Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 01:52 PM JST

PDB ID	:	5B2D
Title	:	Crystal structure of Mumps virus hemagglutinin-neuraminidase bound to 3-sialyllactose
Authors	:	Kubota, M.; Takeuchi, K.; Watanabe, S.; Ohno, S.; Matsuoka, R.; Kohda, D.; Hiramatsu, H.; Suzuki, Y.; Nakayama, T.; Terada, T.; Shimizu, K.; Shimizu, N.; Yanagi, Y.; Hashiguchi, T.
Deposited on	:	2016-01-14
Resolution	:	2.18 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:

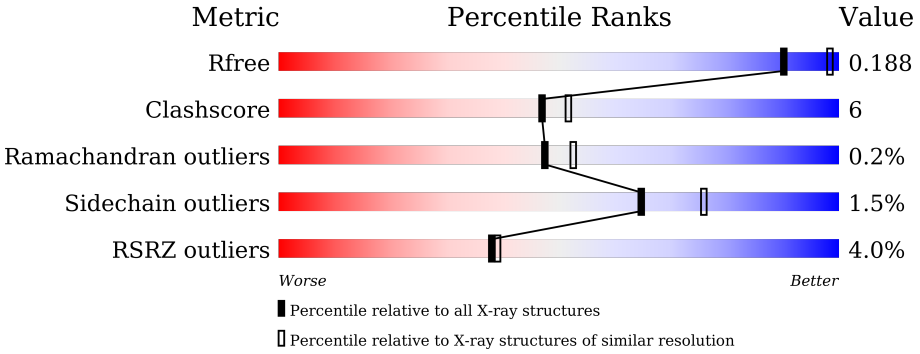
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	489	4%, 75%, 17%, 8%
1	B	489	3%, 77%, 15%, 8%
2	C	3	67%, 33%
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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	602	-	-	-	X
3	NAG	B	602	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7501 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.

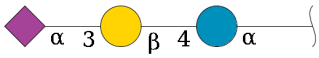
- Molecule 1 is a protein called HN protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3518	2248	582	667	21	0	0	0
1	B	450	3518	2248	582	667	21	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

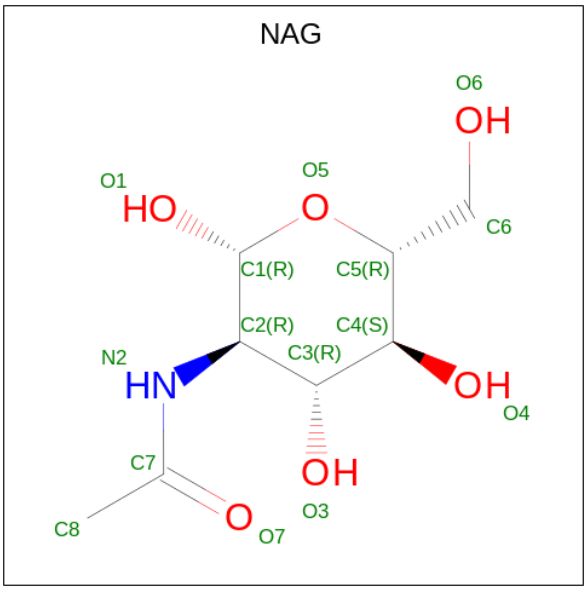
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLU	-	expression tag	UNP Q9WAF5
A	104	THR	-	expression tag	UNP Q9WAF5
A	105	GLY	-	expression tag	UNP Q9WAF5
A	583	GLY	-	expression tag	UNP Q9WAF5
A	584	THR	-	expression tag	UNP Q9WAF5
A	585	LYS	-	expression tag	UNP Q9WAF5
A	586	HIS	-	expression tag	UNP Q9WAF5
A	587	HIS	-	expression tag	UNP Q9WAF5
A	588	HIS	-	expression tag	UNP Q9WAF5
A	589	HIS	-	expression tag	UNP Q9WAF5
A	590	HIS	-	expression tag	UNP Q9WAF5
A	591	HIS	-	expression tag	UNP Q9WAF5
B	103	GLU	-	expression tag	UNP Q9WAF5
B	104	THR	-	expression tag	UNP Q9WAF5
B	105	GLY	-	expression tag	UNP Q9WAF5
B	583	GLY	-	expression tag	UNP Q9WAF5
B	584	THR	-	expression tag	UNP Q9WAF5
B	585	LYS	-	expression tag	UNP Q9WAF5
B	586	HIS	-	expression tag	UNP Q9WAF5
B	587	HIS	-	expression tag	UNP Q9WAF5
B	588	HIS	-	expression tag	UNP Q9WAF5
B	589	HIS	-	expression tag	UNP Q9WAF5
B	590	HIS	-	expression tag	UNP Q9WAF5
B	591	HIS	-	expression tag	UNP Q9WAF5

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-alpha-D-glucopyranose.



