



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:51 AM UTC

PDB ID : 6TWI / pdb_00006twi
Title : Crystal structure of the haemagglutinin mutant (Gln226Leu, Gly228Ser) from an H10N7 seal influenza virus isolated in Germany in complex with avian receptor analogue 3'-SLN
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on : 2020-01-13
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

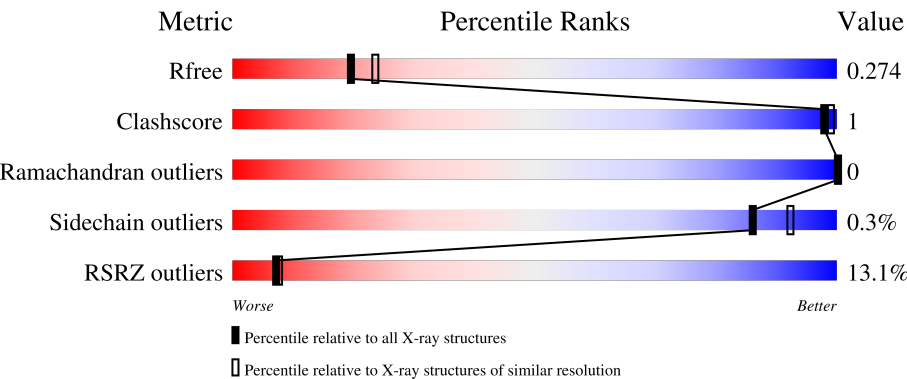
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	8% 95%
1	C	325	6% 97%
1	E	325	32% 98%
2	B	177	6% 94%
2	D	177	6% 95%

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Mol	Chain	Length	Quality of chain
2	F	177	11% 94%
3	G	3	33% 67%
3	H	3	33% 67%
3	J	3	100%
4	I	2	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12267 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2443	1515	442	470	16			
1	C	320	Total	C	N	O	S	0	0	0
			2447	1518	443	470	16			
1	E	323	Total	C	N	O	S	0	0	0
			2471	1534	447	474	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
E	221	SER	GLY	engineered mutation	UNP A0A0A7HR51

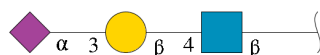
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1382	855	241	278	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	H	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	J	3	Total	C	N	O	0	0	0
			46	25	2	19			

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



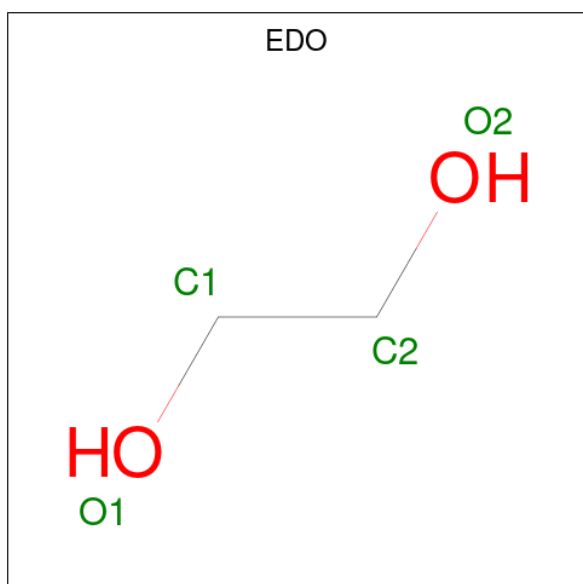
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

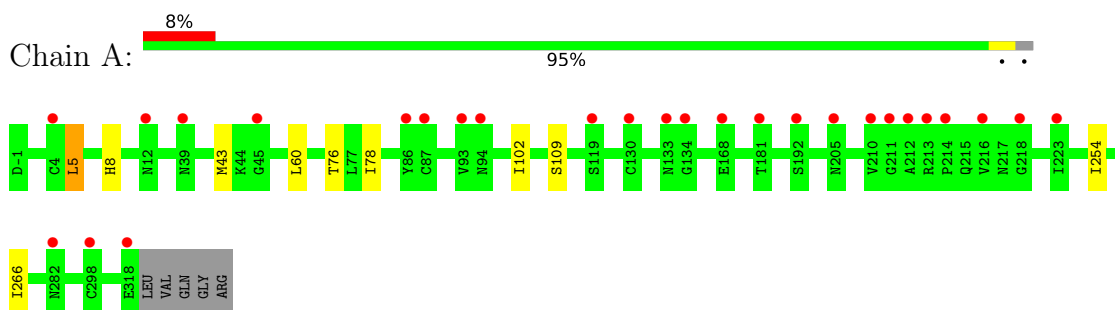
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	110	Total O 110 110	0	0
8	B	58	Total O 58 58	0	0
8	C	122	Total O 122 122	0	0
8	D	94	Total O 94 94	0	0
8	E	53	Total O 53 53	0	0
8	F	60	Total O 60 60	0	0

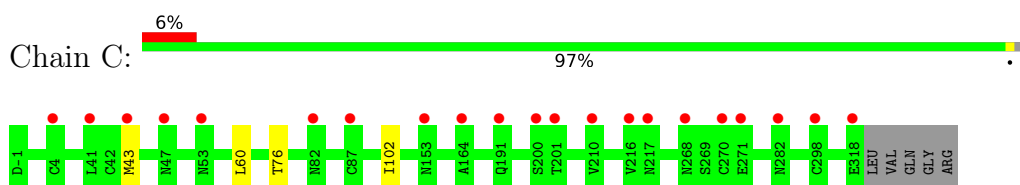
3 Residue-property plots [i](#)

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.

