All	1594/1952 (82%)	1456 (91%)	112 (7%)	26 (2%)	9 31

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	THR
1	A	815	ARG
1	A	737	SER
1	A	778	ASN
1	A	929	THR
1	A	971	TRP
1	B	737	SER
1	B	929	THR
1	B	971	TRP
1	A	373	ALA
1	A	589	ASP
1	A	791	ASP
1	A	975	VAL
1	B	589	ASP
1	B	791	ASP
1	B	815	ARG
1	A	627	ILE
1	A	686	ASP
1	B	627	ILE
1	B	686	ASP
1	B	975	VAL
1	A	100	ASN
1	B	973	GLY
1	A	293	VAL
1	A	297	GLY
1	A	973	GLY

5.3.2 Protein sidechains (i)

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	677/800 (85%)	599 (88%)	78 (12%)	5 17
1	B	677/800 (85%)	604 (89%)	73 (11%)	6 19
All	All	1354/1600 (85%)	1203 (89%)	151 (11%)	6 18

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	46	LEU
1	A	75	LEU
1	A	89	GLN
1	A	104	LEU
1	A	110	GLU
1	A	132	ASP
1	A	138	LEU
1	A	158	LEU
1	A	162	LYS
1	A	166	GLN
1	A	187	LEU
1	A	201	LEU
1	A	203	ARG
1	A	246	ASP
1	A	284	THR
1	A	292	LEU
1	A	293	VAL
1	A	295	MET
1	A	372	THR
1	A	387	GLN
1	A	397	LYS
1	A	493	ASP
1	A	497	SER
1	A	508	GLU
1	A	526	LYS
1	A	534	GLN
1	A	565	LEU
1	A	567	VAL
1	A	572	LEU
1	A	596	ASN
1	A	610	ASP
1	A	634	LEU
1	A	637	PHE
1	A	651	GLN

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Mol	Chain	Res	Type
1	A	659	THR
1	A	669	THR
1	A	674	SER
1	A	679	SER
1	A	703	LEU
1	A	711	ARG
1	A	723	GLU
1	A	724	SER
1	A	727	LYS
1	A	730	ARG
1	A	732	ASN
1	A	736	THR
1	A	738	ASP
1	A	739	ASP
1	A	740	ASN
1	A	744	LYS
1	A	765	PHE
1	A	767	GLU
1	A	778	ASN
1	A	804	LEU
1	A	815	ARG
1	A	825	LEU
1	A	847	THR
1	A	857	SER
1	A	861	PHE
1	A	865	GLU
1	A	896	THR
1	A	928	THR
1	A	940	VAL
1	A	941	GLN
1	A	965	ILE
1	A	966	THR
1	A	968	ASP
1	A	969	GLN
1	A	971	TRP
1	A	974	LYS
1	A	980	ASN
1	A	981	THR
1	A	984	LEU
1	A	986	GLU
1	A	989	ASP
1	A	990	GLN

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Mol	Chain	Res	Type
1	A	998	ARG
1	B	29	LEU
1	B	46	LEU
1	B	50	LEU
1	B	65	VAL
1	B	75	LEU
1	B	89	GLN
1	B	90	ASP
1	B	104	LEU
1	B	132	ASP
1	B	145	ARG
1	B	158	LEU
1	B	162	LYS
1	B	166	GLN
1	B	187	LEU
1	B	201	LEU
1	B	203	ARG
1	B	246	ASP
1	B	284	THR
1	B	292	LEU
1	B	295	MET
1	B	387	GLN
1	B	493	ASP
1	B	497	SER
1	B	508	GLU
1	B	526	LYS
1	B	534	GLN
1	B	565	LEU
1	B	567	VAL
1	B	572	LEU
1	B	596	ASN
1	B	610	ASP
1	B	630	LEU
1	B	634	LEU
1	B	637	PHE
1	B	651	GLN
1	B	659	THR
1	B	669	THR
1	B	674	SER
1	B	679	SER
1	B	703	LEU
1	B	711	ARG

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Mol	Chain	Res	Type
1	B	723	GLU
1	B	724	SER
1	B	727	LYS
1	B	736	THR
1	B	738	ASP
1	B	739	ASP
1	B	740	ASN
1	B	744	LYS
1	B	765	PHE
1	B	767	GLU
1	B	800	PHE
1	B	804	LEU
1	B	825	LEU
1	B	846	SER
1	B	847	THR
1	B	849	LYS
1	B	857	SER
1	B	861	PHE
1	B	865	GLU
1	B	896	THR
1	B	908	LYS
1	B	923	ASN
1	B	928	THR
1	B	940	VAL
1	B	941	GLN
1	B	966	THR
1	B	969	GLN
1	B	971	TRP
1	B	980	ASN
1	B	981	THR
1	B	990	GLN
1	B	997	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	163	GLN
1	A	198	ASN
1	A	902	GLN
1	A	948	GLN
1	B	112	GLN

