Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 06:55 AM EDT

PDB ID	:	3WPC
Title	:	Crystal structure of horse TLR9 in complex with agonistic DNA1668_12mer
Authors	:	Ohto, U.; Tanji, H.; Shimizu, T.
Deposited on	:	2014-01-11
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

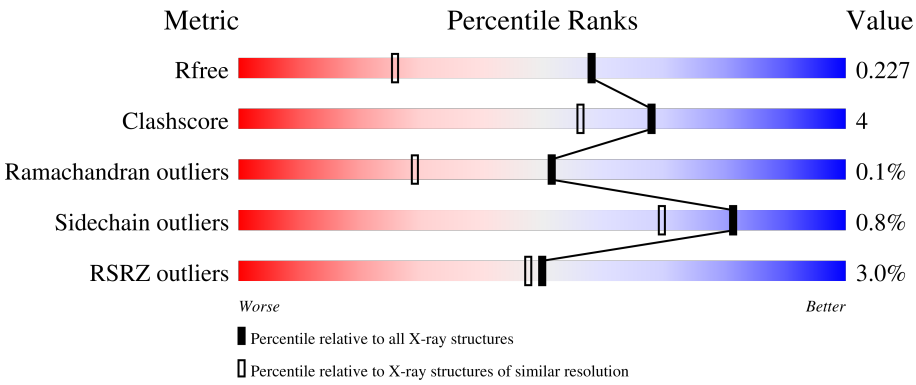
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	802	2%, 86%, 7%, 7%
1	B	802	2%, 86%, 7%, 7%
2	E	12	25%, 58%, 42%
2	F	12	25%, 42%, 58%
3	C	2	100%

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Mol	Chain	Length	Quality of chain
3	D	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14350 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 Toll-like receptor 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	6013	3834	1058	1093	28	7	19	0
1	B	749	6009	3833	1054	1093	29	12	18	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q2EEY0
A	23	SER	-	expression tag	UNP Q2EEY0
A	24	PRO	-	expression tag	UNP Q2EEY0
A	25	TRP	-	expression tag	UNP Q2EEY0
A	818	GLU	-	expression tag	UNP Q2EEY0
A	819	PHE	-	expression tag	UNP Q2EEY0
A	820	LEU	-	expression tag	UNP Q2EEY0
A	821	VAL	-	expression tag	UNP Q2EEY0
A	822	PRO	-	expression tag	UNP Q2EEY0
A	823	ARG	-	expression tag	UNP Q2EEY0
B	22	ARG	-	expression tag	UNP Q2EEY0
B	23	SER	-	expression tag	UNP Q2EEY0
B	24	PRO	-	expression tag	UNP Q2EEY0
B	25	TRP	-	expression tag	UNP Q2EEY0
B	818	GLU	-	expression tag	UNP Q2EEY0
B	819	PHE	-	expression tag	UNP Q2EEY0
B	820	LEU	-	expression tag	UNP Q2EEY0
B	821	VAL	-	expression tag	UNP Q2EEY0
B	822	PRO	-	expression tag	UNP Q2EEY0
B	823	ARG	-	expression tag	UNP Q2EEY0

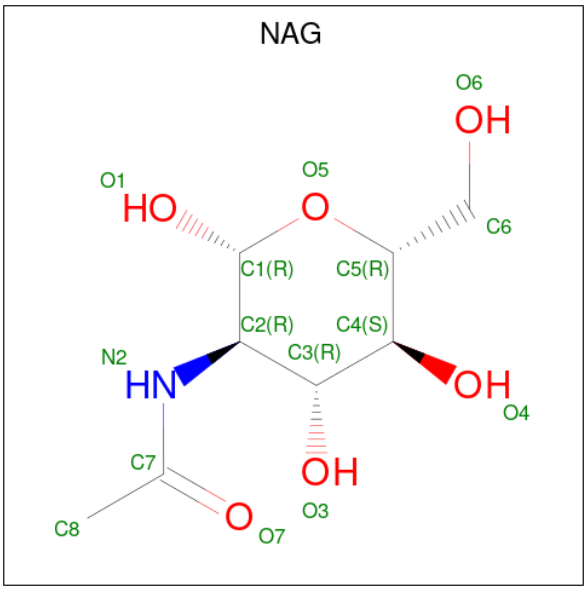
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*TP*GP*AP*CP*GP*TP*TP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	12	239	116	40	72	11	0	0	0
2	E	12	239	116	40	72	11	0	0	0

- 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
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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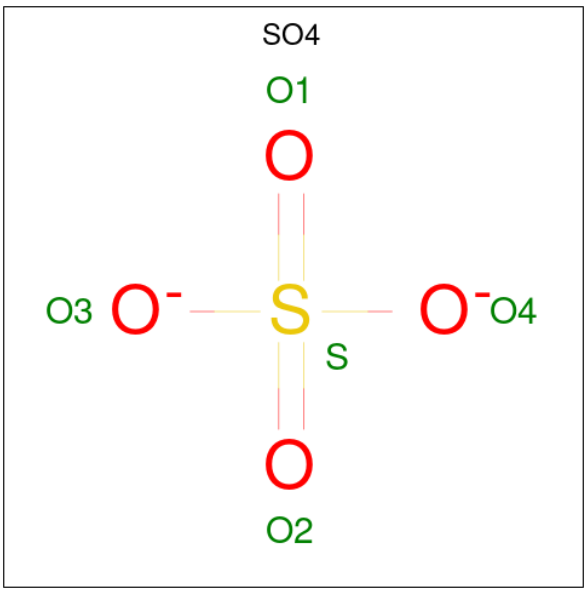
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

