



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:31 PM UTC

PDB ID : 4CQW / pdb_00004cqw
Title : H5 (tyTy) Del133/Ile155Thr Mutant Haemagglutinin in Complex with Avian Receptor Analogue 3'SLN
Authors : Xiong, X.; Xiao, H.; Martin, S.R.; Coombs, P.J.; Liu, J.; Collins, P.J.; Vachieri, S.G.; Walker, P.A.; Lin, Y.P.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-02-21
Resolution : 2.30 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

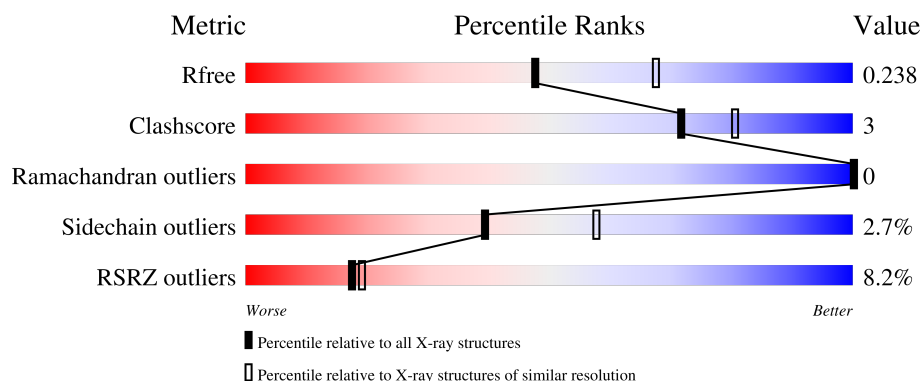
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



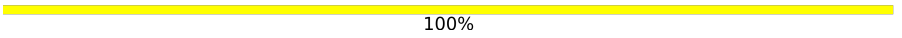
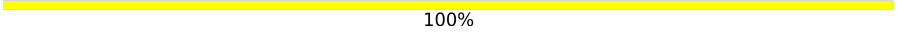
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	327	89% 9% ..
1	C	327	91% 7% .
1	E	327	90% 8% ..
2	B	166	8% 83% 15% .
2	D	166	31% 82% 15% ..

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Mol	Chain	Length	Quality of chain
2	F	166	
3	G	3	
3	H	3	
3	I	3	

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
4	NAG	A	1023	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12709 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 HAEMAGGLUTININ HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2572	1618	449	491	14			
1	C	322	Total	C	N	O	S	0	0	0
			2552	1607	443	488	14			
1	E	322	Total	C	N	O	S	0	0	0
			2552	1607	443	488	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP Q207Z6
A	0	PRO	-	expression tag	UNP Q207Z6
A	?	-	ALA	deletion	UNP Q207Z6
A	150	THR	ILE	engineered mutation	UNP Q207Z6
A	322	ARG	GLY	conflict	UNP Q207Z6
A	324	THR	ARG	conflict	UNP Q207Z6
C	-1	ASP	-	expression tag	UNP Q207Z6
C	0	PRO	-	expression tag	UNP Q207Z6
C	?	-	ALA	deletion	UNP Q207Z6
C	150	THR	ILE	engineered mutation	UNP Q207Z6
C	322	ARG	GLY	conflict	UNP Q207Z6
C	324	THR	ARG	conflict	UNP Q207Z6
E	-1	ASP	-	expression tag	UNP Q207Z6
E	0	PRO	-	expression tag	UNP Q207Z6
E	?	-	ALA	deletion	UNP Q207Z6
E	150	THR	ILE	engineered mutation	UNP Q207Z6
E	322	ARG	GLY	conflict	UNP Q207Z6
E	324	THR	ARG	conflict	UNP Q207Z6

- Molecule 2 is a protein called HAEMAGGLUTININ HA2.