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

- 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
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

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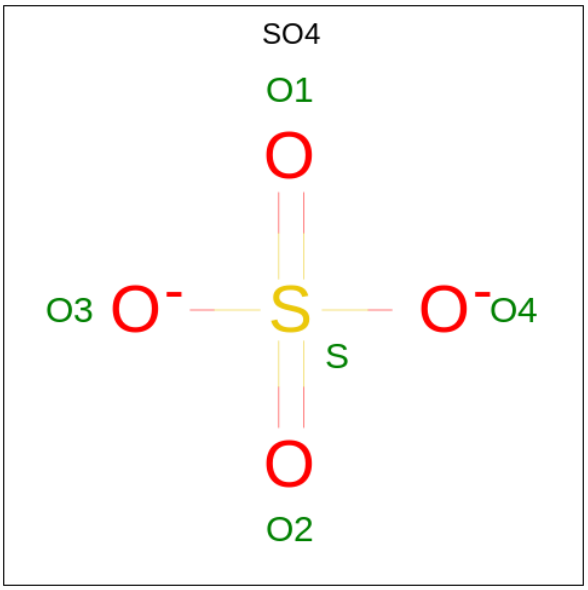
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

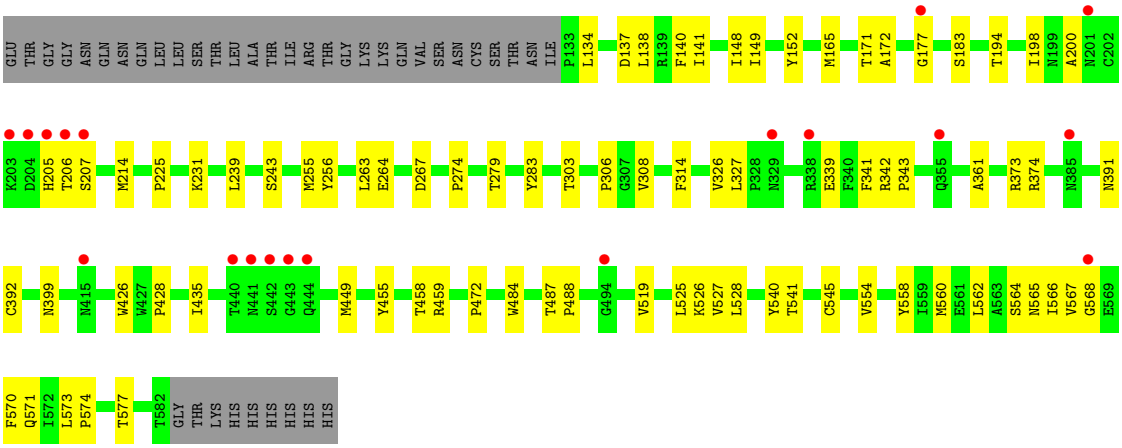
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	120	Total O 120 120	0	0
5	B	114	Total O 114 114	0	0

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.

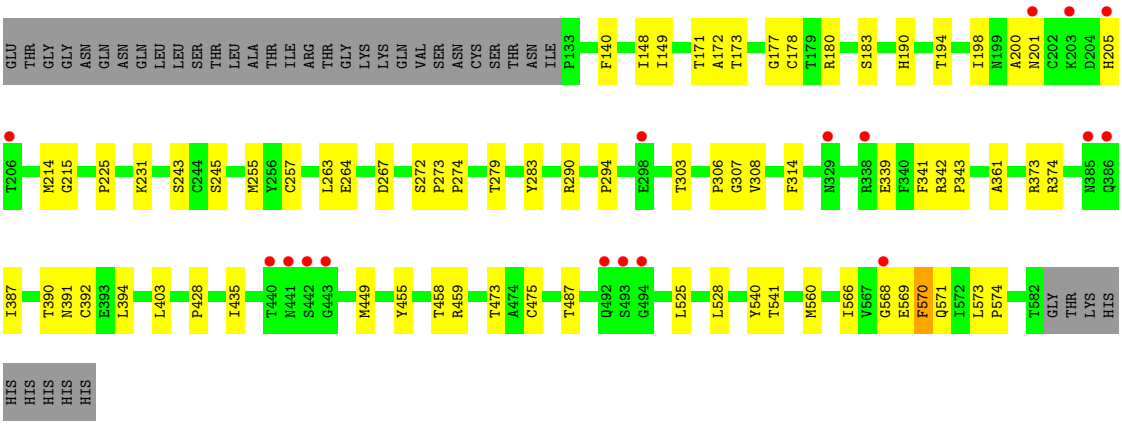
• Molecule 1: HN protein

Chain A:



• Molecule 1: HN protein

Chain B:

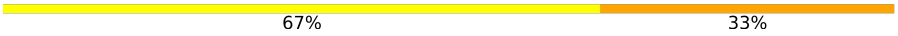


• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	136.88Å 136.88Å 177.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	118.54 – 2.18 118.54 – 2.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (118.54-2.18) 97.3 (118.54-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.176 , 0.191 0.178 , 0.188	Depositor DCC
R_{free} test set	4905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.229 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7501	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 3.66% 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: SO4, SIA, GLC, GAL, 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	0.33	0/3616	0.55	1/4945 (0.0%)
1	B	0.32	0/3616	0.54	0/4945
All	All	0.32	0/7232	0.54	1/9890 (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	134	LEU	CA-CB-CG	7.08	131.59	115.30

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	3518	0	3395	51	0
1	B	3518	0	3395	43	0
2	C	43	0	37	1	0
2	D	43	0	37	1	0
3	A	70	0	65	2	0
3	B	70	0	65	1	0
4	B	5	0	0	0	0
5	A	120	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	114	0	0	0	0
All	All	7501	0	6994	89	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 6.