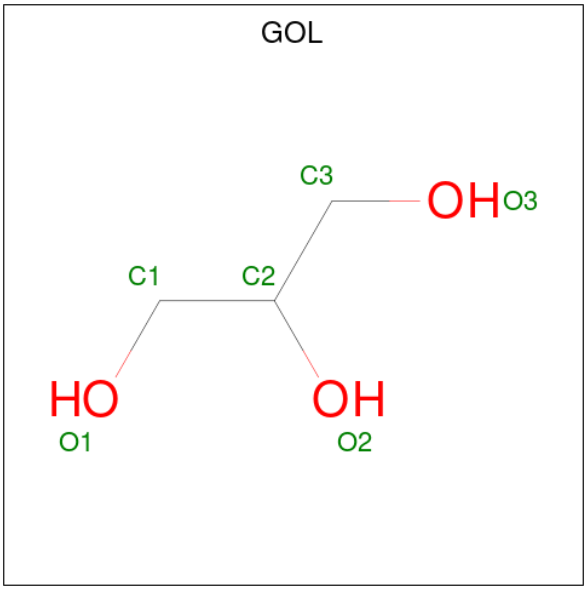


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	B	1	1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	766	766	766	0	0
			Total	O		
8	B	788	788	788	0	0
			Total	O		
8	F	21	21	21	0	0

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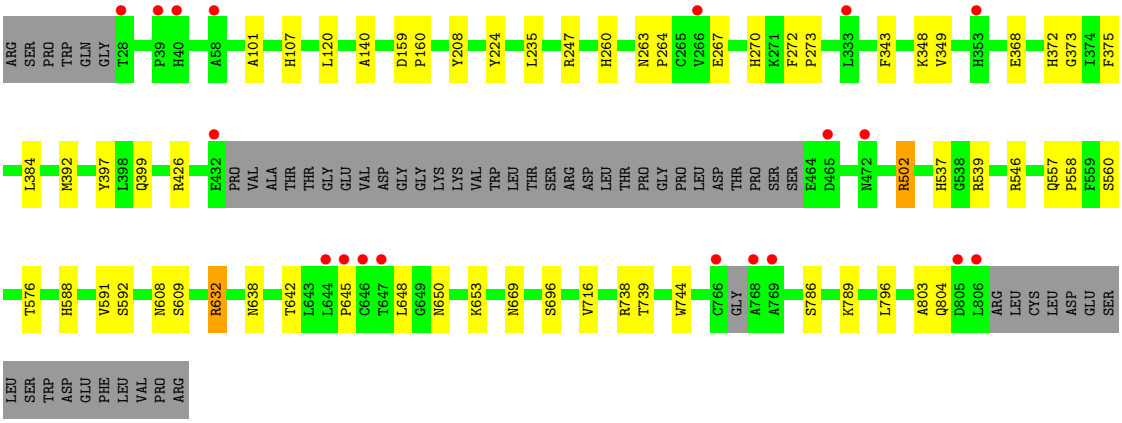
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	E	20	20	20	0	0

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.

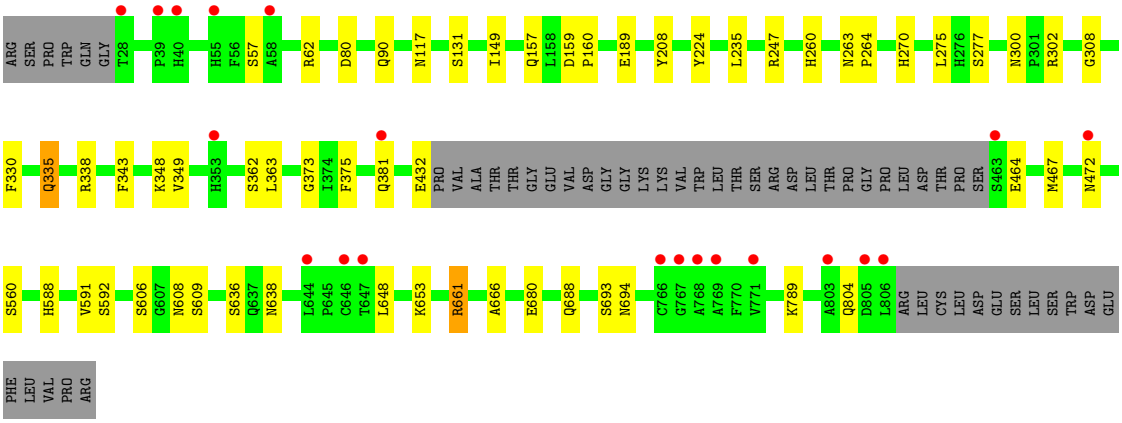
• Molecule 1: Toll-like receptor 9

Chain A:



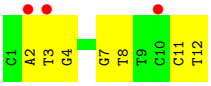
• Molecule 1: Toll-like receptor 9

Chain B:



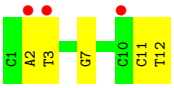
• Molecule 2: DNA (5'-D(*CP*AP*TP*GP*AP*CP*GP*TP*TP*CP*CP*T)-3')

Chain F:



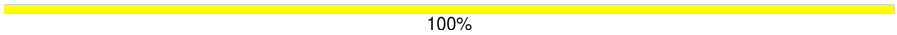
• Molecule 2: DNA (5'-D(*CP*AP*TP*GP*AP*CP*GP*TP*TP*CP*CP*T)-3')

Chain E:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.76Å 81.62Å 81.52Å 87.50° 83.50° 85.98°	Depositor
Resolution (Å)	47.49 – 1.60 44.13 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (47.49-1.60) 95.6 (44.13-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.184 , 0.220 0.193 , 0.227	Depositor DCC
R_{free} test set	11134 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.086 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14350	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, NA, GOL

