Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 11:09 AM GMT

PDB ID	:	6TRF
Title	:	Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) purified from cells treated with kifunensine.
Authors	:	Roversi, P.; Zitzmann, N.
Deposited on	:	2019-12-18
Resolution	:	4.11 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:

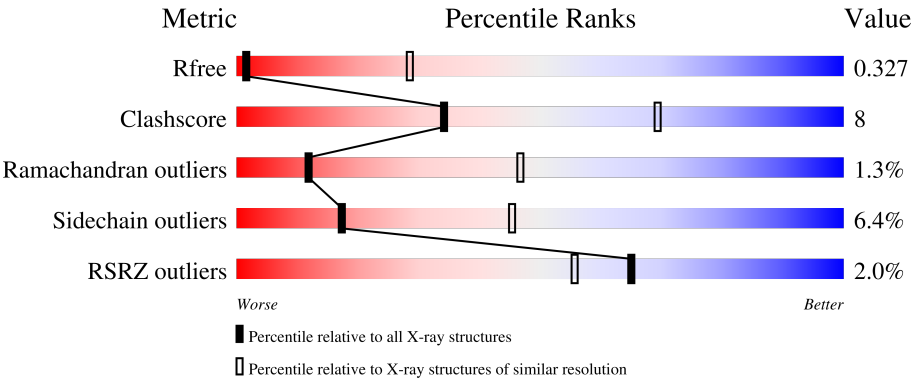
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.11 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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 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 <=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	1494	2% 68% 19% . 12%
2	B	6	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	B	6	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10717 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.

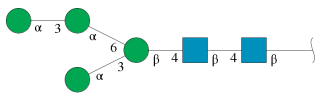
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1319	Total	C	N	O	S	0	0	0
			10616	6785	1806	1993	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

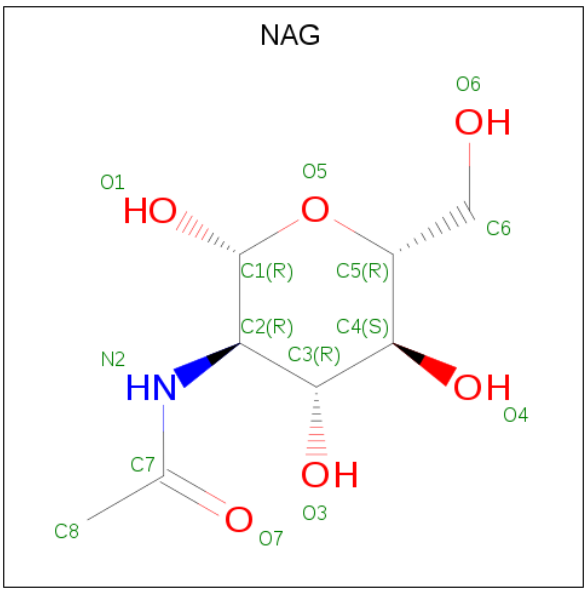
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