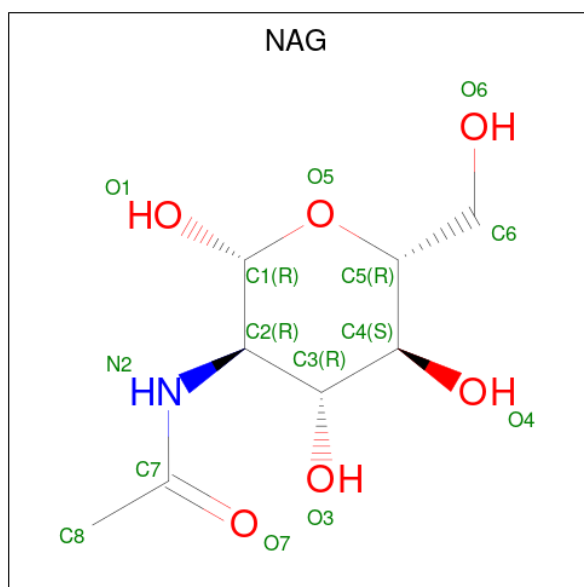
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	163	Total	C	N	O	S	0	0	0
			1320	822	229	261	8			
2	D	163	Total	C	N	O	S	0	0	0
			1320	822	229	261	8			
2	F	163	Total	C	N	O	S	0	0	0
			1320	822	229	261	8			

- 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.



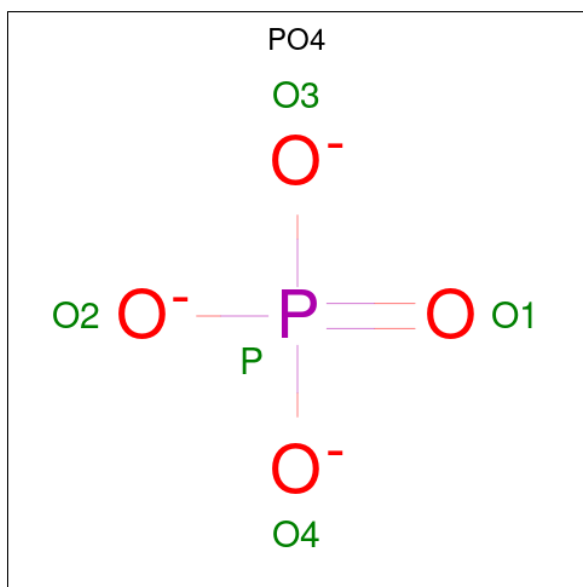
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	H	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	I	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

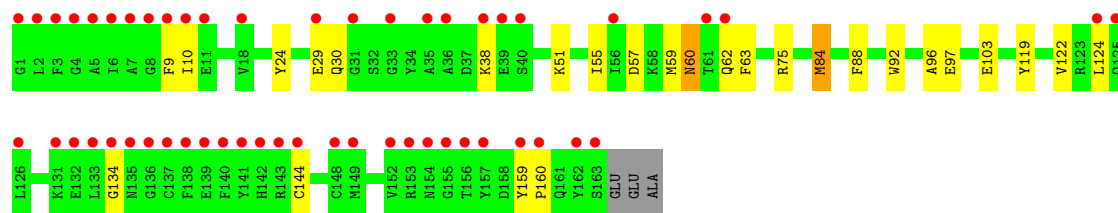
- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



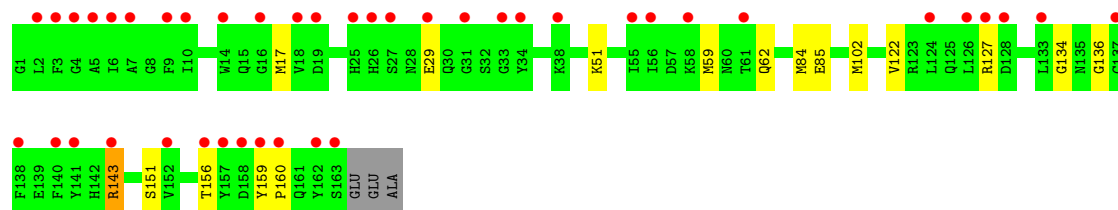
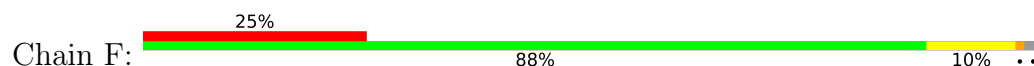
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total 197	O 197	0	0
6	B	64	Total 64	O 64	0	0
6	C	262	Total 262	O 262	0	0
6	D	30	Total 30	O 30	0	0
6	E	225	Total 225	O 225	0	0
6	F	26	Total 26	O 26	0	0