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	0.70	0/6152	0.85	7/8370 (0.1%)
1	B	0.70	0/6149	0.83	3/8366 (0.0%)
2	E	0.77	1/266 (0.4%)	1.04	0/408
2	F	0.64	0/266	1.02	2/408 (0.5%)
All	All	0.70	1/12833 (0.0%)	0.85	12/17552 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	DG	O3'-P	-6.95	1.52	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	432	GLU	CB-CA-C	-6.41	97.57	110.40
1	A	392	MET	CG-SD-CE	-5.96	90.66	100.20
1	A	738	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	426	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	661	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	80	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	502	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	546	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	632	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	632	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	F	8	DT	O5'-P-OP2	-5.03	101.17	105.70
2	F	4	DG	O5'-P-OP1	-5.02	101.18	105.70

There are no chirality outliers.

There are no planarity outliers.

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	6013	0	6008	41	0
1	B	6009	0	6005	40	0
2	E	239	0	138	9	0
2	F	239	0	138	10	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	84	0	78	0	0
4	B	98	0	91	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	B	1	0	0	0	0
7	B	6	0	8	1	0
8	A	766	0	0	13	1
8	B	788	0	0	10	2
8	E	20	0	0	0	0
8	F	21	0	0	0	0
All	All	14350	0	12516	97	2

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 4.