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

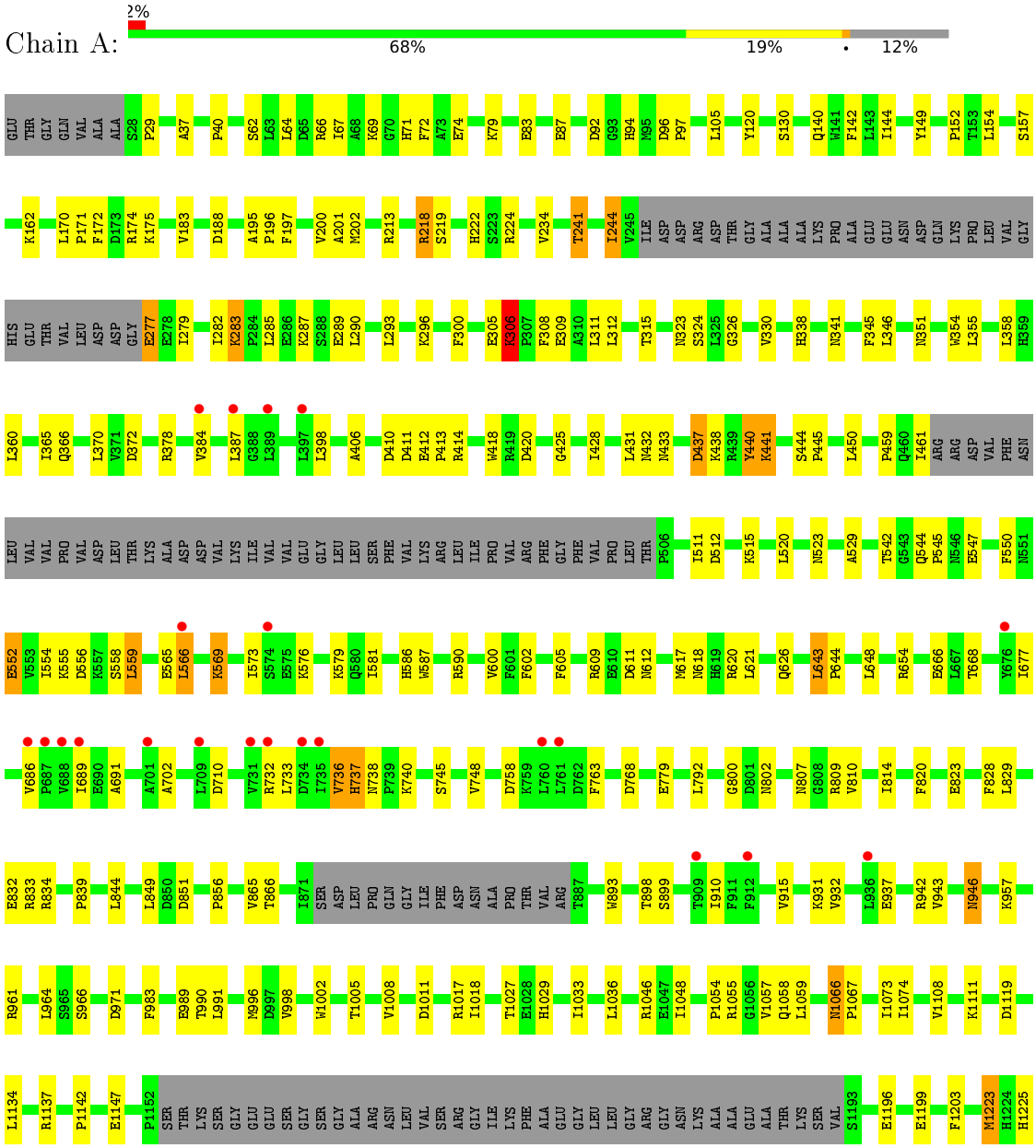
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

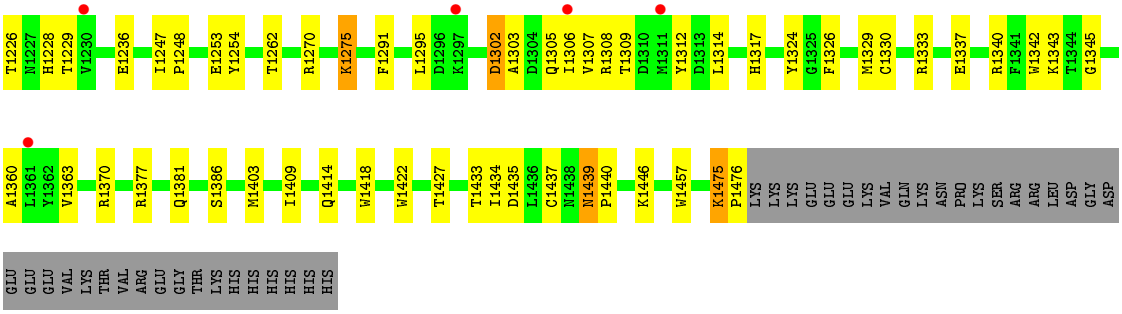
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

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.