● Molecule 2: HAEMAGGLUTININ 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.64Å 117.55Å 101.16Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	101.06 – 2.30 101.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (101.06-2.30) 98.3 (101.06-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.196 , 0.238 0.196 , 0.238	Depositor DCC
R_{free} test set	4479 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12709	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: PO4, NAG, GAL, SIA

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	0.41	0/2634	0.72	0/3580
1	C	0.44	0/2614	0.70	0/3554
1	E	0.44	0/2614	0.72	0/3554
2	B	0.42	0/1347	0.82	0/1813
2	D	0.40	0/1347	0.81	0/1813
2	F	0.42	0/1347	0.83	1/1813 (0.1%)
All	All	0.42	0/11903	0.75	1/16127 (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	F	136	GLY	N-CA-C	-5.41	107.75	115.64

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	2572	0	2504	19	0
1	C	2552	0	2483	12	0
1	E	2552	0	2483	18	0
2	B	1320	0	1224	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1320	0	1224	18	0
2	F	1320	0	1224	11	0
3	G	46	0	40	0	0
3	H	46	0	40	0	0
3	I	46	0	40	0	0
4	A	42	0	39	2	0
4	C	42	0	39	1	0
4	E	42	0	39	4	0
5	A	5	0	0	0	0
6	A	197	0	0	0	0
6	B	64	0	0	2	0
6	C	262	0	0	0	0
6	D	30	0	0	0	0
6	E	225	0	0	0	0
6	F	26	0	0	0	0
All	All	12709	0	11379	77	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 3.