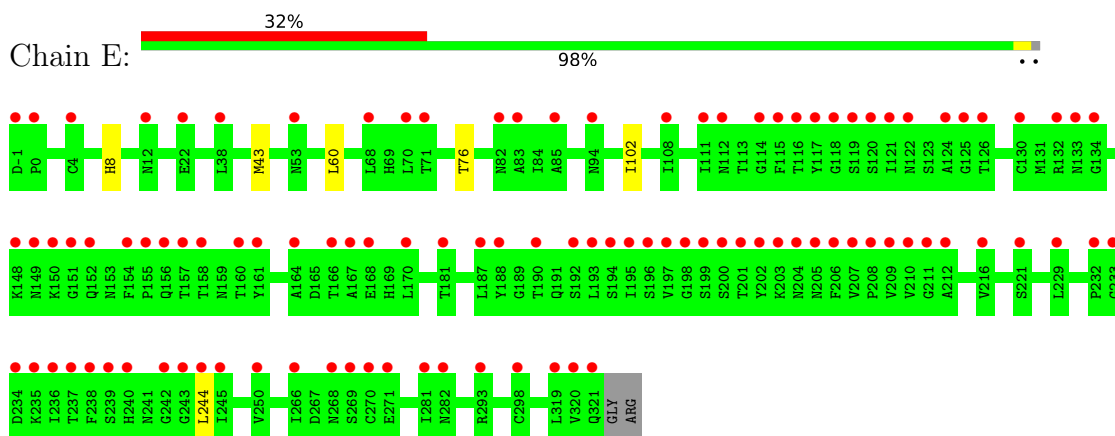
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

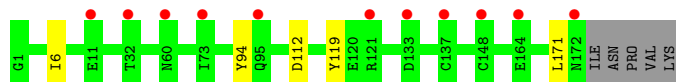


- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin HA2





- Molecule 2: Hemagglutinin HA2



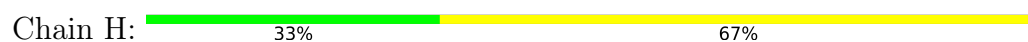
- Molecule 2: Hemagglutinin HA2



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.84Å 215.10Å 78.25Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	73.08 – 2.27 73.08 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (73.08-2.27) 99.7 (73.08-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.245 , 0.273 0.244 , 0.274	Depositor DCC
R_{free} test set	4827 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12267	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, EDO, CA, 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	0.50	0/2493	0.66	0/3379
1	C	0.49	0/2497	0.66	0/3383
1	E	0.52	0/2521	0.66	0/3416
2	B	0.52	0/1411	0.77	0/1903
2	D	0.50	0/1411	0.78	1/1903 (0.1%)
2	F	0.50	0/1407	0.75	0/1898
All	All	0.50	0/11740	0.70	1/15882 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	GLY	N-CA-C	5.28	117.71	110.69

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	2443	0	2400	5	0
1	C	2447	0	2411	3	0
1	E	2471	0	2439	2	0
2	B	1386	0	1291	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1386	0	1291	1	0
2	F	1382	0	1287	5	0
3	G	46	0	40	0	0
3	H	46	0	40	0	0
3	J	46	0	40	0	0
4	I	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	110	0	0	0	0
8	B	58	0	0	0	0
8	C	122	0	0	0	0
8	D	94	0	0	0	0
8	E	53	0	0	0	0
8	F	60	0	0	0	0
All	All	12267	0	11353	17	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 1.

All (17) 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:C:43:MET:HE1	1:C:76:THR:HG21	1.75	0.67
1:E:43:MET:HE1	1:E:76:THR:HG21	1.84	0.59
1:C:60:LEU:HD11	1:C:102:ILE:HD11	1.88	0.55
1:A:60:LEU:HD11	1:A:102:ILE:HD11	1.89	0.54
2:B:94:TYR:OH	2:F:99:LEU:HD22	2.16	0.46
1:A:78:ILE:HD13	1:A:266:ILE:HD11	1.98	0.46
1:A:43:MET:HE1	1:A:76:THR:HG21	1.99	0.44
1:E:60:LEU:HD11	1:E:102:ILE:HD11	1.99	0.43
2:B:171:LEU:HD22	2:F:171:LEU:HD11	2.01	0.43
2:F:115:MET:HA	2:F:115:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:CD1	1:C:102:ILE:HD11	2.49	0.42
2:B:6:ILE:HD12	2:B:112:ASP:HA	2.00	0.42
1:A:5:LEU:HD13	2:B:119:TYR:HA	2.01	0.41
2:F:30:GLN:HE22	2:F:145:ASP:CB	2.34	0.41
1:A:109:SER:OG	1:A:254:ILE:HD11	2.21	0.41
2:D:6:ILE:HD12	2:D:112:ASP:HA	2.02	0.41
2:F:30:GLN:HE22	2:F:145:ASP:HA	1.86	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	318/325 (98%)	315 (99%)	3 (1%)	0	100	100
1	C	318/325 (98%)	311 (98%)	7 (2%)	0	100	100
1	E	321/325 (99%)	315 (98%)	6 (2%)	0	100	100
2	B	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	D	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	F	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
All	All	1467/1506 (97%)	1434 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/276 (98%)	269 (99%)	2 (1%)	76	86
1	C	272/276 (99%)	272 (100%)	0	100	100
1	E	275/276 (100%)	273 (99%)	2 (1%)	76	86
2	B	146/151 (97%)	146 (100%)	0	100	100
2	D	146/151 (97%)	146 (100%)	0	100	100
2	F	145/151 (96%)	145 (100%)	0	100	100
All	All	1255/1281 (98%)	1251 (100%)	4 (0%)	86	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	HIS
1	E	8	HIS
1	E	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	149	ASN
1	A	297	GLN
1	A	303	ASN
2	B	12	ASN
1	C	48	HIS
1	C	100	GLN
1	C	152	GLN
1	C	205	ASN
1	C	268	ASN
1	C	303	ASN
2	D	12	ASN
2	D	95	GLN
1	E	48	HIS
1	E	82	ASN
1	E	133	ASN
1	E	185	ASN
1	E	231	GLN
1	E	268	ASN