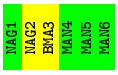
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein





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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.66Å 148.93Å 190.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.15 – 4.11 95.15 – 4.08	Depositor EDS
% Data completeness (in resolution range)	40.7 (95.15-4.11) 40.7 (95.15-4.08)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 4.15Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.255 , 0.315 0.272 , 0.327	Depositor DCC
R_{free} test set	351 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	207.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 257.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10717	wwPDB-VP
Average B, all atoms (Å^2)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: CA, 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	0.28	0/10870	0.59	1/14734 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	GLU	C-N-CA	7.46	140.36	121.70

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	10616	0	10457	178	0
2	B	72	0	61	1	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
All	All	10717	0	10544	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (179) 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:438:LYS:HA	1:A:441:LYS:HG2	1.31	1.12
1:A:643:LEU:HG	1:A:644:PRO:HD3	1.33	1.04
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.76	1.01
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.27	0.97
1:A:309:GLU:HG3	1:A:931:LYS:NZ	1.84	0.91
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.06	0.90
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.08	0.89
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.37	0.89
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.54	0.89
1:A:309:GLU:HG3	1:A:931:LYS:HZ1	1.40	0.83
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.14	0.82
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.63	0.80
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.63	0.79
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.66	0.78
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.66	0.76
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.72	0.72
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.71	0.72
1:A:66:ARG:HA	1:A:69:LYS:HE2	1.72	0.71
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.08	0.71
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.70
1:A:736:VAL:HG23	1:A:737:HIS:H	1.58	0.69
1:A:438:LYS:CA	1:A:441:LYS:HG2	2.17	0.69
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.58	0.69
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.59	0.68
1:A:433:ASN:O	1:A:437:ASP:HB2	1.94	0.67
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.77	0.67
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.76	0.67
1:A:445:PRO:HA	1:A:461:ILE:HG13	1.76	0.66
1:A:1226:THR:OG1	1:A:1228:HIS:ND1	2.28	0.64
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.79	0.64
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.27	0.64
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.59	0.64
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.62	0.63
1:A:554:ILE:O	1:A:558:SER:HB2	1.98	0.63
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.80	0.63
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.80	0.62
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.80	0.62
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.64	0.62
1:A:309:GLU:HG3	1:A:931:LYS:HZ3	1.63	0.62
1:A:1305:GLN:HG2	1:A:1435:ASP:HA	1.82	0.62