All (77) 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:E:19:ILE:HD11	2:F:102:MET:HA	1.57	0.85
4:E:1023:NAG:H83	4:E:1023:NAG:H3	1.66	0.77
1:E:290:PHE:HZ	2:F:59:MET:HG3	1.57	0.69
1:C:290:PHE:HZ	2:D:59:MET:HG3	1.60	0.66
1:E:0:PRO:HA	2:F:143:ARG:HH22	1.60	0.66
1:E:1:ASP:H	2:F:143:ARG:HH12	1.44	0.66
1:A:19:ILE:HD12	2:B:101:LEU:HB3	1.78	0.65
1:C:279:THR:HG22	1:C:297:THR:HG22	1.77	0.65
2:B:131:LYS:HE2	2:F:127:ARG:HH21	1.63	0.63
1:A:290:PHE:HZ	2:B:59:MET:HG3	1.65	0.62
1:C:5:ILE:HD11	2:D:122:VAL:HG21	1.83	0.61
2:B:19:ASP:HB2	6:B:2005:HOH:O	2.01	0.61
4:E:1023:NAG:H3	4:E:1023:NAG:C8	2.31	0.61
2:B:51:LYS:HE3	1:C:20:MET:HE3	1.84	0.59
2:D:57:ASP:O	2:D:60:ASN:HB2	2.03	0.59
1:E:279:THR:HG22	1:E:297:THR:HG22	1.84	0.58
1:C:48:LYS:HG3	1:C:49:PRO:HD2	1.86	0.57
1:A:279:THR:HG22	1:A:297:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:LYS:HE3	1:E:20:MET:HE2	1.89	0.55
2:D:159:TYR:N	2:D:160:PRO:HD2	2.22	0.55
1:C:159:ILE:O	1:C:241:GLU:HA	2.07	0.54
2:B:58:LYS:HE3	2:D:97:GLU:HB3	1.90	0.54
2:F:84:MET:HE2	2:F:85:GLU:HG2	1.90	0.53
2:B:156:THR:O	2:B:156:THR:HG22	2.09	0.52
2:B:25:HIS:HE1	6:B:2015:HOH:O	1.91	0.52
1:E:19:ILE:HD12	1:E:19:ILE:H	1.74	0.52
1:E:280:PRO:HD3	1:E:296:LEU:O	2.10	0.51
1:E:68:ASP:OD2	1:E:144:ARG:NH1	2.44	0.50
1:E:5:ILE:HD11	2:F:122:VAL:HG21	1.92	0.50
1:A:16:VAL:HG21	1:A:313:ALA:HB2	1.93	0.49
1:A:20:MET:HE2	2:F:51:LYS:HE3	1.93	0.49
1:C:16:VAL:HG21	1:C:313:ALA:HB2	1.94	0.48
2:D:62:GLN:HG2	2:D:92:TRP:CE3	2.48	0.48
1:E:235:ASN:HD22	4:E:1164:NAG:H5	1.78	0.48
1:A:159:ILE:O	1:A:241:GLU:HA	2.14	0.47
1:A:-1:ASP:N	1:A:0:PRO:HD2	2.30	0.47
1:E:215:ARG:HH21	1:E:223:GLY:HA2	1.80	0.47
4:A:1023:NAG:H3	4:A:1023:NAG:H83	1.97	0.46
1:A:235:ASN:HD22	4:A:1164:NAG:H5	1.79	0.46
1:C:109:ASN:HB2	1:C:257:LYS:HD3	1.96	0.46
1:C:290:PHE:HE1	2:D:62:GLN:OE1	1.97	0.46
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.97	0.46
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.98	0.46
2:D:55:ILE:HD11	2:D:103:GLU:HG3	1.98	0.45
1:A:2:GLN:HB2	2:B:138:PHE:O	2.17	0.45
1:A:93:GLY:HA3	1:A:225:MET:O	2.17	0.45
1:C:5:ILE:HG13	2:D:119:TYR:HA	1.99	0.45
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.52	0.44
1:A:280:PRO:HD3	1:A:296:LEU:O	2.18	0.44
1:C:93:GLY:HA3	1:C:225:MET:O	2.18	0.44
2:D:59:MET:HE2	2:D:96:ALA:HB2	2.00	0.43
1:A:215:ARG:HH21	1:A:223:GLY:HA2	1.83	0.43
2:B:124:LEU:HD22	2:D:134:GLY:HA2	2.00	0.43
1:A:47:VAL:HB	1:A:77:SER:HB3	2.01	0.43
2:B:68:ARG:HD2	2:B:81:ASN:OD1	2.19	0.43
2:D:63:PHE:CZ	2:D:84:MET:HE1	2.53	0.43
1:E:159:ILE:O	1:E:241:GLU:HA	2.19	0.43
1:E:235:ASN:ND2	4:E:1164:NAG:H5	2.33	0.43
1:A:5:ILE:HG13	2:B:119:TYR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.53	0.42
2:B:129:ASN:OD1	2:B:163:SER:HB3	2.19	0.42
1:A:63:GLY:O	1:A:144:ARG:HD2	2.20	0.42
2:D:63:PHE:CZ	2:D:84:MET:CE	3.02	0.42
1:E:93:GLY:HA3	1:E:225:MET:O	2.20	0.42
1:E:15:GLN:O	1:E:309:ARG:NH2	2.53	0.42
1:E:75:GLU:OE2	1:E:257:LYS:HE2	2.19	0.42
2:F:59:MET:HE3	2:F:62:GLN:OE1	2.19	0.42
1:A:48:LYS:HG2	1:A:49:PRO:HD2	2.02	0.41
2:D:124:LEU:HD22	2:F:134:GLY:HA2	2.01	0.41
1:C:53:ARG:HB3	1:C:54:ASP:H	1.63	0.41
2:D:62:GLN:HG2	2:D:92:TRP:CD2	2.56	0.41
2:D:84:MET:HE3	2:D:88:PHE:CD2	2.56	0.41
1:A:214:THR:O	1:E:239:ASN:HB2	2.21	0.41
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.55	0.41
4:C:1023:NAG:C8	4:C:1023:NAG:H3	2.51	0.41
1:A:5:ILE:HD11	2:B:122:VAL:HG21	2.03	0.41
1:A:8:HIS:O	1:A:316:LEU:HD11	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/327 (98%)	312 (97%)	10 (3%)	0	100	100
1	C	320/327 (98%)	308 (96%)	12 (4%)	0	100	100
1	E	320/327 (98%)	311 (97%)	9 (3%)	0	100	100
2	B	161/166 (97%)	156 (97%)	5 (3%)	0	100	100
2	D	161/166 (97%)	155 (96%)	6 (4%)	0	100	100
2	F	161/166 (97%)	158 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1445/1479 (98%)	1400 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	291/294 (99%)	285 (98%)	6 (2%)	47	66
1	C	289/294 (98%)	282 (98%)	7 (2%)	43	62
1	E	289/294 (98%)	283 (98%)	6 (2%)	47	66
2	B	139/141 (99%)	136 (98%)	3 (2%)	45	65
2	D	139/141 (99%)	131 (94%)	8 (6%)	18	26
2	F	139/141 (99%)	134 (96%)	5 (4%)	31	47
All	All	1286/1305 (98%)	1251 (97%)	35 (3%)	39	58