All (89) 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:267:ASP:HB3	1:A:303:THR:HG21	1.50	0.94
1:B:267:ASP:HB3	1:B:303:THR:HG21	1.48	0.94
1:A:274:PRO:HD3	1:A:303:THR:HG22	1.63	0.80
1:A:165:MET:SD	5:A:793:HOH:O	2.45	0.74
1:A:571:GLN:NE2	1:B:171:THR:HG21	2.01	0.74
1:A:177:GLY:O	1:A:568:GLY:HA3	1.89	0.72
1:B:274:PRO:HD3	1:B:303:THR:HG22	1.73	0.69
1:A:571:GLN:HE22	1:B:171:THR:HG21	1.57	0.68
1:B:149:ILE:HB	1:B:487:THR:HG22	1.77	0.67
1:A:525:LEU:HD13	1:A:528:LEU:HD21	1.76	0.66
1:B:525:LEU:HD13	1:B:528:LEU:HD21	1.77	0.65
1:A:373:ARG:HH12	3:A:602:NAG:H4	1.62	0.65
1:B:177:GLY:O	1:B:568:GLY:HA3	1.96	0.64
1:A:198:ILE:HG22	1:A:200:ALA:H	1.62	0.64
1:A:526:LYS:NZ	5:A:702:HOH:O	2.32	0.62
1:B:339:GLU:O	1:B:374:ARG:NH2	2.31	0.61
1:A:562:LEU:O	1:A:570:PHE:HA	2.01	0.61
1:A:171:THR:HG23	1:A:172:ALA:O	2.01	0.60
1:B:435:ILE:HG22	1:B:449:MET:HB3	1.82	0.60
1:A:573:LEU:HD12	1:A:574:PRO:HD2	1.84	0.58
1:B:198:ILE:HG22	1:B:200:ALA:H	1.68	0.58
1:A:171:THR:HG21	1:B:571:GLN:OE1	2.02	0.58
1:B:171:THR:HG23	1:B:172:ALA:O	2.03	0.58
1:A:428:PRO:HB2	1:A:458:THR:OG1	2.04	0.57
1:A:327:LEU:HD22	3:A:602:NAG:H61	1.86	0.56
1:B:180:ARG:HG2	1:B:570:PHE:HD2	1.71	0.55
1:B:428:PRO:HB2	1:B:458:THR:OG1	2.06	0.55
1:A:206:THR:HG23	1:A:207:SER:H	1.72	0.55
1:A:558:TYR:HE1	1:A:577:THR:HG21	1.71	0.55
1:A:149:ILE:HB	1:A:487:THR:HG22	1.90	0.54
1:A:435:ILE:HG22	1:A:449:MET:HB3	1.90	0.54
1:A:214:MET:HG2	1:A:231:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HG3	1:B:361:ALA:HB2	1.89	0.53
1:A:256:TYR:CD2	1:A:306:PRO:HB3	2.44	0.53
1:A:152:TYR:HE1	1:A:488:PRO:HG2	1.74	0.53
1:B:391:ASN:O	1:B:392:CYS:HB2	2.09	0.52
1:B:541:THR:HG22	1:B:560:MET:HB3	1.90	0.51
1:A:342:ARG:HG3	1:A:361:ALA:HB2	1.92	0.51
1:A:564:SER:HB2	1:B:566:ILE:HD11	1.92	0.51
1:B:294:PRO:HB2	1:B:394:LEU:HG	1.91	0.51
1:A:138:LEU:HD23	1:A:141:ILE:HD12	1.95	0.49
1:A:243:SER:O	1:A:306:PRO:HG2	2.12	0.49
1:A:558:TYR:HE1	1:A:577:THR:CG2	2.26	0.49
1:B:573:LEU:HD12	1:B:574:PRO:HD2	1.95	0.49
1:B:148:ILE:HG13	1:B:149:ILE:HG13	1.94	0.49
1:B:214:MET:HG2	1:B:231:LYS:HB2	1.95	0.49
1:A:264:GLU:O	1:A:267:ASP:HB2	2.12	0.48