1:A:188:ASP:OD1	1:A:219:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:PHE:HB3	1:A:1295:LEU:HD21	1.80	0.61
1:A:1418:TRP:HB3	1:A:1434:ILE:CD1	2.30	0.61
1:A:668:THR:HG23	1:A:810:VAL:HG13	1.82	0.61
1:A:1340:ARG:HD2	1:A:1343:LYS:HZ2	1.66	0.60
1:A:241:THR:HG21	1:A:957:LYS:HD3	1.82	0.60
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.84	0.60
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.84	0.60
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.48	0.60
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.32	0.59
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.90	0.59
1:A:702:ALA:HB1	1:A:732:ARG:HH21	1.68	0.59
1:A:67:ILE:CG2	1:A:72:PHE:HD2	2.12	0.59
1:A:365:ILE:HG23	1:A:370:LEU:HD11	1.85	0.58
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.85	0.58
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.67	0.58
1:A:1439:ASN:HB2	1:A:1440:PRO:HA	1.86	0.58
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.86	0.57
1:A:1055:ARG:HH12	1:A:1377:ARG:HH12	1.53	0.57
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.40	0.56
1:A:643:LEU:HG	1:A:644:PRO:CD	2.22	0.56
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.88	0.56
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.40	0.56
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.23	0.56
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.20	0.56
1:A:1475:LYS:HG3	1:A:1476:PRO:HD3	1.88	0.55
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.85	0.55
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.88	0.55
1:A:244:ILE:HG13	1:A:285:LEU:HD12	1.89	0.54
1:A:66:ARG:O	1:A:71:HIS:HB3	2.07	0.54
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.90	0.54
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.39	0.53
1:A:834:ARG:O	1:A:839:PRO:HD3	2.08	0.53
1:A:736:VAL:HG23	1:A:737:HIS:N	2.21	0.52
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.90	0.52
1:A:306:LYS:HA	1:A:306:LYS:NZ	2.25	0.52
1:A:686:VAL:HG11	1:A:736:VAL:HG12	1.92	0.52
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.74	0.51
1:A:1422:TRP:HZ3	1:A:1437:CYS:HB3	1.76	0.51
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.12	0.51
1:A:899:SER:HA	1:A:943:VAL:O	2.11	0.51
1:A:174:ARG:O	1:A:213:ARG:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:HA	1:A:931:LYS:NZ	2.27	0.50
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.92	0.50
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.12	0.50
1:A:1340:ARG:HD2	1:A:1343:LYS:NZ	2.26	0.50
1:A:413:PRO:HB3	1:A:605:PHE:HE1	1.77	0.50
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.94	0.50
1:A:1360:ALA:HB1	1:A:1435:ASP:OD1	2.11	0.49
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.94	0.49
1:A:277:GLU:N	1:A:324:SER:HG	2.11	0.49
1:A:829:LEU:O	1:A:833:ARG:HB2	2.13	0.49
1:A:1027:THR:HG22	1:A:1029:HIS:H	1.78	0.49
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.48	0.49
1:A:1223:MET:SD	1:A:1254:TYR:HB3	2.53	0.48
1:A:432:ASN:ND2	1:A:440:TYR:OH	2.46	0.48
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.94	0.48
1:A:130:SER:HB3	1:A:162:LYS:O	2.12	0.48
1:A:828:PHE:O	1:A:832:GLU:HB2	2.13	0.48
1:A:1418:TRP:HB3	1:A:1434:ILE:HD13	1.94	0.48
1:A:600:VAL:CG2	1:A:609:ARG:HG3	2.43	0.48
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.96	0.48
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.95	0.47
1:A:1418:TRP:HB3	1:A:1434:ILE:HD12	1.96	0.47
1:A:62:SER:OG	1:A:66:ARG:NH1	2.48	0.47
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.97	0.46
1:A:702:ALA:H	1:A:807:ASN:ND2	2.13	0.46
1:A:296:LYS:HG2	1:A:330:VAL:HG22	1.97	0.46
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.81	0.46