All (97) 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:642[B]:THR:OG1	2:F:7:DG:H5"	1.57	1.01
2:F:11:DC:OP1	2:F:12:DT:H73	1.82	0.79
1:B:277[A]:SER:OG	1:B:302:ARG:NH1	2.17	0.78
1:B:653:LYS:HA	1:B:653:LYS:HE2	1.69	0.72
2:E:11:DC:OP1	2:E:12:DT:H73	1.92	0.69
1:B:224:TYR:OH	1:B:247:ARG:NH2	2.21	0.69
1:A:642[B]:THR:HG1	2:F:7:DG:H5"	1.56	0.68
2:E:2:DA:N3	2:E:2:DA:H5"	2.09	0.68
1:A:537:HIS:HD2	1:A:539:ARG:H	1.42	0.65
2:F:2:DA:H5"	2:F:2:DA:N3	2.11	0.65
1:A:120:LEU:HD21	1:A:140:ALA:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:DA:N3	2:E:2:DA:H3'	2.12	0.64
1:A:120:LEU:HD21	1:A:140:ALA:CB	2.28	0.63
1:B:666:ALA:HB2	1:B:688:GLN:HG3	1.81	0.62
1:A:560:SER:OG	8:A:1504:HOH:O	2.05	0.62
1:B:789:LYS:NZ	8:B:1573:HOH:O	2.33	0.61
2:F:11:DC:P	2:F:12:DT:H73	2.41	0.61
8:A:1634:HOH:O	1:B:260:HIS:HD2	1.82	0.60
1:A:120:LEU:HD22	8:A:1022:HOH:O	2.01	0.59
1:B:277[B]:SER:OG	1:B:300:ASN:ND2	2.34	0.59
1:A:537:HIS:CD2	1:A:539:ARG:H	2.20	0.59
2:E:11:DC:OP2	2:E:12:DT:O4	2.22	0.58
1:A:739:THR:HG22	8:A:1571:HOH:O	2.03	0.57
1:B:117[A]:ASN:ND2	8:B:1495:HOH:O	2.37	0.57
1:B:90:GLN:NE2	8:B:1509:HOH:O	2.27	0.56
2:E:11:DC:P	2:E:12:DT:H73	2.47	0.55
1:B:560:SER:OG	8:B:1435:HOH:O	2.08	0.54
1:A:796[B]:LEU:HD22	1:A:804:GLN:OE1	2.07	0.54
1:A:696:SER:OG	8:A:1707:HOH:O	2.16	0.54
1:A:260:HIS:HE1	8:A:1495:HOH:O	1.91	0.54
1:B:159:ASP:HB2	1:B:160:PRO:CD	2.38	0.53
1:A:796[A]:LEU:HD12	1:A:796[A]:LEU:N	2.24	0.53
1:B:648:LEU:HD12	8:B:1111:HOH:O	2.09	0.53
1:A:669:ASN:ND2	8:A:1600:HOH:O	2.41	0.52
1:A:224:TYR:OH	1:A:247:ARG:NH2	2.43	0.52
1:A:650:ASN:ND2	8:A:1369:HOH:O	2.39	0.52
1:B:260:HIS:HE1	8:B:1407:HOH:O	1.93	0.52
1:B:693[A]:SER:O	1:B:694:ASN:HB2	2.09	0.52
1:B:235:LEU:HB3	1:B:275:LEU:HD23	1.92	0.51
2:F:11:DC:OP2	2:F:12:DT:O4	2.28	0.51
1:A:632:ARG:NH2	8:A:1661:HOH:O	2.24	0.48
2:F:2:DA:N3	2:F:2:DA:H3'	2.29	0.48
1:A:159[A]:ASP:HB2	1:A:160:PRO:CD	2.44	0.48
1:A:576[B]:THR:HG22	1:A:576[B]:THR:O	2.14	0.48
1:A:208:TYR:CZ	2:E:12:DT:H71	2.50	0.47
7:B:912:GOL:H12	8:B:1197:HOH:O	2.13	0.47
2:E:11:DC:P	2:E:12:DT:O4	2.72	0.47
1:A:557:GLN:HB3	1:A:558:PRO:HD3	1.96	0.47
1:A:786:SER:O	1:A:789:LYS:NZ	2.45	0.47
1:A:804:GLN:N	1:A:804:GLN:CD	2.69	0.46
1:B:588:HIS:HB3	1:B:609[A]:SER:HB2	1.97	0.46
1:B:653:LYS:HE2	1:B:653:LYS:CA	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:DT:H6	2:F:3:DT:H5"	1.80	0.46
1:A:502:ARG:HB3	8:A:1536:HOH:O	2.14	0.46
1:A:588:HIS:HB3	1:A:609[A]:SER:HB2	1.98	0.45
1:B:591:VAL:HG22	1:B:592:SER:N	2.31	0.45
1:B:348:LYS:HB2	1:B:349:VAL:HG13	1.97	0.45
1:B:464:GLU:HA	1:B:467:MET:O	2.17	0.45
2:E:2:DA:N3	2:E:2:DA:C3'	2.79	0.45
1:A:591:VAL:HG22	1:A:592:SER:N	2.32	0.44
1:B:653:LYS:CA	1:B:653:LYS:CE	2.95	0.44
1:A:803:ALA:HB3	1:A:804:GLN:OE1	2.18	0.44
1:B:308:GLY:O	1:B:335:GLN:HG3	2.16	0.44
1:A:645:PRO:HG3	1:A:669:ASN:HD22	1.82	0.44
1:A:368:GLU:HG3	1:A:397:TYR:HE2	1.83	0.44
1:A:272:PHE:HB3	1:A:273:PRO:HA	2.00	0.43
1:A:267:GLU:CD	8:A:1370:HOH:O	2.56	0.43
2:F:11:DC:P	2:F:12:DT:O4	2.77	0.43
1:A:372:HIS:HB2	1:A:399:GLN:O	2.18	0.43
1:B:263:ASN:HB2	1:B:264:PRO:HD2	1.99	0.43
1:B:208:TYR:CZ	2:F:12:DT:H71	2.54	0.43
1:B:263:ASN:HB2	1:B:264:PRO:CD	2.49	0.43
1:A:591:VAL:HG22	1:A:592:SER:H	1.84	0.43
1:B:608:ASN:O	1:B:638:ASN:HA	2.19	0.43
1:B:693[A]:SER:O	1:B:694:ASN:CB	2.67	0.42
1:A:608:ASN:O	1:A:638:ASN:HA	2.19	0.42
1:B:653:LYS:HA	1:B:653:LYS:CE	2.40	0.42
8:A:1634:HOH:O	1:B:260:HIS:CD2	2.66	0.42
1:B:804:GLN:N	1:B:804:GLN:CD	2.73	0.42
1:A:348:LYS:HB2	1:A:349:VAL:HG13	2.02	0.41
1:B:606:SER:HA	1:B:636:SER:O	2.20	0.41
1:B:591:VAL:HG22	1:B:592:SER:H	1.85	0.41
1:B:131:SER:HB3	1:B:149[B]:ILE:HG22	2.02	0.41
1:A:120:LEU:HD21	1:A:140:ALA:HB1	2.02	0.41
1:B:338:ARG:NH1	8:B:1712:HOH:O	2.54	0.41
1:B:472:ASN:OD1	1:B:472:ASN:N	2.43	0.41
1:A:101:ALA:O	1:A:107:HIS:HA	2.20	0.41
1:A:263:ASN:HB2	1:A:264:PRO:CD	2.51	0.41
1:A:384:LEU:HB2	8:A:1749:HOH:O	2.21	0.41
1:A:343:PHE:HA	1:A:373:GLY:O	2.20	0.41
1:A:716:VAL:HB	1:A:744:TRP:CE2	2.55	0.41
1:B:330:PHE:HB3	1:B:363:LEU:HD21	2.01	0.41
1:B:661:ARG:NH2	8:B:1492:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLN:HA	1:B:189:GLU:O	2.22	0.40
1:B:343:PHE:HA	1:B:373:GLY:O	2.22	0.40
1:B:680:GLU:OE1	8:B:1650:HOH:O	2.22	0.40
2:E:3:DT:H6	2:E:3:DT:H5"	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1286:HOH:O	8:B:1285:HOH:O[1_655]	1.71	0.49
8:B:1218:HOH:O	8:B:1753:HOH:O[1_556]	2.13	0.07

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	760/802 (95%)	729 (96%)	30 (4%)	1 (0%)	51	29
1	B	763/802 (95%)	723 (95%)	39 (5%)	1 (0%)	51	29
All	All	1523/1604 (95%)	1452 (95%)	69 (4%)	2 (0%)	51	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	PHE
1	A	375	PHE

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	683/712 (96%)	678 (99%)	5 (1%)	84	73
1	B	683/712 (96%)	676 (99%)	7 (1%)	76	61
All	All	1366/1424 (96%)	1354 (99%)	12 (1%)	81	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	270[A]	HIS
1	A	270[B]	HIS
1	A	648	LEU
1	A	653	LYS
1	B	57	SER
1	B	62	ARG
1	B	270	HIS
1	B	335	GLN
1	B	362[A]	SER
1	B	362[B]	SER
1	B	381	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	HIS
1	A	650	ASN
1	B	260	HIS
1	B	270	HIS
1	B	641	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	C	1	1,3	14,14,15	0.82	0	17,19,21	1.14	2 (11%)
3	NAG	C	2	3	14,14,15	0.48	0	17,19,21	1.55	3 (17%)
3	NAG	D	1	1,3	14,14,15	0.74	0	17,19,21	1.04	1 (5%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	1.43	4 (23%)