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Mol	Chain	Res	Type
1	B	850	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 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	BGC	C	1	2	12,12,12	0.28	0	17,17,17	0.49	0
2	GAL	C	2	2	11,11,12	0.38	0	15,15,17	0.49	0
2	SIA	C	3	2	17,20,21	0.24	0	21,28,31	0.91	0
2	BGC	D	1	2	12,12,12	0.34	0	17,17,17	0.99	1 (5%)
2	GAL	D	2	2	11,11,12	0.38	0	15,15,17	0.69	0
2	SIA	D	3	2	17,20,21	0.24	0	21,28,31	0.88	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	SIA	C	3	2	-	1/14/34/38	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	1/14/34/38	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(^{o})	Ideal(^{o})
2	D	1	BGC	C1-O5-C5	3.25	119.80	113.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

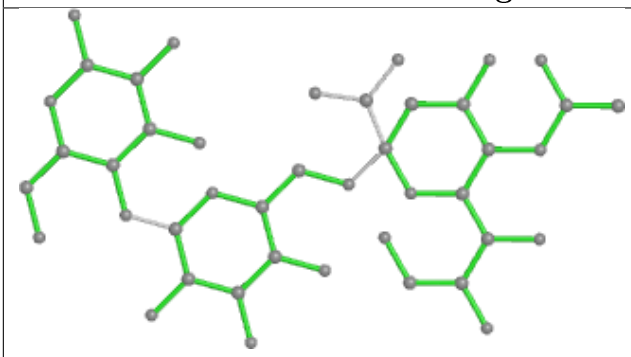
Mol	Chain	Res	Type	Atoms
2	C	3	SIA	C6-C7-C8-O8
2	D	3	SIA	C6-C7-C8-O8

There are no ring outliers.

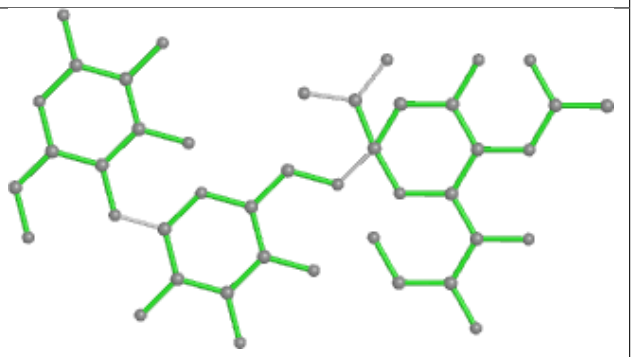
No monomer is involved in short contacts.