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.86	0.46
2:B:2:NAG:H62	2:B:3:BMA:C1	2.45	0.46
1:A:79:LYS:O	1:A:83:GLU:HG2	2.16	0.46
1:A:174:ARG:O	1:A:213:ARG:CB	2.64	0.46
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.51	0.45
1:A:1302:ASP:OD1	1:A:1302:ASP:C	2.54	0.45
1:A:542:THR:HG22	1:A:544:GLN:H	1.81	0.45
1:A:552:GLU:HA	1:A:555:LYS:NZ	2.32	0.45
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.99	0.45
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.98	0.45
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.35	0.45
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.99	0.45
1:A:544:GLN:HG3	1:A:545:PRO:HD2	1.98	0.45
1:A:654:ARG:HH11	1:A:823:GLU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.99	0.45
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.33	0.45
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.99	0.45
1:A:586:HIS:O	1:A:590:ARG:HB2	2.17	0.45
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.99	0.45
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.52	0.45
1:A:234:VAL:HG22	1:A:996:MET:CE	2.47	0.44
1:A:691:ALA:HB3	1:A:856:PRO:HG2	1.98	0.44
1:A:736:VAL:CG2	1:A:737:HIS:H	2.25	0.44
1:A:306:LYS:HA	1:A:306:LYS:HZ3	1.82	0.44
1:A:338:HIS:O	1:A:341:ASN:HB2	2.17	0.44
1:A:1314:LEU:HG	1:A:1363:VAL:HG21	1.99	0.44
1:A:600:VAL:HG23	1:A:609:ARG:HG3	2.00	0.44
1:A:428:ILE:HD11	1:A:587:TRP:NE1	2.33	0.44
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.99	0.44
1:A:1439:ASN:HB2	1:A:1440:PRO:CA	2.48	0.43
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.18	0.43
1:A:64:LEU:HD12	1:A:67:ILE:HD11	2.00	0.43
1:A:69:LYS:HE3	1:A:71:HIS:HB2	2.01	0.43
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.83	0.43
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	2.01	0.43
1:A:1329:MET:SD	1:A:1342:TRP:NE1	2.92	0.43
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.53	0.43
1:A:552:GLU:HA	1:A:555:LYS:HZ1	1.84	0.43
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.42	0.43
1:A:740:LYS:HB2	1:A:800:GLY:HA3	2.00	0.43
1:A:961:ARG:HD3	1:A:961:ARG:HA	1.92	0.43
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.47	0.42
1:A:195:ALA:HB3	1:A:196:PRO:HD3	2.00	0.42
1:A:1306:ILE:CD1	1:A:1457:TRP:HD1	2.30	0.42
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	3.07	0.42
1:A:311:LEU:O	1:A:315:THR:HG22	2.18	0.42
1:A:573:ILE:HB	1:A:576:LYS:CB	2.47	0.42
1:A:120:TYR:CG	1:A:218:ARG:HG2	2.55	0.42
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.02	0.42
1:A:745:SER:O	1:A:748:VAL:HG22	2.20	0.42
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.39	0.42
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.52	0.41
1:A:702:ALA:H	1:A:807:ASN:HD21	1.68	0.41
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.34	0.41
1:A:296:LYS:HE2	1:A:330:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD11	1:A:910:ILE:HG23	2.03	0.41
1:A:105:LEU:HD13	1:A:966:SER:HA	2.03	0.41
1:A:1275:LYS:HB3	1:A:1275:LYS:HE2	1.92	0.41
1:A:1340:ARG:HD3	1:A:1342:TRP:CZ2	2.56	0.41
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.85	0.41
1:A:413:PRO:HB3	1:A:605:PHE:CE1	2.56	0.41
1:A:523:ASN:OD1	1:A:566:LEU:HA	2.20	0.41
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.61	0.40
1:A:283:LYS:HD2	1:A:283:LYS:O	2.22	0.40
1:A:406:ALA:HB2	1:A:839:PRO:HG2	2.04	0.40
1:A:346:LEU:HD11	1:A:354:TRP:HH2	1.87	0.40
1:A:450:LEU:HD23	1:A:459:PRO:HB2	2.04	0.40
1:A:351:ASN:HA	1:A:915:VAL:O	2.21	0.40
1:A:37:ALA:HA	1:A:1036:LEU:HB3	2.03	0.40
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.37	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	1309/1494 (88%)	1235 (94%)	57 (4%)	17 (1%)	12 47