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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	O5-C1-C2	-3.77	105.45	111.29
3	C	2	NAG	O5-C1-C2	-3.45	105.95	111.29
3	C	2	NAG	C1-O5-C5	3.10	116.34	112.19
3	C	2	NAG	C1-C2-N2	2.74	114.75	110.43
3	D	1	NAG	C3-C4-C5	-2.34	105.99	110.23
3	D	2	NAG	O5-C5-C6	2.31	112.16	107.66
3	C	1	NAG	O5-C5-C6	2.27	112.07	107.66
3	C	1	NAG	O7-C7-C8	-2.19	118.15	122.05
3	D	2	NAG	O3-C3-C2	2.11	113.79	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C1-C2-N2	2.03	113.62	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

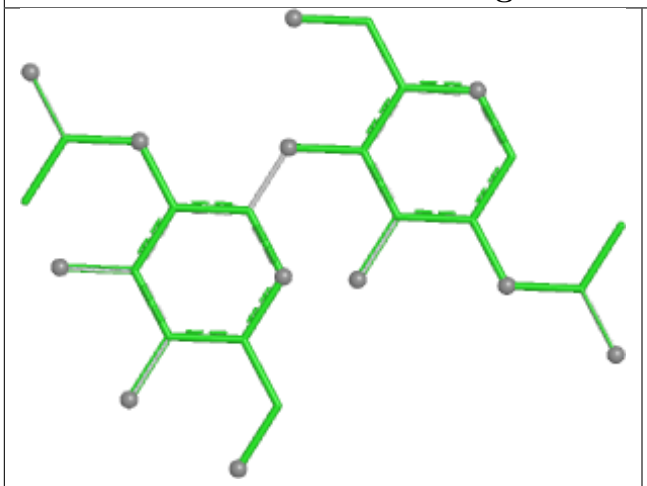
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

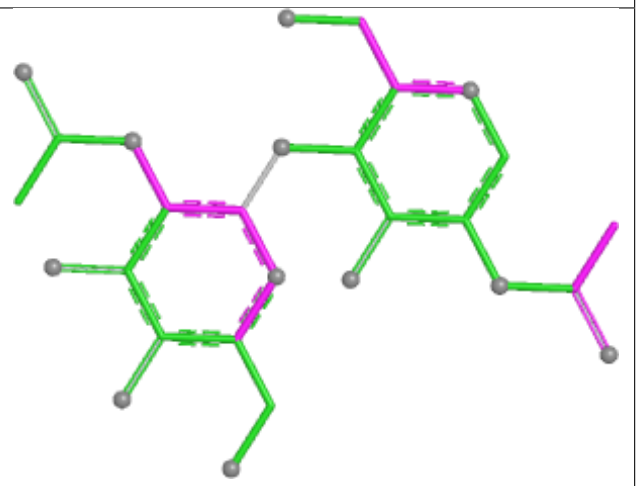
No monomer is involved in short contacts.