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Mol	Chain	Res	Type
2	F	12	ASN
2	F	95	GLN
2	F	125	GLN
2	F	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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	G	1	3	15,15,15	0.43	0	21,21,21	1.08	2 (9%)
3	GAL	G	2	3	11,11,12	0.29	0	15,15,17	0.56	0
3	SIA	G	3	3	20,20,21	0.63	0	21,28,31	1.16	3 (14%)
3	NAG	H	1	3	15,15,15	0.45	0	21,21,21	0.95	2 (9%)
3	GAL	H	2	3	11,11,12	0.31	0	15,15,17	0.54	0
3	SIA	H	3	3	20,20,21	0.60	0	21,28,31	1.20	4 (19%)
4	NAG	I	1	2,4,7	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
4	NAG	I	2	4	14,14,15	0.37	0	17,19,21	0.77	0
3	NAG	J	1	3	15,15,15	0.43	0	21,21,21	1.09	2 (9%)
3	GAL	J	2	3	11,11,12	0.34	0	15,15,17	0.77	1 (6%)
3	SIA	J	3	3	20,20,21	0.58	0	21,28,31	1.09	2 (9%)

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	G	1	3	-	0/6/26/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1
3	SIA	G	3	3	-	0/18/34/38	0/1/1/1
3	NAG	H	1	3	-	0/6/26/26	0/1/1/1
3	GAL	H	2	3	-	2/2/19/22	0/1/1/1
3	SIA	H	3	3	-	0/18/34/38	0/1/1/1
4	NAG	I	1	2,4,7	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3	-	0/6/26/26	0/1/1/1
3	GAL	J	2	3	-	0/2/19/22	0/1/1/1
3	SIA	J	3	3	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-C2-N2	-3.38	106.81	110.73
3	J	1	NAG	C1-C2-N2	-3.31	106.89	110.73
3	H	1	NAG	C1-C2-N2	-3.07	107.17	110.73
3	J	3	SIA	O1B-C1-C2	2.68	119.67	112.71
3	H	3	SIA	O1B-C1-C2	2.53	119.30	112.71
3	G	3	SIA	O1B-C1-C2	2.49	119.18	112.71
3	G	1	NAG	C3-C2-N2	-2.43	106.13	110.62
3	G	3	SIA	C4-C5-N5	-2.43	105.66	110.44
3	H	3	SIA	C4-C5-N5	-2.29	105.93	110.44
3	J	3	SIA	C4-C5-N5	-2.20	106.11	110.44
3	H	1	NAG	C3-C2-N2	-2.08	106.79	110.62
3	J	1	NAG	C3-C2-N2	-2.05	106.83	110.62
3	G	3	SIA	O6-C2-C1	2.05	111.58	107.72
3	H	3	SIA	O6-C2-C1	2.03	111.54	107.72
4	I	1	NAG	C1-O5-C5	2.02	114.89	112.19
3	J	2	GAL	C1-C2-C3	2.00	112.56	109.64
3	H	3	SIA	C6-C5-N5	-2.00	107.71	110.91

There are no chirality outliers.

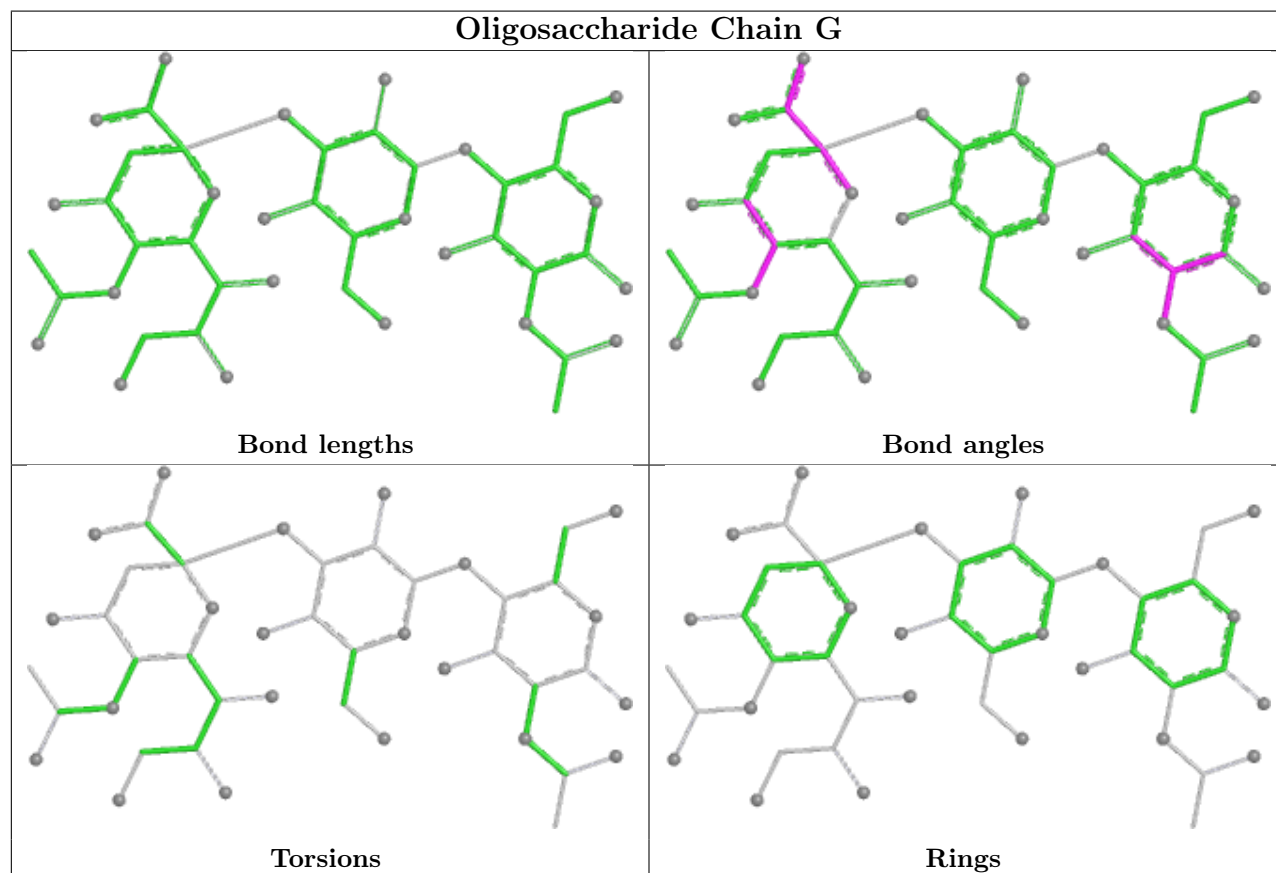
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	GAL	C4-C5-C6-O6
3	H	2	GAL	O5-C5-C6-O6