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	89	LEU
1	A	104	LEU
1	A	144	ARG
1	A	273	CYS
1	A	279	THR
2	B	22	TYR
2	B	30	GLN
2	B	39	GLU
1	C	19	ILE
1	C	89	LEU
1	C	104	LEU
1	C	107	ARG
1	C	161	ARG

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Mol	Chain	Res	Type
1	C	212	ILE
1	C	316	LEU
2	D	24	TYR
2	D	29	GLU
2	D	30	GLN
2	D	38	LYS
2	D	60	ASN
2	D	75	ARG
2	D	84	MET
2	D	144	CYS
1	E	84	ASN
1	E	89	LEU
1	E	104	LEU
1	E	139	ARG
1	E	144	ARG
1	E	279	THR
2	F	17	MET
2	F	29	GLU
2	F	143	ARG
2	F	151	SER
2	F	156	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	103	HIS
1	A	235	ASN
2	B	25	HIS
2	B	42	GLN
2	B	154	ASN
1	C	72	ASN
1	C	110	HIS
2	D	42	GLN
2	D	60	ASN
2	D	161	GLN
1	E	8	HIS
1	E	84	ASN
1	E	94	ASN
1	E	110	HIS
1	E	137	GLN
1	E	154	ASN

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Mol	Chain	Res	Type
1	E	235	ASN
1	E	272	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	0.47	0	21,21,21	1.30	2 (9%)
3	GAL	G	2	3	11,11,12	0.33	0	15,15,17	0.99	1 (6%)
3	SIA	G	3	3	20,20,21	0.58	0	21,28,31	1.31	3 (14%)
3	NAG	H	1	3	15,15,15	0.45	0	21,21,21	2.02	4 (19%)
3	GAL	H	2	3	11,11,12	0.30	0	15,15,17	0.77	0
3	SIA	H	3	3	20,20,21	0.62	0	21,28,31	1.25	2 (9%)
3	NAG	I	1	3	15,15,15	0.47	0	21,21,21	1.23	2 (9%)
3	GAL	I	2	3	11,11,12	0.35	0	15,15,17	1.08	3 (20%)
3	SIA	I	3	3	20,20,21	0.65	0	21,28,31	1.28	3 (14%)