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

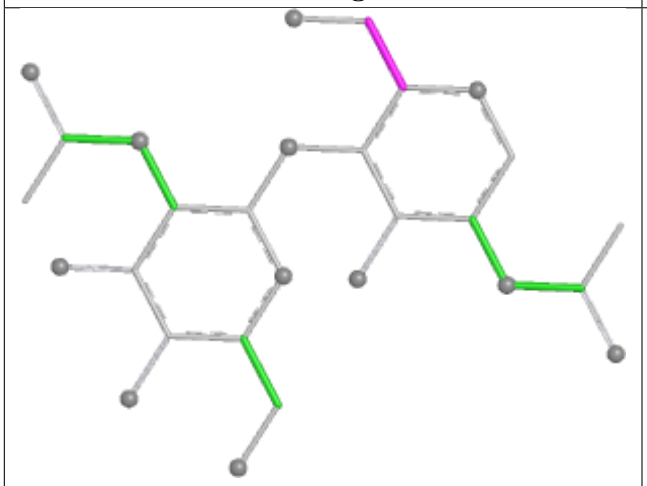
Oligosaccharide Chain C



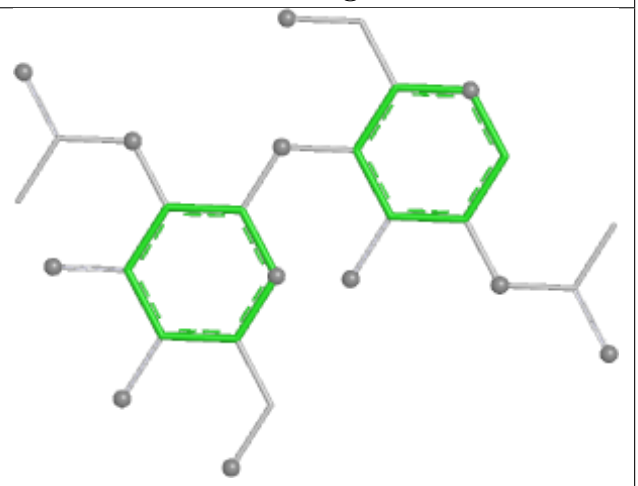
Bond lengths



Bond angles

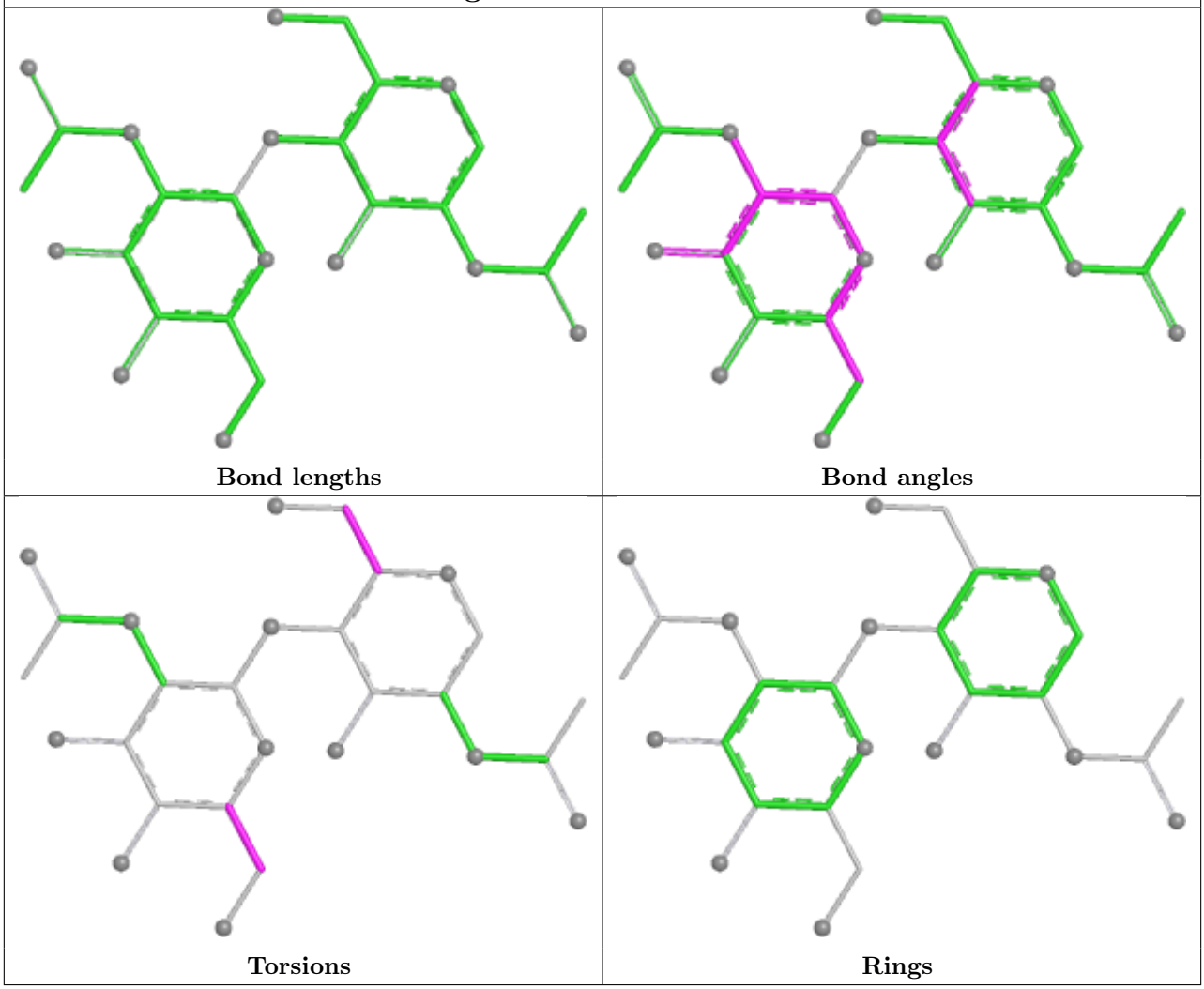


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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	902	1	14,14,15	0.79	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	B	901	1	14,14,15	0.69	0	17,19,21	1.31	1 (5%)
4	NAG	B	907	1	14,14,15	0.62	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	902	1	14,14,15	0.71	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	A	906	1	14,14,15	0.58	0	17,19,21	0.92	0
4	NAG	A	905	1	14,14,15	0.81	1 (7%)	17,19,21	1.06	0
4	NAG	A	901	1	14,14,15	0.44	0	17,19,21	1.23	3 (17%)
4	NAG	B	904	1	14,14,15	0.78	0	17,19,21	1.46	3 (17%)
4	NAG	B	905	1	14,14,15	0.76	0	17,19,21	0.98	0
4	NAG	A	904	1	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
4	NAG	B	906	1	14,14,15	0.74	0	17,19,21	1.63	5 (29%)
5	SO4	A	909	-	4,4,4	0.68	0	6,6,6	0.22	0
5	SO4	B	911	-	4,4,4	0.66	0	6,6,6	0.33	0
4	NAG	B	903	1	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
7	GOL	B	912	-	5,5,5	0.27	0	5,5,5	0.59	0
4	NAG	A	903	1	14,14,15	0.41	0	17,19,21	1.34	2 (11%)