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ILE
1	A	287	LYS
1	A	306	LYS
1	A	444	SER
1	A	737	HIS
1	A	1303	ALA

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Mol	Chain	Res	Type
1	A	1439	ASN
1	A	569	LYS
1	A	736	VAL
1	A	1345	GLY
1	A	559	LEU
1	A	666	GLU
1	A	611	ASP
1	A	1475	LYS
1	A	279	ILE
1	A	1142	PRO
1	A	1337	GLU

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	1151/1297 (89%)	1077 (94%)	74 (6%)	17 45

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	87	GLU
1	A	140	GLN
1	A	154	LEU
1	A	175	LYS
1	A	202	MET
1	A	218	ARG
1	A	222	HIS
1	A	241	THR
1	A	277	GLU
1	A	283	LYS
1	A	289	GLU
1	A	300	PHE
1	A	306	LYS
1	A	308	PHE

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Mol	Chain	Res	Type
1	A	323	ASN
1	A	358	LEU
1	A	360	LEU
1	A	366	GLN
1	A	372	ASP
1	A	378	ARG
1	A	387	LEU
1	A	410	ASP
1	A	411	ASP
1	A	412	GLU
1	A	414	ARG
1	A	431	LEU
1	A	437	ASP
1	A	440	TYR
1	A	441	LYS
1	A	552	GLU
1	A	556	ASP
1	A	559	LEU
1	A	565	GLU
1	A	566	LEU
1	A	569	LYS
1	A	579	LYS
1	A	612	ASN
1	A	617	MET
1	A	618	ASN
1	A	620	ARG
1	A	626	GLN
1	A	643	LEU
1	A	677	ILE
1	A	710	ASP
1	A	758	ASP
1	A	779	GLU
1	A	809	ARG
1	A	820	PHE
1	A	851	ASP
1	A	937	GLU
1	A	942	ARG
1	A	946	ASN
1	A	971	ASP
1	A	989	GLU
1	A	1011	ASP
1	A	1046	ARG

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Mol	Chain	Res	Type
1	A	1066	ASN
1	A	1147	GLU
1	A	1196	GLU
1	A	1203	PHE
1	A	1223	MET
1	A	1253	GLU
1	A	1262	THR
1	A	1275	LYS
1	A	1302	ASP
1	A	1309	THR
1	A	1312	TYR
1	A	1317	HIS
1	A	1330	CYS
1	A	1333	ARG
1	A	1370	ARG
1	A	1414	GLN
1	A	1446	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	432	ASN
1	A	679	ASN
1	A	807	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.

There are no bond length outliers.

There are no bond angle outliers.