1:A:231:LYS:HE3	1:A:283:TYR:O	2.13	0.48
1:B:341:PHE:CE2	1:B:343:PRO:HG3	2.49	0.48
1:B:569:GLU:O	1:B:570:PHE:HB2	2.13	0.48
1:B:243:SER:O	1:B:306:PRO:HB2	2.13	0.47
1:A:519:VAL:HB	1:A:527:VAL:HG12	1.96	0.47
1:B:255:MET:HB3	1:B:279:THR:CG2	2.45	0.47
1:B:540:TYR:OH	2:D:3:SIA:H31	2.15	0.47
1:A:148:ILE:HD13	1:A:554:VAL:HG13	1.96	0.46
1:A:206:THR:HG23	1:A:207:SER:N	2.30	0.46
1:B:178:CYS:HB3	1:B:198:ILE:HB	1.98	0.46
1:B:264:GLU:O	1:B:267:ASP:HB2	2.15	0.46
1:A:541:THR:HG22	1:A:560:MET:HB3	1.97	0.45
1:A:374:ARG:HH21	1:A:399:ASN:HB2	1.81	0.45
1:A:140:PHE:CZ	1:A:225:PRO:HB3	2.51	0.45
1:A:573:LEU:HD11	1:B:173:THR:HA	1.98	0.45
1:B:290:ARG:NH2	1:B:390:THR:O	2.30	0.45
1:B:373:ARG:NH1	3:B:602:NAG:O7	2.51	0.45
1:A:183:SER:HB3	1:A:194:THR:HG22	2.00	0.44
1:A:484:TRP:CD1	1:A:545:CYS:HB2	2.53	0.44
1:A:540:TYR:OH	2:C:3:SIA:H31	2.18	0.44
1:A:171:THR:OG1	1:A:567:VAL:HG21	2.18	0.44
1:B:290:ARG:NH1	1:B:387:ILE:O	2.50	0.44
1:B:473:THR:HG23	1:B:475:CYS:SG	2.57	0.44
1:B:272:SER:HA	1:B:273:PRO:HD3	1.92	0.44
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.85	0.44
1:A:391:ASN:O	1:A:392:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:HIS:HB2	1:B:215:GLY:O	2.19	0.43
1:B:341:PHE:CD2	1:B:403:LEU:HD22	2.54	0.42
1:B:257:CYS:HA	1:B:306:PRO:HG2	2.01	0.42
1:B:341:PHE:HD2	1:B:403:LEU:HD22	1.84	0.42
1:B:183:SER:HB3	1:B:194:THR:HG22	2.02	0.42
1:A:255:MET:HB3	1:A:279:THR:CG2	2.50	0.42
1:A:137:ASP:HB3	1:A:140:PHE:CD1	2.55	0.42
1:A:198:ILE:HG22	1:A:200:ALA:N	2.32	0.42
1:B:307:GLY:O	1:B:308:VAL:HB	2.20	0.42
1:A:565:ASN:CG	1:A:566:ILE:HG23	2.41	0.41
1:B:140:PHE:CZ	1:B:225:PRO:HB3	2.56	0.41
1:A:339:GLU:O	1:A:374:ARG:NH2	2.45	0.41
1:A:341:PHE:CE2	1:A:343:PRO:HG3	2.55	0.41
1:A:426:TRP:CD2	1:A:472:PRO:HA	2.56	0.41
1:B:231:LYS:HE3	1:B:283:TYR:O	2.21	0.40
1:A:326:VAL:HB	1:A:374:ARG:HB3	2.03	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	448/489 (92%)	424 (95%)	23 (5%)	1 (0%)	47	52
1	B	448/489 (92%)	430 (96%)	17 (4%)	1 (0%)	47	52
All	All	896/978 (92%)	854 (95%)	40 (4%)	2 (0%)	47	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	570	PHE
1	A	308	VAL