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

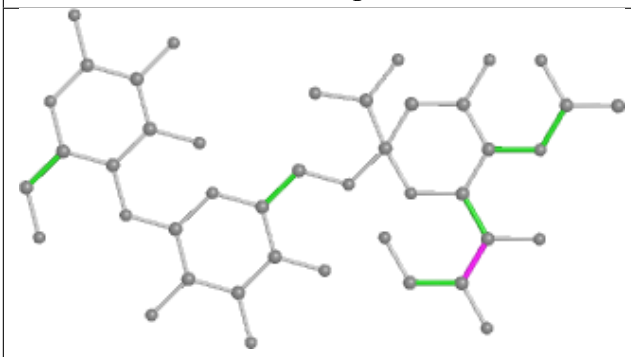
Oligosaccharide Chain C



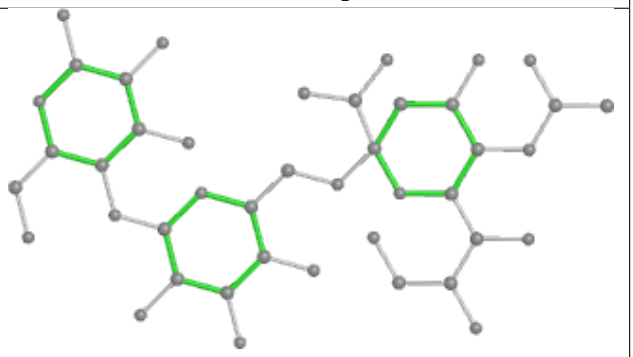
Bond lengths



Bond angles

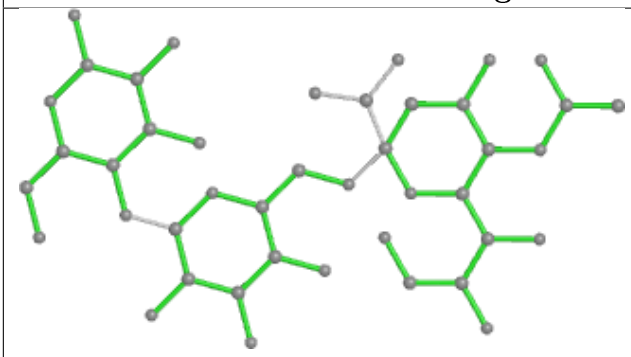


Torsions

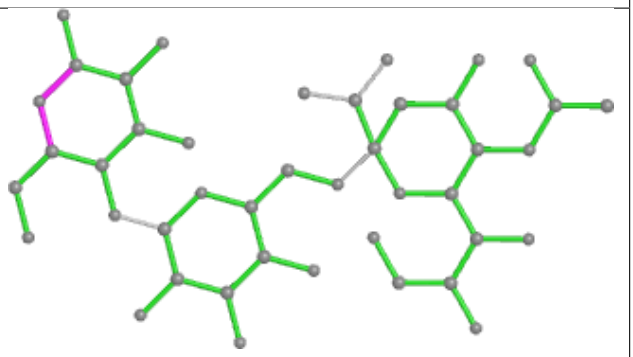


Rings

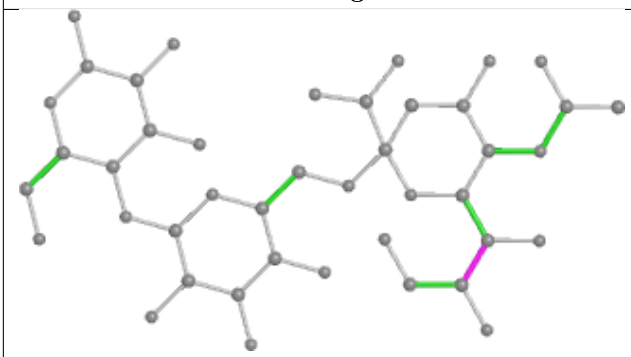
Oligosaccharide Chain D



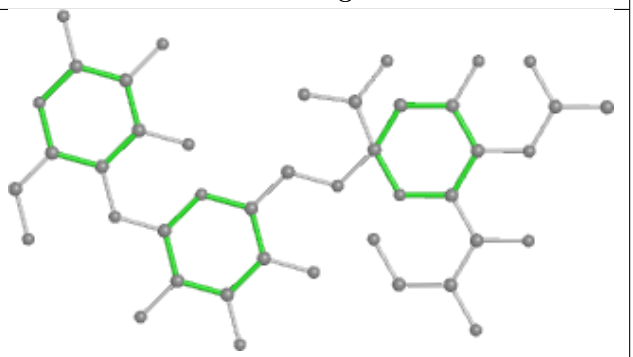
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	811/976 (83%)	0.09	28 (3%)	44	34	55, 91, 139, 201	0
1	B	811/976 (83%)	0.12	32 (3%)	39	29	59, 91, 137, 200	0
All	All	1622/1952 (83%)	0.10	60 (3%)	41	31	55, 91, 139, 201	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	972	THR	5.6
1	A	847	THR	5.0
1	B	109	GLN	4.7
1	B	968	ASP	4.4
1	B	662	VAL	4.4
1	B	83	LEU	4.1
1	A	296	VAL	3.8
1	A	747	TRP	3.4
1	B	847	THR	3.3
1	A	537	PHE	3.3
1	A	633	LEU	3.3
1	B	222	TRP	3.2
1	A	295	MET	3.1
1	B	555	LEU	3.1
1	B	726	LEU	3.0
1	A	968	ASP	3.0
1	B	661	PRO	3.0
1	B	996	LYS	3.0
1	B	207	VAL	2.9
1	B	296	VAL	2.9
1	A	395	LEU	2.7
1	A	726	LEU	2.7
1	B	582	VAL	2.6
1	B	641	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	145	ARG	2.6
1	A	972	THR	2.6
1	A	398	TRP	2.6
1	B	747	TRP	2.6
1	A	487	ILE	2.5
1	A	91	THR	2.5
1	B	703	LEU	2.5
1	A	559	ALA	2.5
1	A	183	LEU	2.4
1	A	599	LEU	2.4
1	A	574	PHE	2.4
1	A	638	ALA	2.4
1	A	635	ASP	2.4
1	A	582	VAL	2.3
1	A	131	GLN	2.3
1	B	944	ILE	2.3
1	A	768	ALA	2.3
1	A	701	PHE	2.3
1	A	584	TYR	2.2
1	A	931	LEU	2.2
1	B	633	LEU	2.2
1	B	574	PHE	2.2
1	B	381	THR	2.2
1	B	176	LYS	2.1
1	A	498	LEU	2.1
1	B	537	PHE	2.1
1	B	630	LEU	2.1
1	A	397	LYS	2.1
1	B	208	ALA	2.1
1	B	656	VAL	2.1
1	B	183	LEU	2.0
1	B	737	SER	2.0
1	B	746	LYS	2.0
1	A	70	VAL	2.0
1	B	990	GLN	2.0
1	B	610	ASP	2.0