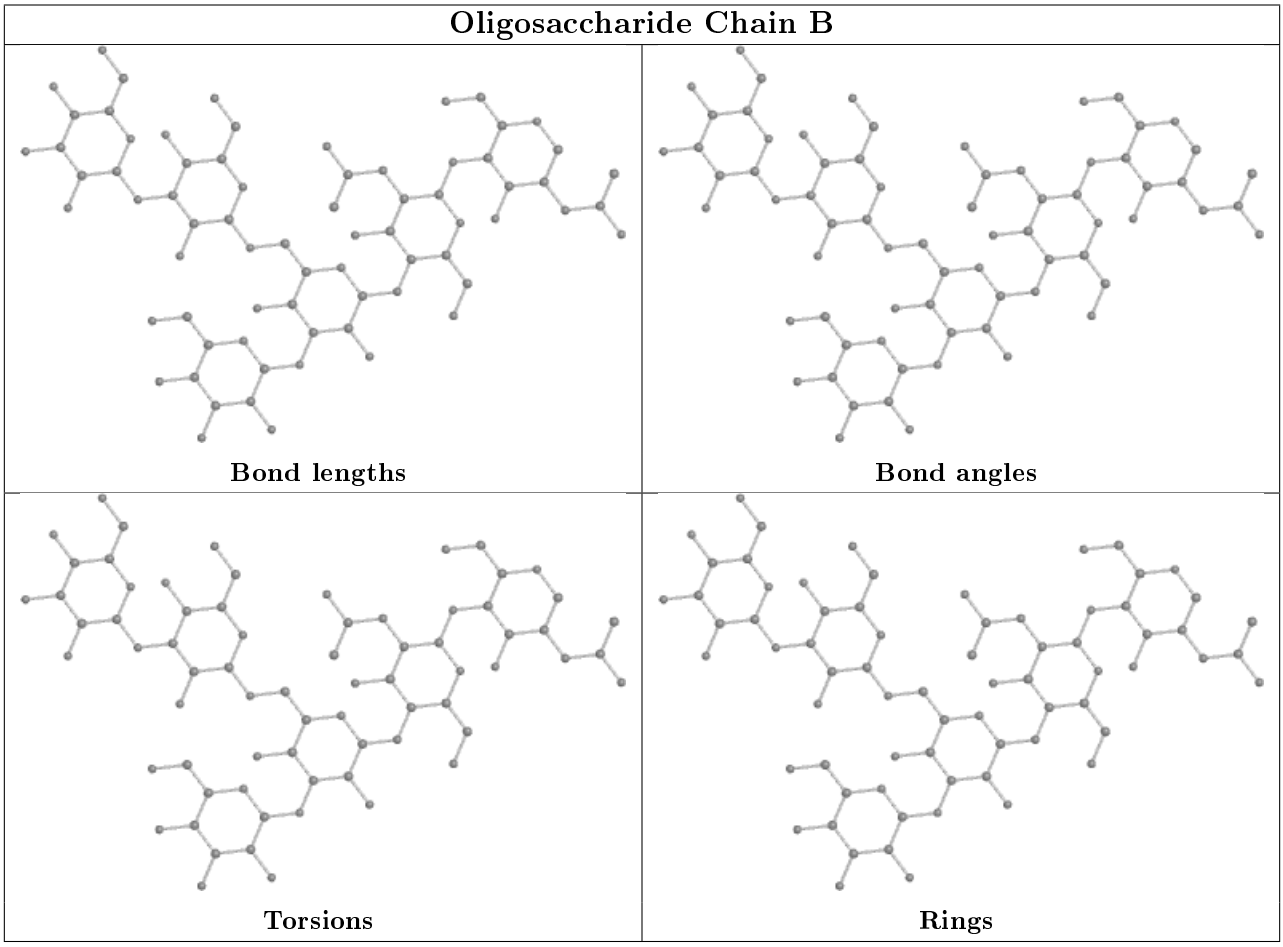
There are no chirality outliers.

There are no torsion outliers.

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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	1319/1494 (88%)	-0.22	27 (2%) 65 56	94, 284, 300, 300	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	761	LEU	4.0
1	A	686	VAL	4.0
1	A	687	PRO	3.9
1	A	734	ASP	3.4
1	A	1361	LEU	3.2
1	A	912	PHE	3.2
1	A	1230	VAL	3.0
1	A	760	LEU	2.9
1	A	387	LEU	2.8
1	A	701	ALA	2.7
1	A	909	THR	2.6
1	A	735	ILE	2.5
1	A	688	VAL	2.5
1	A	1306	ILE	2.4
1	A	574	SER	2.3
1	A	1297	LYS	2.3
1	A	709	LEU	2.1
1	A	676	TYR	2.1
1	A	936	LEU	2.1
1	A	566	LEU	2.1
1	A	731	VAL	2.1
1	A	384	VAL	2.1
1	A	1311	MET	2.1
1	A	689	ILE	2.1
1	A	397	LEU	2.1
1	A	389	LEU	2.0
1	A	732	ARG	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)