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	398/432 (92%)	393 (99%)	5 (1%)	69	79
1	B	398/432 (92%)	391 (98%)	7 (2%)	59	70
All	All	796/864 (92%)	784 (98%)	12 (2%)	65	76

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

Mol	Chain	Res	Type
1	A	205	HIS
1	A	263	LEU
1	A	314	PHE
1	A	455	TYR
1	A	459	ARG
1	B	201	ASN
1	B	205	HIS
1	B	245	SER
1	B	263	LEU
1	B	314	PHE
1	B	455	TYR
1	B	459	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN

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)

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	GLC	C	1	2	12,12,12	1.66	4 (33%)	17,17,17	0.78	0
2	GAL	C	2	2	11,11,12	1.56	3 (27%)	15,15,17	0.89	0
2	SIA	C	3	2	20,20,21	2.28	5 (25%)	24,28,31	1.58	6 (25%)
2	GLC	D	1	2	12,12,12	1.66	4 (33%)	17,17,17	0.78	0
2	GAL	D	2	2	11,11,12	1.45	3 (27%)	15,15,17	0.86	0
2	SIA	D	3	2	20,20,21	2.29	6 (30%)	24,28,31	1.54	6 (25%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	SIA	C	3	2	-	0/18/34/38	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	SIA	C4-C5	-6.54	1.47	1.53
2	D	3	SIA	C4-C5	-6.04	1.47	1.53
2	D	3	SIA	C2-C1	-4.55	1.48	1.52
2	C	3	SIA	C2-C1	-4.05	1.48	1.52
2	C	3	SIA	C10-N5	3.56	1.46	1.34
2	C	1	GLC	O3-C3	3.44	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C10-N5	3.42	1.46	1.34
2	D	1	GLC	O3-C3	3.31	1.50	1.43
2	C	2	GAL	O5-C1	3.02	1.48	1.43
2	D	1	GLC	O4-C4	2.78	1.49	1.43
2	C	1	GLC	O4-C4	2.68	1.49	1.43
2	D	2	GAL	O5-C1	2.64	1.47	1.43
2	D	3	SIA	O6-C6	2.54	1.47	1.44
2	D	3	SIA	C3-C4	-2.53	1.48	1.52
2	C	3	SIA	O6-C6	2.52	1.47	1.44
2	D	2	GAL	O3-C3	2.47	1.48	1.43
2	C	2	GAL	O3-C3	2.46	1.48	1.43
2	D	1	GLC	C4-C3	-2.43	1.46	1.52
2	C	3	SIA	C3-C4	-2.36	1.48	1.52
2	C	1	GLC	C4-C3	-2.30	1.46	1.52
2	D	1	GLC	C3-C2	-2.22	1.46	1.52
2	C	1	GLC	C3-C2	-2.09	1.47	1.52
2	C	2	GAL	O5-C5	2.06	1.47	1.43
2	D	2	GAL	O5-C5	2.04	1.47	1.43
2	D	3	SIA	C3-C2	-2.04	1.49	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	SIA	O6-C2-C3	3.13	114.77	110.46
2	C	3	SIA	C4-C3-C2	3.02	115.22	109.81
2	D	3	SIA	O6-C2-C3	2.82	114.34	110.46
2	D	3	SIA	C4-C3-C2	2.67	114.60	109.81
2	C	3	SIA	O6-C2-C1	2.43	112.46	107.70
2	C	3	SIA	O1B-C1-C2	2.42	119.94	113.03
2	D	3	SIA	O1B-C1-C2	2.35	119.73	113.03
2	D	3	SIA	O6-C2-C1	2.33	112.27	107.70
2	D	3	SIA	C11-C10-N5	2.20	119.82	116.10
2	C	3	SIA	C8-C7-C6	-2.17	108.92	113.03
2	C	3	SIA	C11-C10-N5	2.15	119.73	116.10
2	D	3	SIA	C8-C7-C6	-2.03	109.18	113.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	2	GAL	O5-C5-C6-O6
2	C	2	GAL	O5-C5-C6-O6

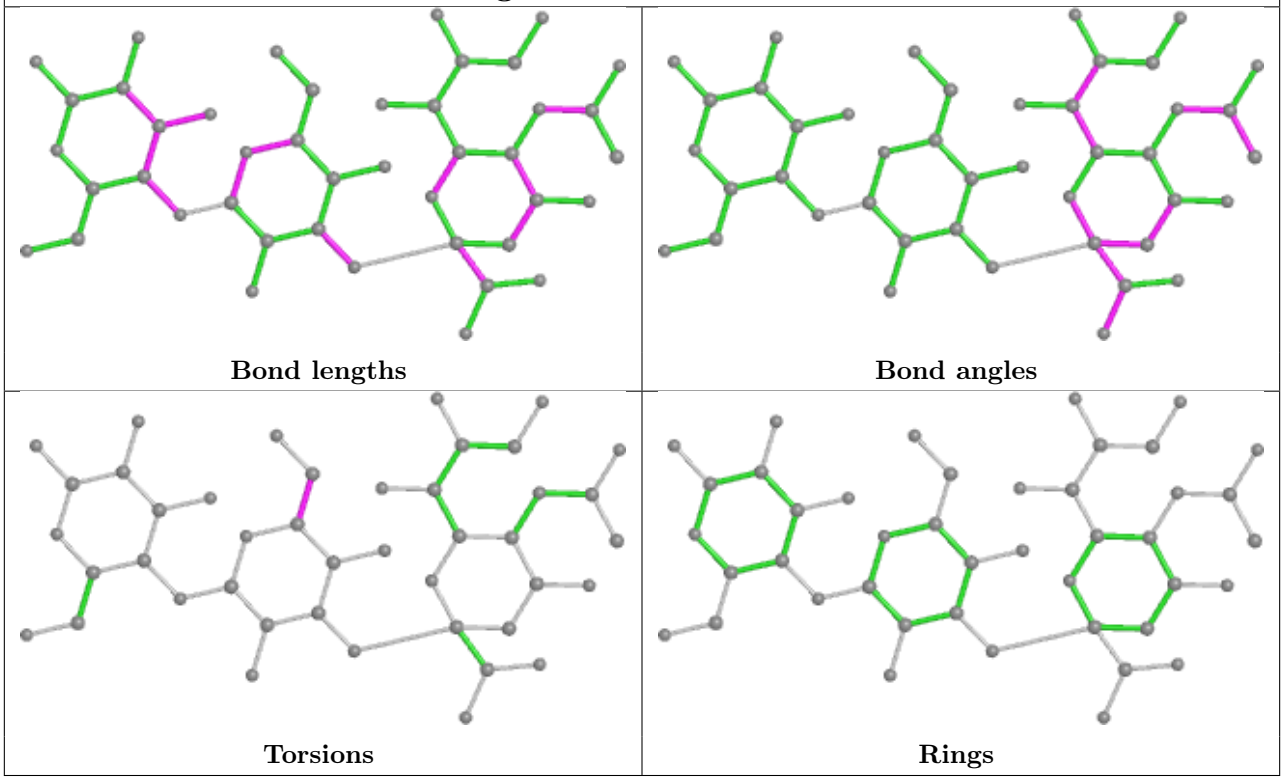
There are no ring outliers.