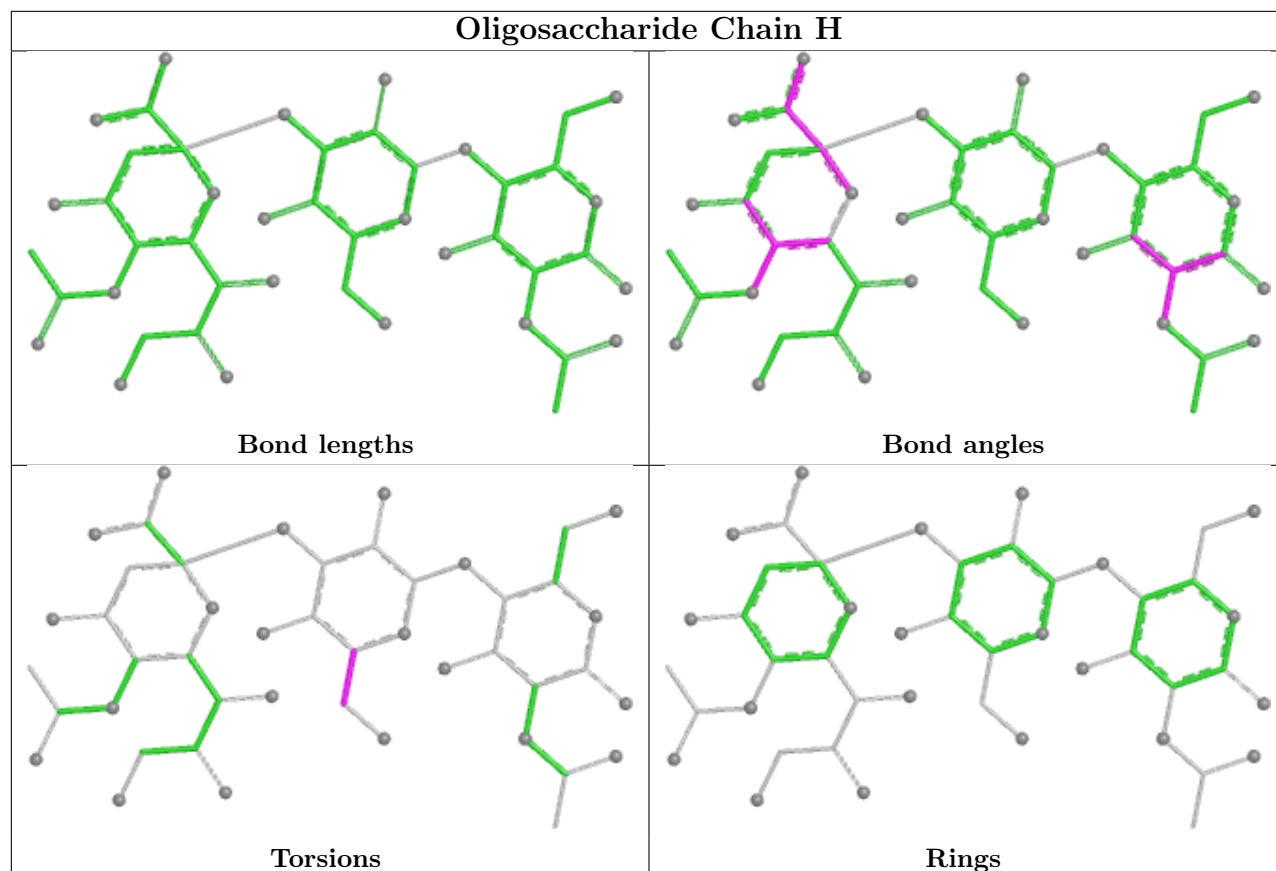
There are no ring outliers.

No monomer is involved in short contacts.