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

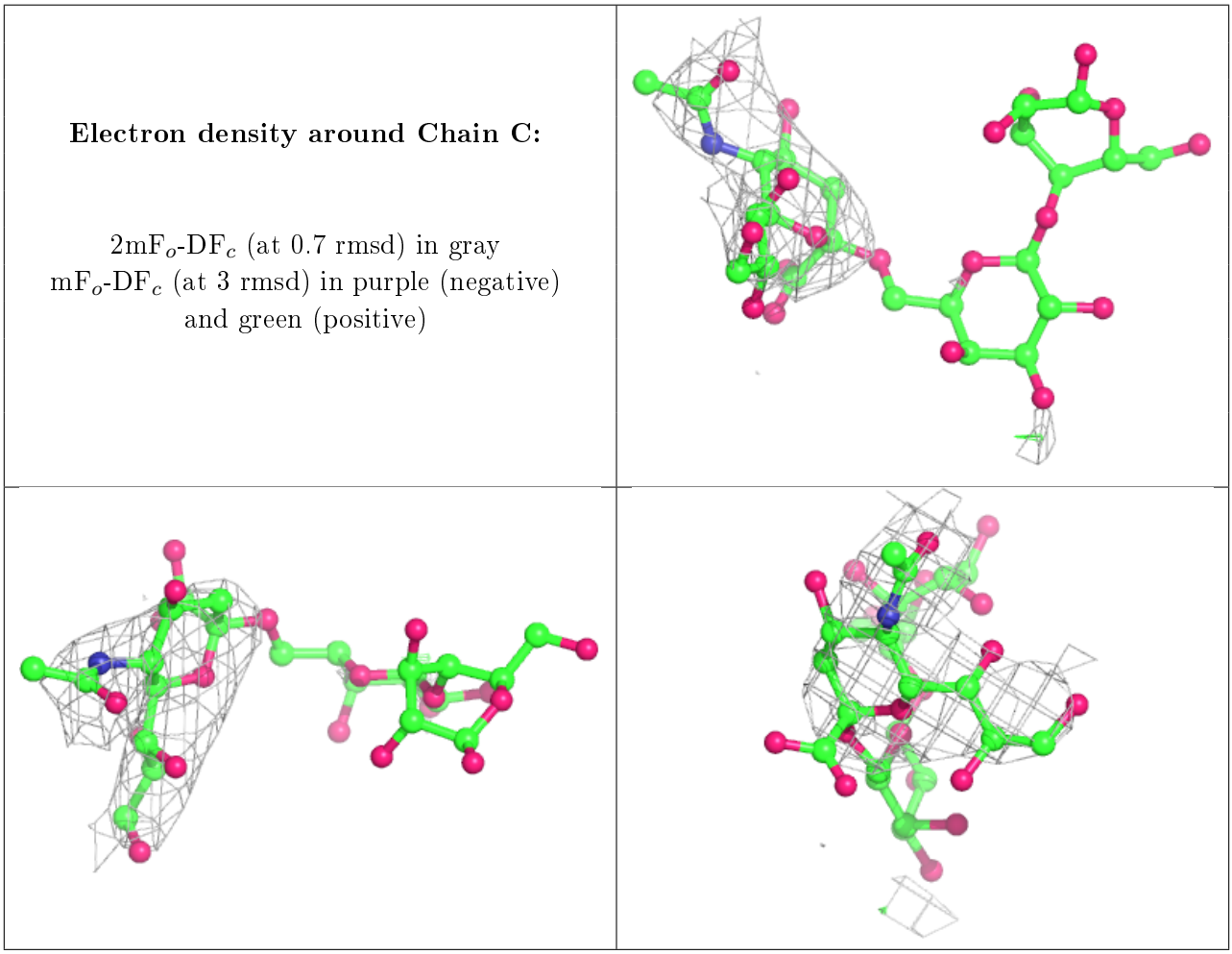
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} 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.