2 monomers are involved in 2 short contacts:

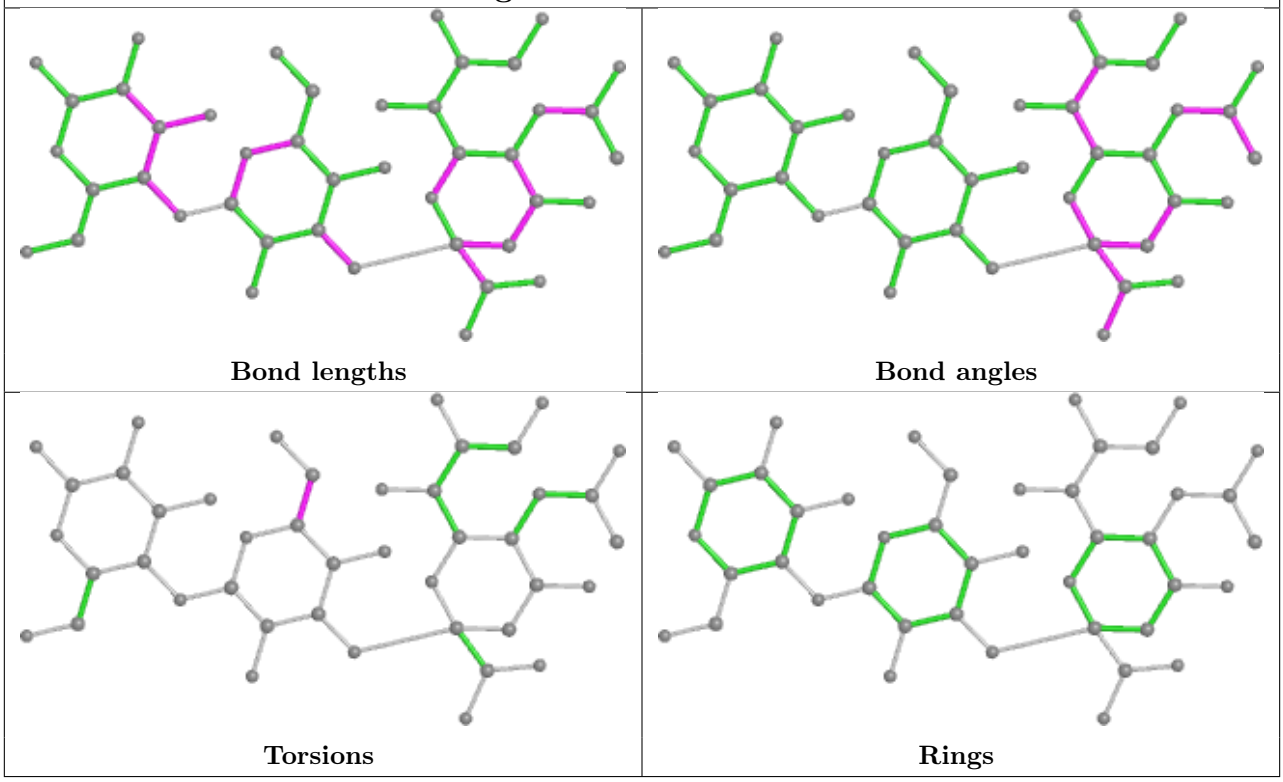
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	1	0
2	C	3	SIA	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
3	NAG	B	605	1	14,14,15	1.02	1 (7%)	17,19,21	1.55	3 (17%)
3	NAG	B	604	1	14,14,15	1.12	2 (14%)	17,19,21	1.48	2 (11%)
3	NAG	A	602	1	14,14,15	1.00	2 (14%)	17,19,21	1.47	4 (23%)
3	NAG	B	601	1	14,14,15	1.03	2 (14%)	17,19,21	1.46	3 (17%)
3	NAG	A	603	1	14,14,15	1.14	2 (14%)	17,19,21	1.13	1 (5%)
3	NAG	A	604	1	14,14,15	1.05	2 (14%)	17,19,21	1.10	1 (5%)
3	NAG	A	601	1	14,14,15	1.12	2 (14%)	17,19,21	1.49	3 (17%)
3	NAG	B	603	1	14,14,15	1.14	3 (21%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	607	-	4,4,4	0.16	0	6,6,6	0.22	0
3	NAG	B	602	1	14,14,15	1.10	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	A	605	1	14,14,15	1.05	1 (7%)	17,19,21	1.31	1 (5%)