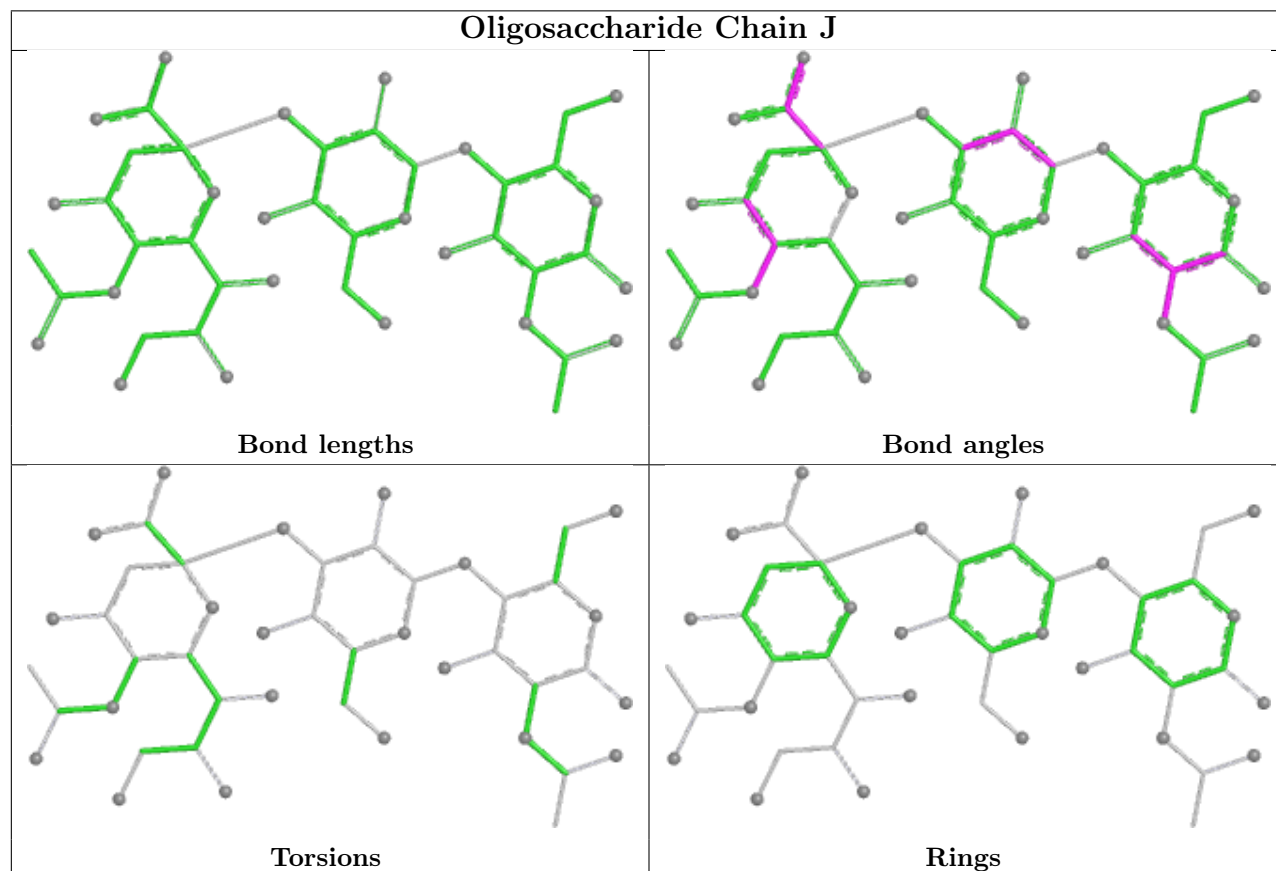
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