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	902	1	-	1/6/23/26	0/1/1/1
4	NAG	B	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	1/6/23/26	0/1/1/1
4	NAG	B	902	1	-	1/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	0/6/23/26	0/1/1/1
4	NAG	B	905	1	-	2/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	2/6/23/26	0/1/1/1
4	NAG	B	903	1	-	2/6/23/26	0/1/1/1
7	GOL	B	912	-	-	4/4/4/4	-
4	NAG	A	903	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	905	NAG	O5-C1	-2.32	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	NAG	C1-C2	2.18	1.55	1.52
4	A	902	NAG	O5-C1	-2.07	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	NAG	C1-O5-C5	3.80	117.28	112.19
4	B	906	NAG	C1-O5-C5	3.77	117.25	112.19
4	A	903	NAG	C1-O5-C5	3.67	117.11	112.19
4	B	904	NAG	C2-N2-C7	-3.46	118.26	122.90
4	B	902	NAG	O7-C7-C8	-3.19	116.38	122.05
4	B	903	NAG	O5-C1-C2	-2.89	106.83	111.29
4	B	906	NAG	O7-C7-C8	-2.73	117.20	122.05
4	A	904	NAG	C1-C2-N2	-2.54	106.44	110.43
4	B	906	NAG	C1-C2-N2	-2.53	106.45	110.43
4	B	902	NAG	O5-C5-C6	2.39	112.32	107.66
4	B	907	NAG	C6-C5-C4	-2.39	107.16	113.02
4	A	902	NAG	O7-C7-C8	-2.36	117.84	122.05
4	A	901	NAG	O5-C5-C6	2.36	112.25	107.66
4	B	906	NAG	O7-C7-N2	2.23	125.92	121.98
4	A	903	NAG	C6-C5-C4	-2.23	107.55	113.02
4	B	904	NAG	O5-C5-C4	-2.19	105.50	110.83
4	B	907	NAG	C4-C3-C2	2.19	114.23	111.02
4	B	904	NAG	O5-C1-C2	-2.16	107.94	111.29
4	A	901	NAG	O7-C7-C8	-2.07	118.37	122.05
4	A	901	NAG	C1-C2-N2	-2.03	107.23	110.43
4	B	906	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	912	GOL	O1-C1-C2-C3
7	B	912	GOL	C1-C2-C3-O3
4	B	905	NAG	O5-C5-C6-O6
4	B	906	NAG	O5-C5-C6-O6
4	B	905	NAG	C4-C5-C6-O6
4	B	906	NAG	C4-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6
7	B	912	GOL	O1-C1-C2-O2
7	B	912	GOL	O2-C2-C3-O3
4	A	903	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	902	NAG	C4-C5-C6-O6
4	B	903	NAG	C4-C5-C6-O6
4	B	902	NAG	C4-C5-C6-O6
4	B	907	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	912	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	747/802 (93%)	0.02	19 (2%)	57	55	10, 19, 35, 64	1 (0%)
1	B	749/802 (93%)	0.01	20 (2%)	54	52	10, 18, 37, 58	2 (0%)
2	E	12/12 (100%)	1.02	3 (25%)	0	0	27, 32, 65, 82	0
2	F	12/12 (100%)	0.98	3 (25%)	0	0	23, 32, 62, 102	0
All	All	1520/1628 (93%)	0.03	45 (2%)	50	48	10, 18, 37, 102	3 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	CYS	10.0
1	B	646	CYS	6.5
1	B	806	LEU	5.3
1	B	766	CYS	5.2
1	A	766	CYS	4.7
2	F	2	DA	4.4
2	E	2	DA	4.4
1	B	644	LEU	4.0
1	A	806	LEU	3.8
1	B	39	PRO	3.6
1	A	769	ALA	3.6
1	B	769	ALA	3.6
1	A	40	HIS	3.5
1	B	58	ALA	3.2
1	A	644	LEU	3.1
1	A	432	GLU	3.1
1	A	39	PRO	3.0
1	A	266	VAL	3.0
1	A	645	PRO	3.0
1	B	803	ALA	2.7
1	A	805	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	767	GLY	2.7
1	B	647	THR	2.7
2	F	3	DT	2.6
1	A	647	THR	2.6
1	B	28	THR	2.6
1	A	768	ALA	2.6
2	E	3	DT	2.5
1	B	353	HIS	2.5
1	B	805	ASP	2.4
1	B	40	HIS	2.4
1	B	463	SER	2.3
1	B	381	GLN	2.3
1	A	58	ALA	2.2
1	B	768	ALA	2.2
1	B	55	HIS	2.2
1	A	28	THR	2.2
1	A	333	LEU	2.2
1	A	353	HIS	2.1
2	F	10	DC	2.1
1	B	771	VAL	2.1
1	A	465	ASP	2.1
1	A	472	ASN	2.1
1	B	472	ASN	2.0
2	E	10	DC	2.0

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

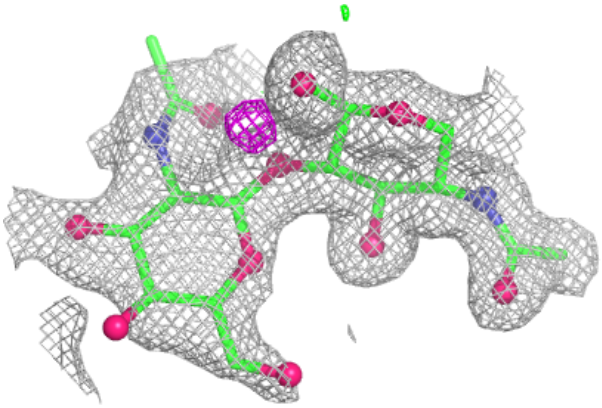
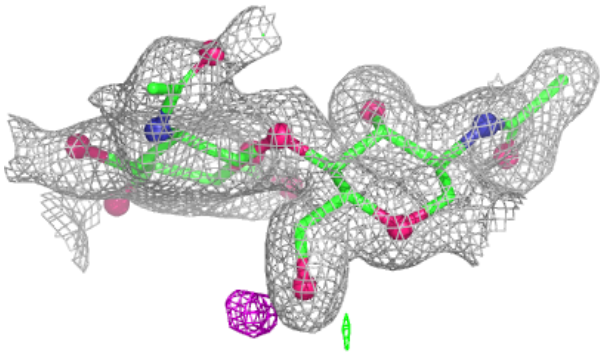
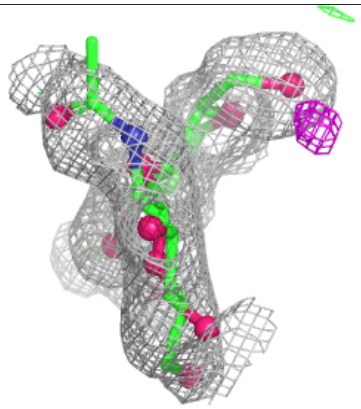
There are no non-standard protein/DNA/RNA residues in this entry.