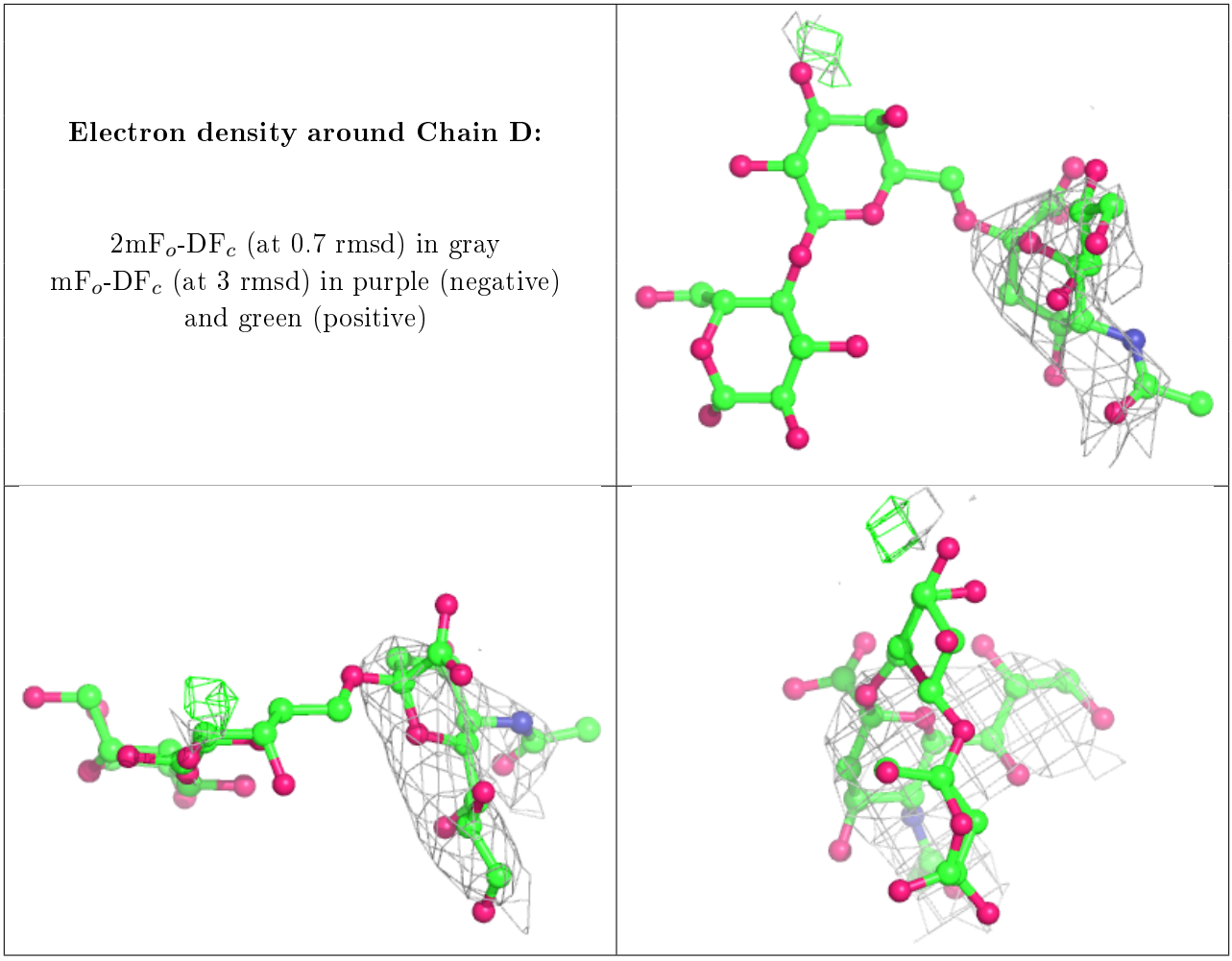
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	D	1	12/12	-0.00	1.62	118,121,121,122	12
2	BGC	C	1	12/12	0.12	1.80	115,117,119,119	12
2	GAL	D	2	11/12	0.43	0.62	116,118,118,119	11
2	GAL	C	2	11/12	0.49	0.73	116,117,118,119	11
2	SIA	D	3	20/21	0.82	0.44	104,113,119,120	20
2	SIA	C	3	20/21	0.83	0.41	105,114,119,121	20

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 D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.