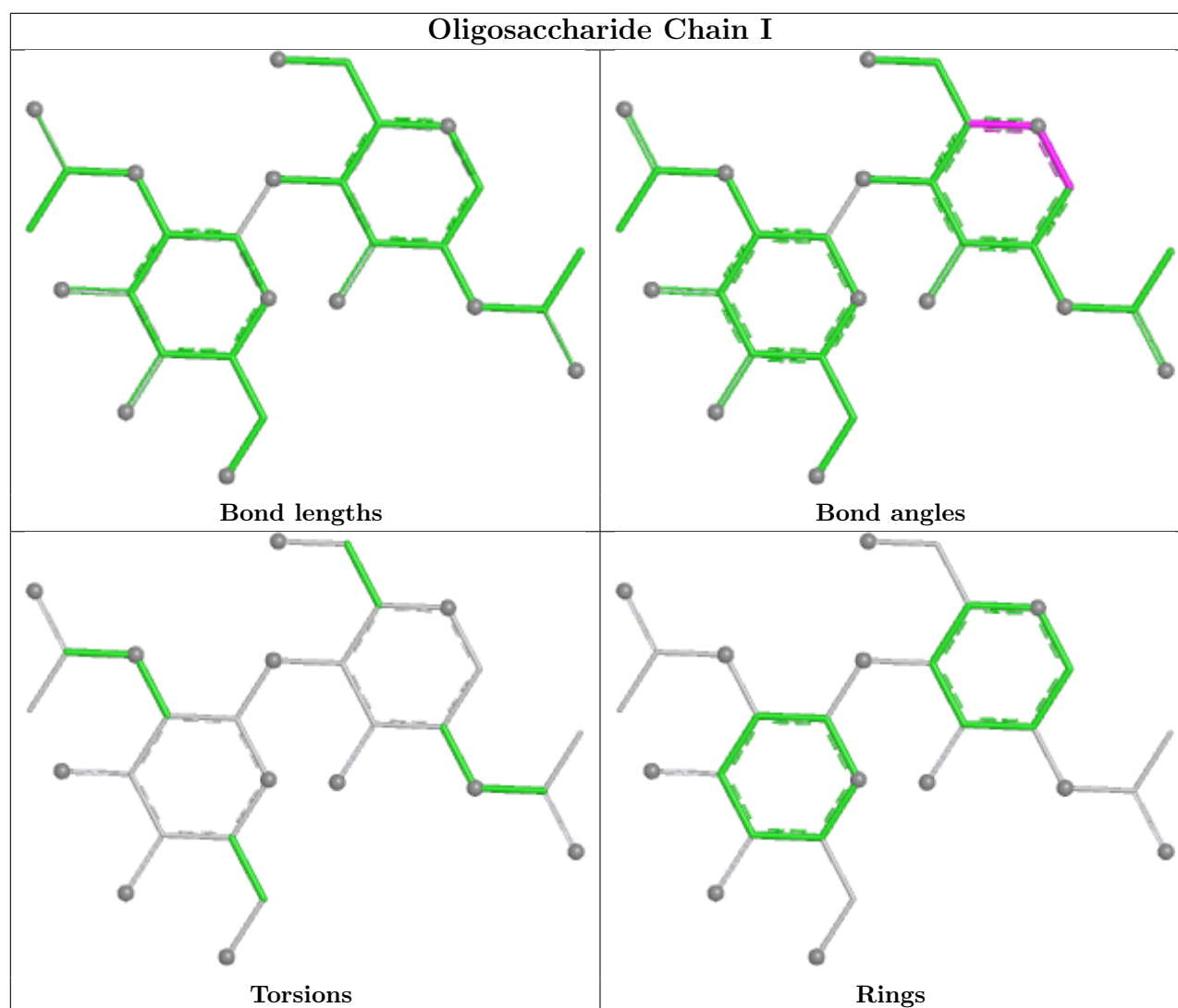


Oligosaccharide Chain H



Oligosaccharide Chain J





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
5	NAG	F	201	2,7	14,14,15	0.35	0	17,19,21	0.70	0
6	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.25	0
6	EDO	B	202	-	3,3,3	0.44	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.32	0
5	NAG	B	201	2,7	14,14,15	0.30	0	17,19,21	0.92	1 (5%)
6	EDO	A	405	-	3,3,3	0.40	0	2,2,2	0.47	0
5	NAG	A	404	1	14,14,15	0.34	0	17,19,21	1.21	2 (11%)
5	NAG	C	401	1	14,14,15	0.36	0	17,19,21	0.81	0
5	NAG	E	404	1	14,14,15	0.54	0	17,19,21	1.28	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
5	NAG	F	201	2,7	-	0/6/23/26	0/1/1/1
6	EDO	A	406	-	-	0/1/1/1	-
6	EDO	B	202	-	-	0/1/1/1	-
6	EDO	C	405	-	-	0/1/1/1	-
5	NAG	B	201	2,7	-	1/6/23/26	0/1/1/1
6	EDO	A	405	-	-	1/1/1/1	-
5	NAG	A	404	1	-	3/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	404	NAG	C1-O5-C5	4.56	118.29	112.19
5	A	404	NAG	O5-C1-C2	-3.03	106.60	111.29
5	B	201	NAG	C1-O5-C5	2.62	115.70	112.19
5	A	404	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	NAG	O5-C5-C6-O6
5	B	201	NAG	O5-C5-C6-O6
5	A	404	NAG	C3-C2-N2-C7
6	A	405	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	404	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/325 (98%)	0.81	27 (8%) 17 17	31, 41, 61, 75	0
1	C	320/325 (98%)	0.77	21 (6%) 24 25	28, 41, 56, 67	0
1	E	323/325 (99%)	1.68	104 (32%) 1 1	36, 60, 84, 92	0
2	B	172/177 (97%)	0.84	11 (6%) 25 26	32, 42, 58, 67	0
2	D	172/177 (97%)	0.56	11 (6%) 25 26	27, 37, 51, 63	0
2	F	172/177 (97%)	0.92	20 (11%) 9 10	31, 45, 60, 67	0
All	All	1479/1506 (98%)	0.98	194 (13%) 7 8	27, 44, 73, 92	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	ALA	5.1
1	E	197	VAL	4.8
1	E	233	GLY	4.7
1	A	210	VAL	4.6
1	E	119	SER	4.5
1	E	134	GLY	4.4
1	E	158	THR	4.2
1	E	157	THR	4.2
1	E	210	VAL	4.1
1	E	209	VAL	4.1
1	E	212	ALA	4.0
1	E	150	LYS	3.9
1	E	266	ILE	3.7
1	E	270	CYS	3.7
1	E	202	TYR	3.7
1	E	194	SER	3.6
1	E	167	ALA	3.6
1	E	118	GLY	3.6
1	E	207	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	94	TYR	3.6
1	E	244	LEU	3.4
1	C	282	ASN	3.4
1	E	156	GLN	3.4
1	C	268	ASN	3.4
1	E	193	LEU	3.4
1	E	130	CYS	3.3
1	E	116	THR	3.3
1	E	126	THR	3.3
1	E	70	LEU	3.3
1	E	234	ASP	3.2
1	C	270	CYS	3.2
1	E	117	TYR	3.2
2	F	72	GLU	3.2
1	E	181	THR	3.2
1	A	216	VAL	3.1
1	E	12	ASN	3.1
1	E	155	PRO	3.1
2	D	95	GLN	3.1
1	E	242	GLY	3.1
1	E	211	GLY	3.1
1	E	121	ILE	3.1
1	A	211	GLY	3.1
2	B	148	CYS	3.1
2	F	121	ARG	3.1
2	D	103	GLU	3.0
1	E	236	ILE	3.0
1	E	245	ILE	3.0
1	E	-1	ASP	3.0
2	D	137	CYS	3.0
2	F	75	HIS	3.0
1	A	282	ASN	3.0
2	F	144	CYS	3.0
1	E	168	GLU	3.0
1	E	195	ILE	3.0
1	E	196	SER	3.0
1	E	203	LYS	3.0
1	E	71	THR	2.9
1	E	38	LEU	2.9
2	B	32	THR	2.9
1	A	39	ASN	2.9
1	A	133	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	282	ASN	2.9
2	F	16	GLY	2.9
2	F	18	VAL	2.9
1	E	0	PRO	2.9
2	B	164	GLU	2.9
1	E	199	SER	2.8
1	E	111	ILE	2.8
1	E	201	THR	2.8
2	B	137	CYS	2.8
1	E	243	GLY	2.8
1	E	298	CYS	2.8
1	E	125	GLY	2.8
2	F	164	GLU	2.8
1	E	232	PRO	2.8
1	E	154	PHE	2.8
1	A	205	ASN	2.7
1	E	53	ASN	2.7
1	E	94	ASN	2.7
2	F	32	THR	2.7
1	E	149	ASN	2.7
1	E	151	GLY	2.7
1	E	206	PHE	2.6
1	A	94	ASN	2.6
1	E	268	ASN	2.6
2	B	172	ASN	2.6
1	A	192	SER	2.6
2	F	30	GLN	2.6
1	C	4	CYS	2.6
2	F	137	CYS	2.6
1	C	153	ASN	2.6
1	E	239	SER	2.6
1	E	122	ASN	2.6
1	E	114	GLY	2.6
1	A	223	ILE	2.6
1	E	205	ASN	2.5
1	E	166	THR	2.5
2	D	77	ILE	2.5
1	E	83	ALA	2.5
1	C	210	VAL	2.5
1	E	120	SER	2.5
1	E	152	GLN	2.5
1	E	187	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	229	LEU	2.5
1	E	164	ALA	2.5
1	A	87	CYS	2.5
1	A	134	GLY	2.5
1	A	214	PRO	2.5
1	E	188	TYR	2.5
1	E	124	ALA	2.5
1	C	87	CYS	2.4
1	E	4	CYS	2.4
1	E	237	THR	2.4
2	B	11	GLU	2.4
2	D	148	CYS	2.4
1	C	53	ASN	2.4
1	C	191	GLN	2.4
1	E	192	SER	2.4
1	E	115	PHE	2.4
1	E	238	PHE	2.4
1	E	68	LEU	2.4
1	E	170	LEU	2.4
1	C	47	ASN	2.4
1	A	45	GLY	2.4
1	E	269	SER	2.4
1	C	216	VAL	2.4
2	B	73	ILE	2.4
2	D	94	TYR	2.4
1	E	320	VAL	2.4
1	E	319	LEU	2.4
1	C	271	GLU	2.4
1	C	217	ASN	2.3
1	E	208	PRO	2.3
2	F	73	ILE	2.3
1	E	271	GLU	2.3
1	E	321	GLN	2.3
1	A	218	GLY	2.3
1	A	181	THR	2.3
1	C	200	SER	2.3
1	A	213	ARG	2.3
2	D	164	GLU	2.3
2	F	148	CYS	2.3
1	E	82	ASN	2.3
2	D	73	ILE	2.3
1	E	148	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	235	LYS	2.3
2	D	133	ASP	2.3
2	F	152	ILE	2.3
1	E	216	VAL	2.3
1	A	168	GLU	2.2
1	C	201	THR	2.2
2	F	171	LEU	2.2
2	F	70	PHE	2.2
1	E	190	THR	2.2
2	B	60	ASN	2.2
1	A	4	CYS	2.2
1	C	298	CYS	2.2
1	E	161	TYR	2.2
1	C	41	LEU	2.2
1	E	108	ILE	2.2
1	E	132	ARG	2.2
2	F	1	GLY	2.2
1	A	119	SER	2.2
1	E	85	ALA	2.2
1	E	281	ILE	2.1
1	C	43	MET	2.1
1	E	133	ASN	2.1
1	E	204	ASN	2.1
2	B	133	ASP	2.1
1	C	164	ALA	2.1
2	D	54	ARG	2.1
1	A	86	TYR	2.1
1	A	12	ASN	2.1
1	E	250	VAL	2.1
1	A	298	CYS	2.1
1	C	318	GLU	2.1
1	E	198	GLY	2.1
1	A	130	CYS	2.1
1	E	200	SER	2.1
1	A	318	GLU	2.1
1	E	22	GLU	2.1
2	F	168	LEU	2.1
1	E	293	ARG	2.1
1	E	240	HIS	2.0
1	E	112	ASN	2.0
2	F	60	ASN	2.0
1	A	93	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	160	THR	2.0
1	E	221	SER	2.0
2	F	62	GLU	2.0
2	B	95	GLN	2.0
1	C	82	ASN	2.0
2	D	171	LEU	2.0
2	B	121	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](#)