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.

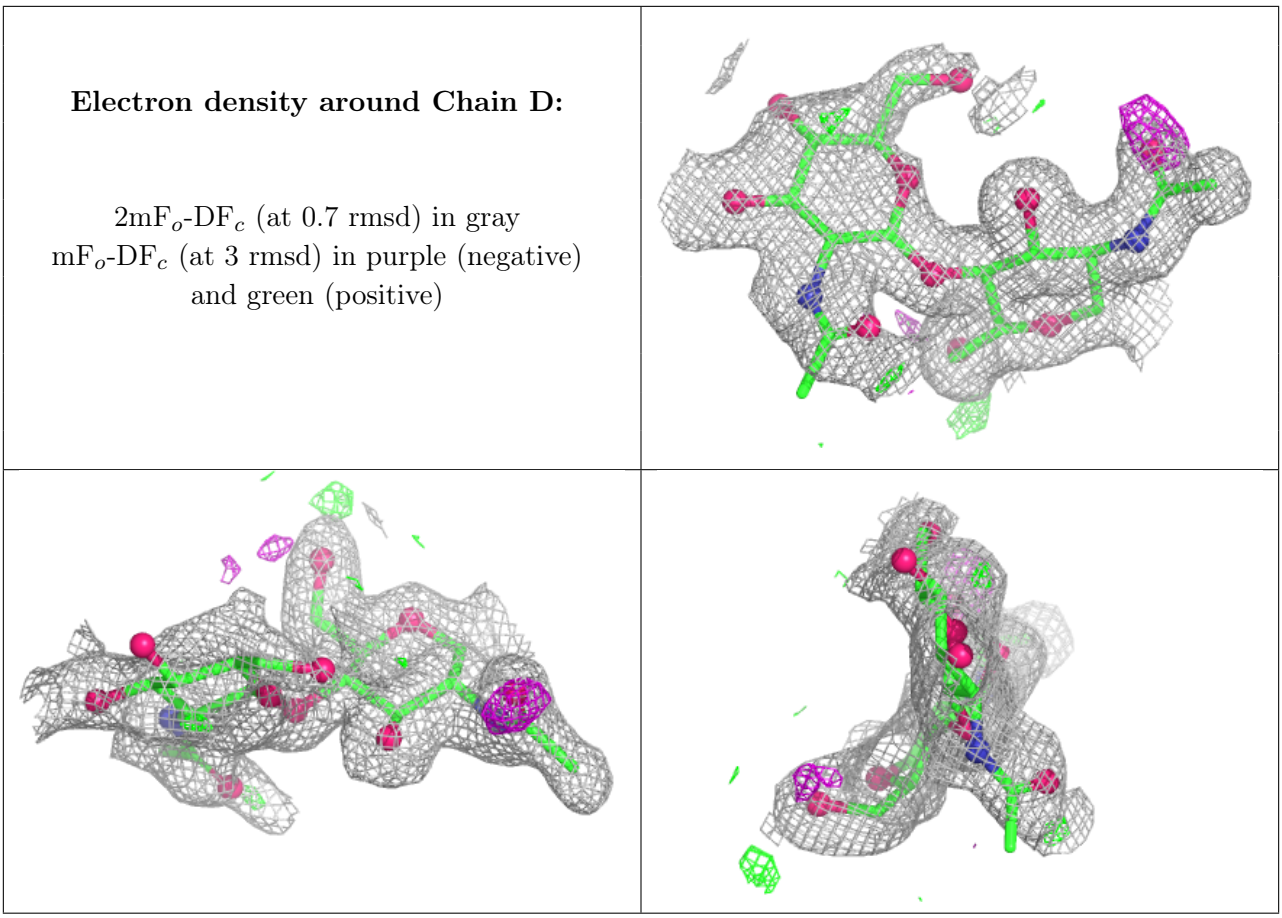
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.78	0.20	38,53,63,69	0
3	NAG	C	2	14/15	0.86	0.17	42,56,70,76	0
3	NAG	D	1	14/15	0.88	0.11	17,24,31,33	0
3	NAG	C	1	14/15	0.93	0.12	16,23,28,32	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

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 (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	A	905	14/15	0.76	0.17	35,49,53,58	0
7	GOL	B	912	6/6	0.80	0.15	39,46,47,49	0
4	NAG	A	903	14/15	0.81	0.28	36,42,46,62	0
4	NAG	A	901	14/15	0.82	0.23	33,38,46,53	0
4	NAG	B	903	14/15	0.82	0.25	29,35,44,57	0
4	NAG	B	905	14/15	0.82	0.13	31,34,45,47	0
4	NAG	A	904	14/15	0.82	0.12	30,40,48,54	0
4	NAG	B	906	14/15	0.83	0.24	33,46,58,63	0
5	SO4	B	911	5/5	0.85	0.29	21,34,45,51	0
4	NAG	B	904	14/15	0.85	0.15	22,31,37,45	0
4	NAG	B	901	14/15	0.87	0.23	34,39,50,56	0
5	SO4	A	909	5/5	0.87	0.28	21,35,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	907	14/15	0.90	0.12	23,29,35,37	0
4	NAG	A	906	14/15	0.92	0.10	22,26,36,38	0
4	NAG	A	902	14/15	0.93	0.10	19,23,28,33	0
4	NAG	B	902	14/15	0.93	0.10	16,20,30,33	0
6	NA	B	910	1/1	0.98	0.17	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.