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	605	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	1/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	NAG	C7-N2	2.58	1.43	1.34
3	A	605	NAG	C7-N2	2.46	1.42	1.34
3	B	603	NAG	C7-N2	2.45	1.42	1.34
3	B	605	NAG	C7-N2	2.45	1.42	1.34
3	B	602	NAG	C7-N2	2.42	1.42	1.34
3	A	602	NAG	C7-N2	2.40	1.42	1.34
3	B	601	NAG	C7-N2	2.38	1.42	1.34
3	B	604	NAG	C7-N2	2.30	1.42	1.34
3	A	601	NAG	C2-N2	-2.29	1.42	1.46
3	A	604	NAG	C7-N2	2.26	1.42	1.34
3	A	601	NAG	C7-N2	2.26	1.42	1.34
3	B	604	NAG	O5-C1	-2.13	1.40	1.43
3	A	603	NAG	O5-C1	-2.09	1.40	1.43
3	A	602	NAG	C2-N2	-2.09	1.42	1.46
3	B	603	NAG	C2-N2	-2.08	1.42	1.46
3	B	603	NAG	O5-C1	-2.05	1.40	1.43
3	A	604	NAG	C2-N2	-2.05	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	C2-N2	-2.04	1.42	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	605	NAG	C1-O5-C5	4.60	118.43	112.19
3	A	601	NAG	C1-O5-C5	4.51	118.31	112.19
3	B	601	NAG	C1-O5-C5	3.83	117.38	112.19
3	A	605	NAG	C1-O5-C5	3.78	117.31	112.19
3	B	604	NAG	C4-C3-C2	3.69	116.43	111.02
3	A	602	NAG	C2-N2-C7	-2.71	119.05	122.90
3	B	605	NAG	C6-C5-C4	-2.66	106.77	113.00
3	A	602	NAG	O5-C5-C6	2.60	111.28	107.20
3	A	603	NAG	C8-C7-N2	2.50	120.33	116.10
3	A	602	NAG	C8-C7-N2	2.48	120.30	116.10
3	B	603	NAG	C8-C7-N2	2.30	119.99	116.10
3	B	601	NAG	C8-C7-N2	2.23	119.88	116.10
3	B	604	NAG	C1-C2-N2	-2.15	106.81	110.49
3	A	601	NAG	C8-C7-N2	2.14	119.72	116.10
3	B	601	NAG	C6-C5-C4	-2.14	108.00	113.00
3	A	601	NAG	C2-N2-C7	-2.13	119.88	122.90
3	B	602	NAG	C8-C7-N2	2.12	119.69	116.10
3	A	602	NAG	C4-C3-C2	-2.12	107.91	111.02
3	B	605	NAG	C8-C7-N2	2.06	119.59	116.10
3	A	604	NAG	C8-C7-N2	2.04	119.56	116.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	A	605	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAG	2	0
3	B	602	NAG	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	450/489 (92%)	0.22	19 (4%)	36	37	17, 29, 50, 93	0
1	B	450/489 (92%)	0.22	17 (3%)	40	41	17, 29, 50, 95	0
All	All	900/978 (92%)	0.22	36 (4%)	38	39	17, 29, 51, 95	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	THR	10.3
1	A	440	THR	10.1
1	B	442	SER	6.5
1	A	443	GLY	6.3
1	B	443	GLY	6.3
1	B	206	THR	5.7
1	A	442	SER	5.6
1	B	205	HIS	4.8
1	A	441	ASN	4.7
1	A	203	LYS	4.0
1	A	329	ASN	3.9
1	B	441	ASN	3.7
1	B	329	ASN	3.7
1	B	338	ARG	3.2
1	A	204	ASP	3.2
1	A	206	THR	3.1
1	A	201	ASN	3.1
1	B	568	GLY	3.1
1	A	205	HIS	3.1
1	B	492	GLN	3.0
1	A	568	GLY	2.8
1	B	201	ASN	2.8
1	B	298	GLU	2.8
1	A	338	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	494	GLY	2.5
1	B	494	GLY	2.5
1	B	203	LYS	2.4
1	A	385	ASN	2.3
1	B	386	GLN	2.2
1	A	415	ASN	2.2
1	B	385	ASN	2.2
1	A	177	GLY	2.2
1	A	355	GLN	2.1
1	A	444	GLN	2.1
1	A	207	SER	2.1
1	B	493	SER	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)

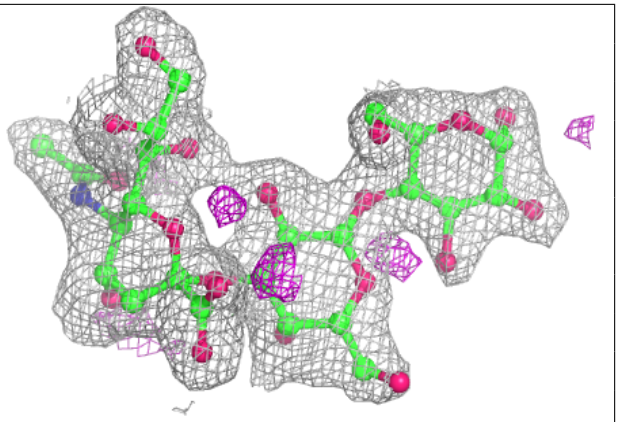
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