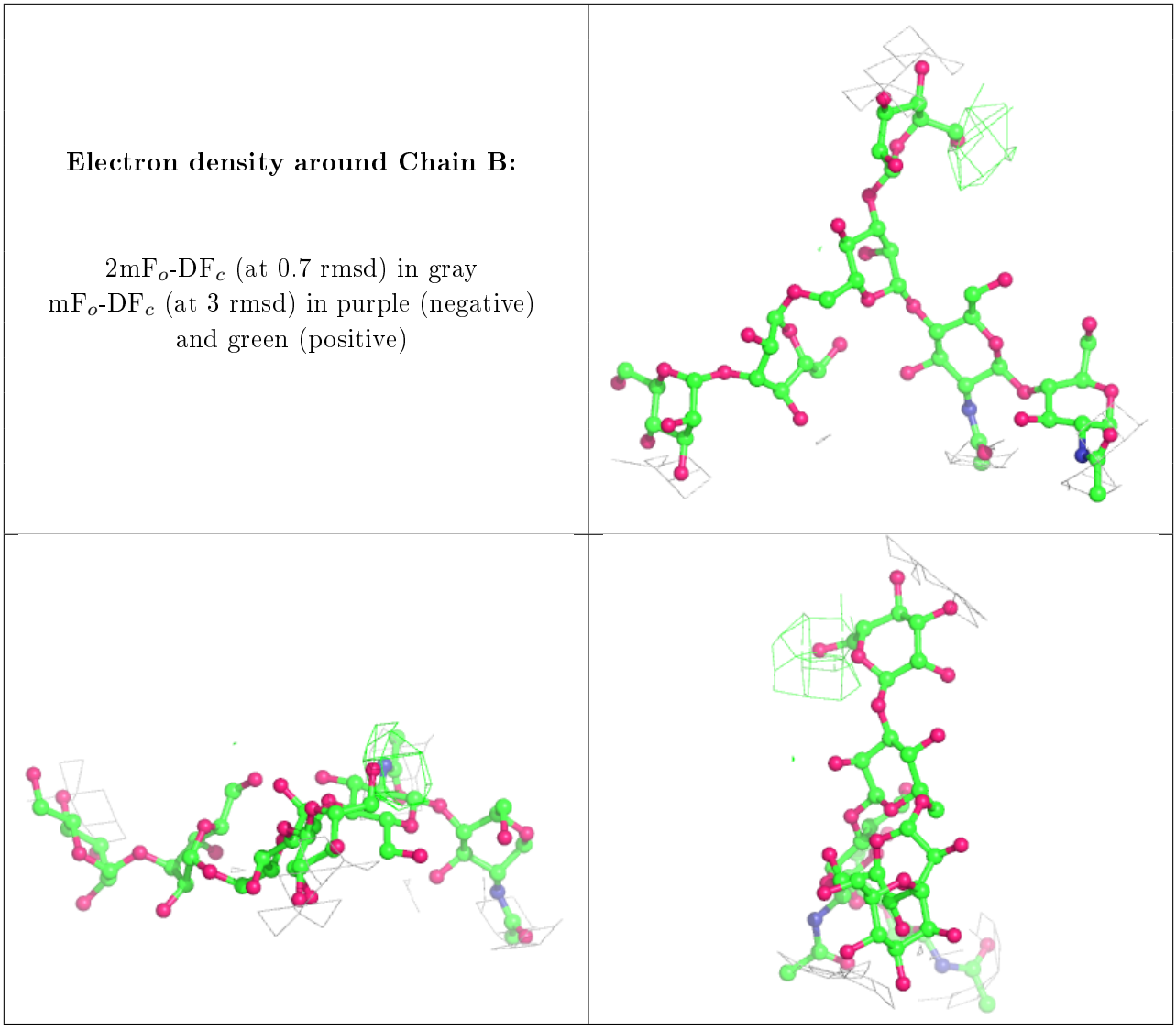
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MAN	B	5	11/12	0.77	0.21	292,293,295,295	0
2	MAN	B	6	11/12	0.79	0.40	300,300,300,300	0
2	BMA	B	3	11/12	0.83	0.27	298,300,300,300	0
2	MAN	B	4	11/12	0.92	0.25	293,295,297,297	0
2	NAG	B	2	14/15	0.96	0.18	290,295,300,300	0
2	NAG	B	1	14/15	0.98	0.20	286,292,296,298	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

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
4	CA	A	1603	1/1	0.78	0.14	298,298,298,298	1
3	NAG	A	1601	14/15	0.86	0.21	240,268,285,290	0
3	NAG	A	1602	14/15	0.89	0.19	300,300,300,300	0

6.5 Other polymers

There are no such residues in this entry.