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	-	0/2/19/22	0/1/1/1
3	SIA	H	3	3	-	0/18/34/38	0/1/1/1
3	NAG	I	1	3	-	0/6/26/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	SIA	I	3	3	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-C2-N2	-6.05	103.72	110.73
3	G	1	NAG	C1-C2-N2	-4.79	105.18	110.73
3	H	1	NAG	C3-C2-N2	-4.50	102.33	110.62
3	I	1	NAG	C1-C2-N2	-3.57	106.59	110.73
3	I	3	SIA	C4-C5-N5	-3.34	103.85	110.44
3	H	1	NAG	O5-C1-C2	2.97	112.50	109.52
3	H	3	SIA	C4-C5-N5	-2.84	104.85	110.44
3	G	3	SIA	C4-C5-N5	-2.66	105.19	110.44
3	G	3	SIA	O1B-C1-C2	2.54	119.31	112.71
3	G	1	NAG	C3-C2-N2	-2.51	105.99	110.62
3	H	3	SIA	O1B-C1-C2	2.51	119.23	112.71
3	G	2	GAL	C1-C2-C3	2.44	113.19	109.64
3	I	3	SIA	O1B-C1-C2	2.33	118.76	112.71
3	G	3	SIA	O6-C2-C1	2.28	112.02	107.72
3	I	3	SIA	C6-C5-N5	-2.19	107.42	110.91
3	I	2	GAL	C1-C2-C3	2.15	112.77	109.64
3	I	2	GAL	C1-O5-C5	2.10	115.00	112.19
3	I	1	NAG	C3-C2-N2	-2.09	106.76	110.62
3	H	1	NAG	C1-C2-C3	2.08	113.38	110.54
3	I	2	GAL	O3-C3-C2	-2.05	105.86	110.05

There are no chirality outliers.

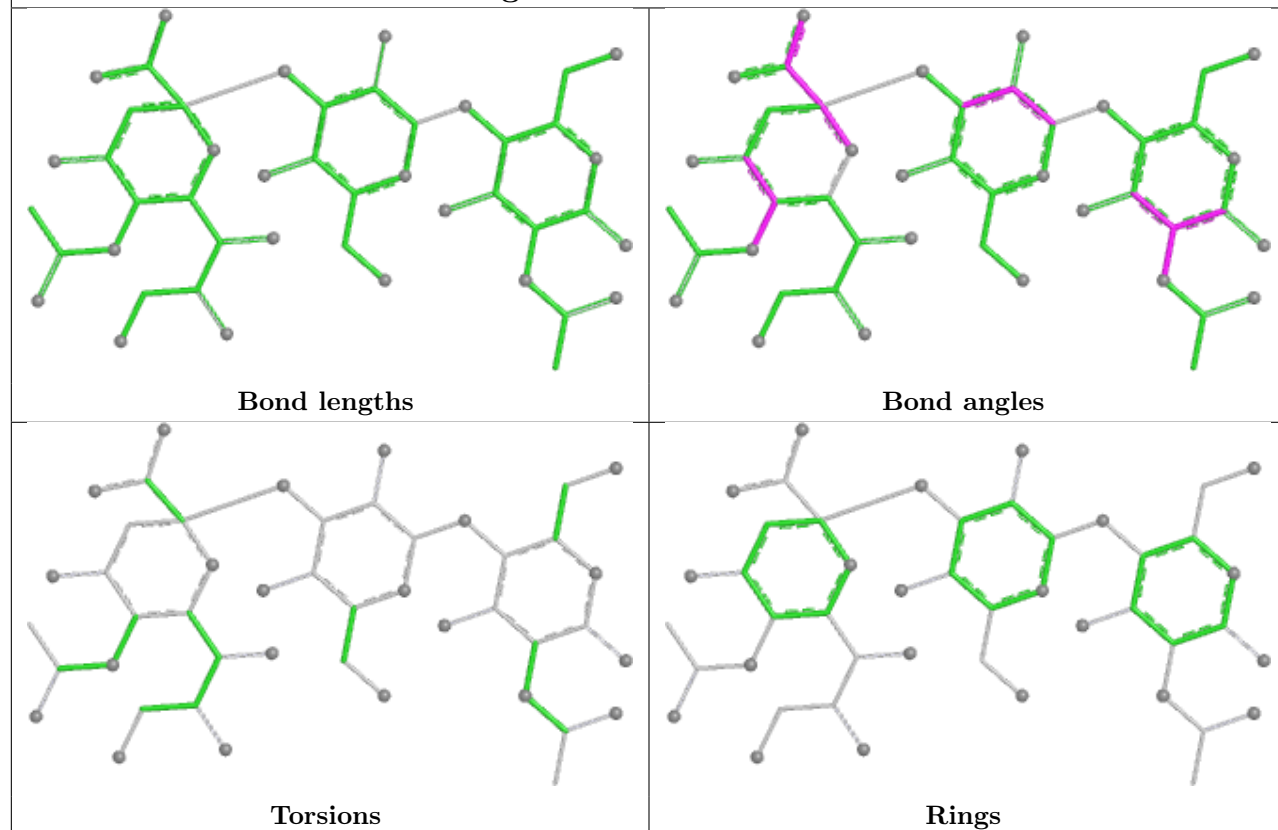
There are no torsion outliers.