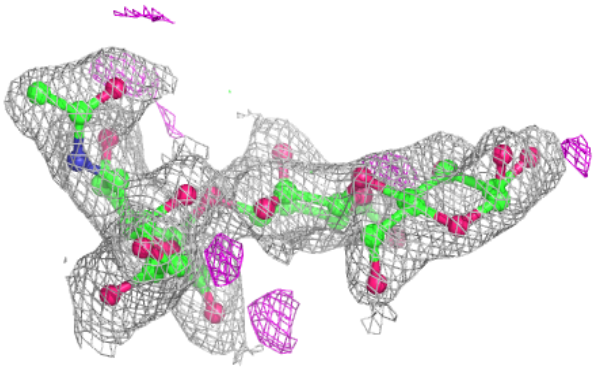
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	12/12	0.89	0.26	44,49,53,58	0
2	GAL	C	2	11/12	0.92	0.18	32,38,44,56	0
2	GLC	C	1	12/12	0.92	0.19	41,46,49,50	0
2	GAL	D	2	11/12	0.92	0.18	35,42,47,56	0
2	SIA	C	3	20/21	0.96	0.11	22,25,29,29	0
2	SIA	D	3	20/21	0.96	0.12	22,30,31,32	0

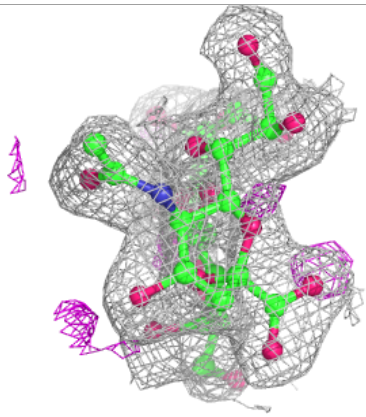
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

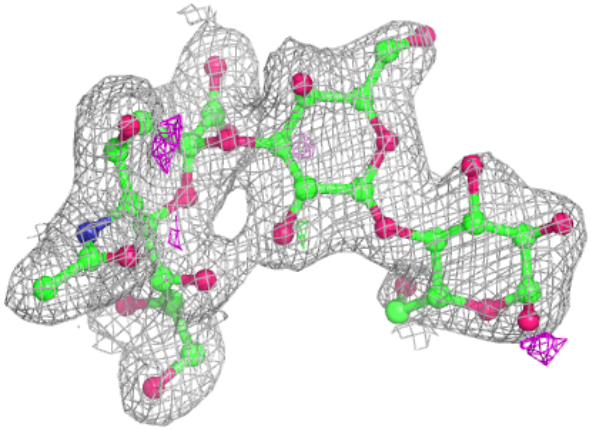


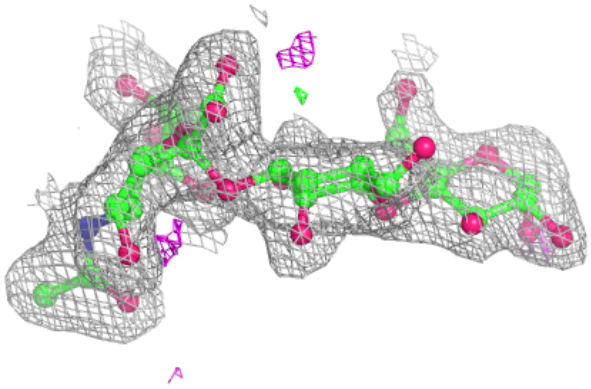


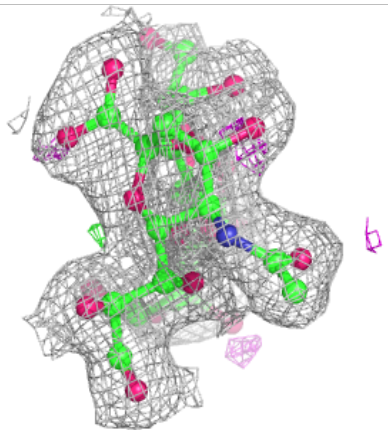


Electron density around Chain D:

$2mF_o$-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
3	NAG	B	602	14/15	0.62	0.70	69,72,76,77	0
3	NAG	A	604	14/15	0.77	0.28	48,58,61,65	0
3	NAG	A	602	14/15	0.77	0.58	62,71,74,77	0
3	NAG	A	603	14/15	0.83	0.15	47,53,60,61	0
3	NAG	B	604	14/15	0.83	0.27	40,52,59,59	0
3	NAG	B	603	14/15	0.85	0.18	52,55,59,63	0
3	NAG	B	605	14/15	0.85	0.15	36,45,57,64	0
3	NAG	B	601	14/15	0.88	0.17	37,43,50,52	0
3	NAG	A	601	14/15	0.89	0.17	40,47,54,56	0
3	NAG	A	605	14/15	0.94	0.12	27,42,53,54	0
4	SO4	B	607	5/5	0.98	0.12	36,39,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.