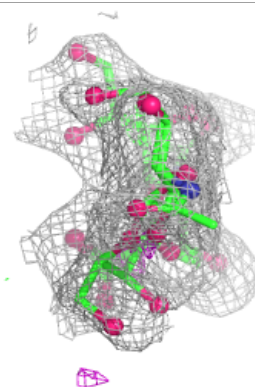
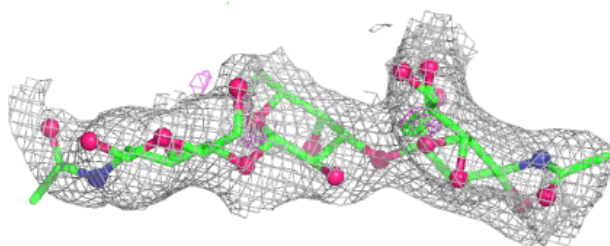
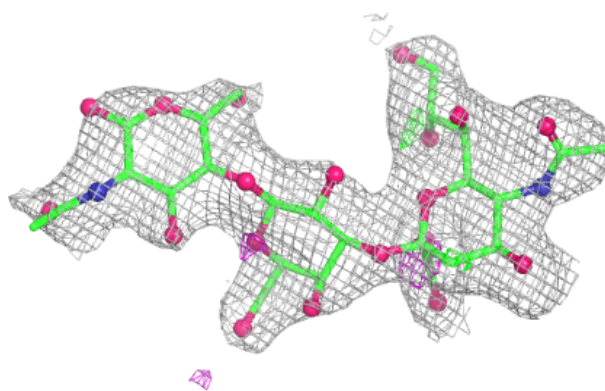
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	I	2	14/15	0.66	0.17	67,70,71,71	0
3	NAG	G	1	15/15	0.69	0.18	75,79,81,81	0
3	GAL	G	2	11/12	0.73	0.15	64,71,73,73	0
3	NAG	J	1	15/15	0.77	0.20	66,70,72,73	0
3	NAG	H	1	15/15	0.80	0.15	61,65,66,67	0
3	GAL	J	2	11/12	0.81	0.15	67,68,69,69	0
3	SIA	J	3	20/21	0.84	0.14	63,65,66,66	0
4	NAG	I	1	14/15	0.85	0.11	51,55,57,62	0
3	SIA	G	3	20/21	0.87	0.14	53,55,59,60	0
3	GAL	H	2	11/12	0.90	0.10	51,56,58,58	0
3	SIA	H	3	20/21	0.92	0.10	43,44,47,47	0

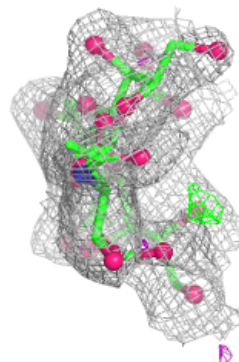
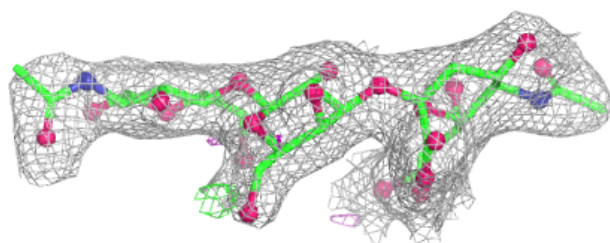
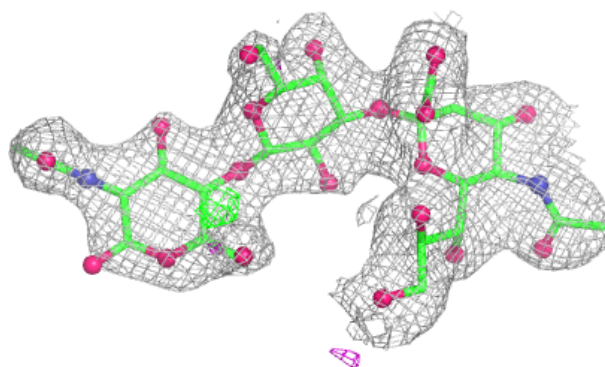
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

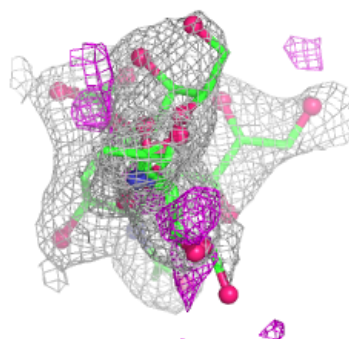
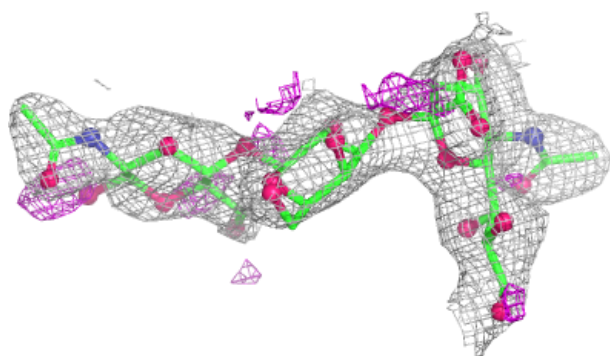
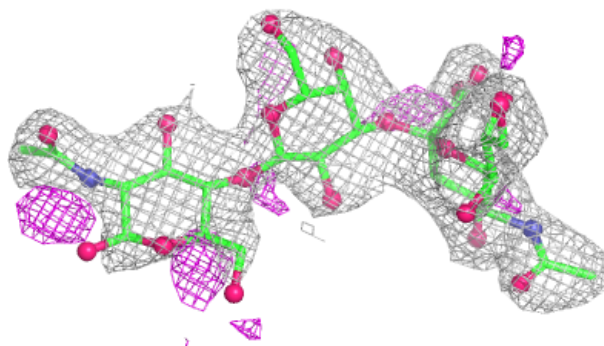
**Electron density around Chain H:**

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

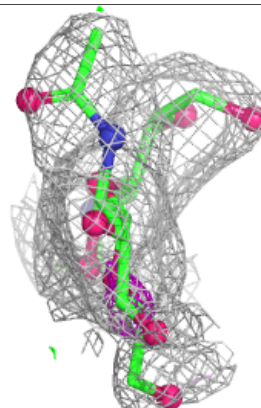
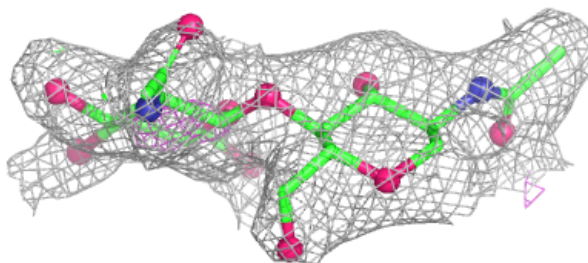
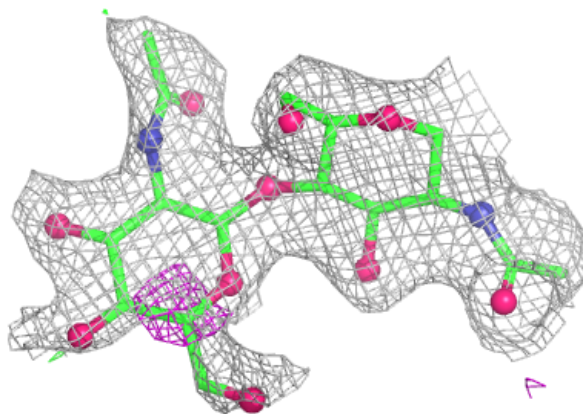


Electron density around Chain J:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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
5	NAG	E	404	14/15	0.55	0.23	76,80,82,83	0
5	NAG	C	401	14/15	0.60	0.18	54,57,58,58	0
6	EDO	B	202	4/4	0.63	0.29	73,73,73,73	0
5	NAG	A	404	14/15	0.72	0.15	59,62,63,63	0
5	NAG	B	201	14/15	0.76	0.14	49,52,54,54	0
5	NAG	F	201	14/15	0.77	0.14	53,56,59,61	0
6	EDO	C	405	4/4	0.86	0.19	55,55,56,57	0
7	CA	E	405	1/1	0.87	0.09	59,59,59,59	0
6	EDO	A	406	4/4	0.88	0.15	48,48,48,49	0
6	EDO	A	405	4/4	0.90	0.19	48,49,50,50	0
7	CA	C	406	1/1	0.91	0.10	65,65,65,65	0
7	CA	A	407	1/1	0.96	0.10	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.