There are no ring outliers.

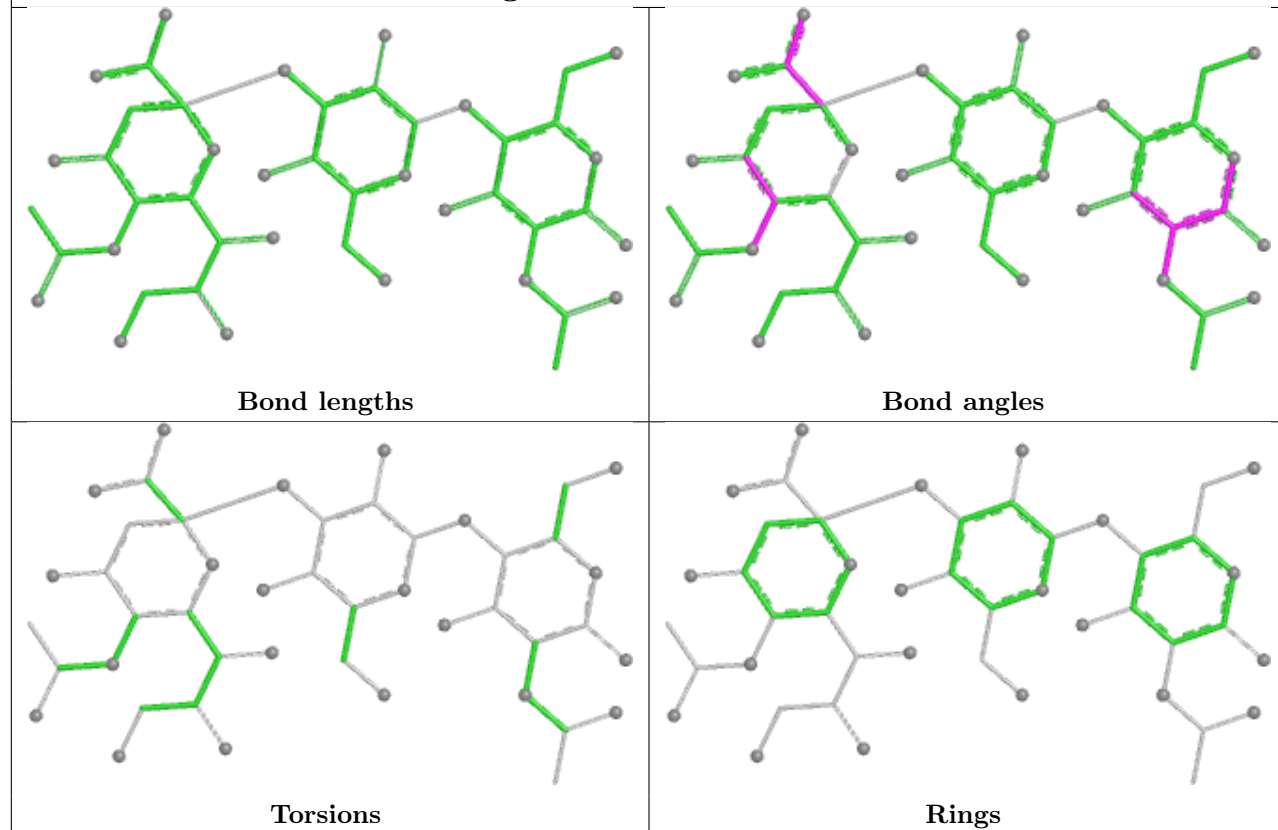
No monomer is involved in short contacts.

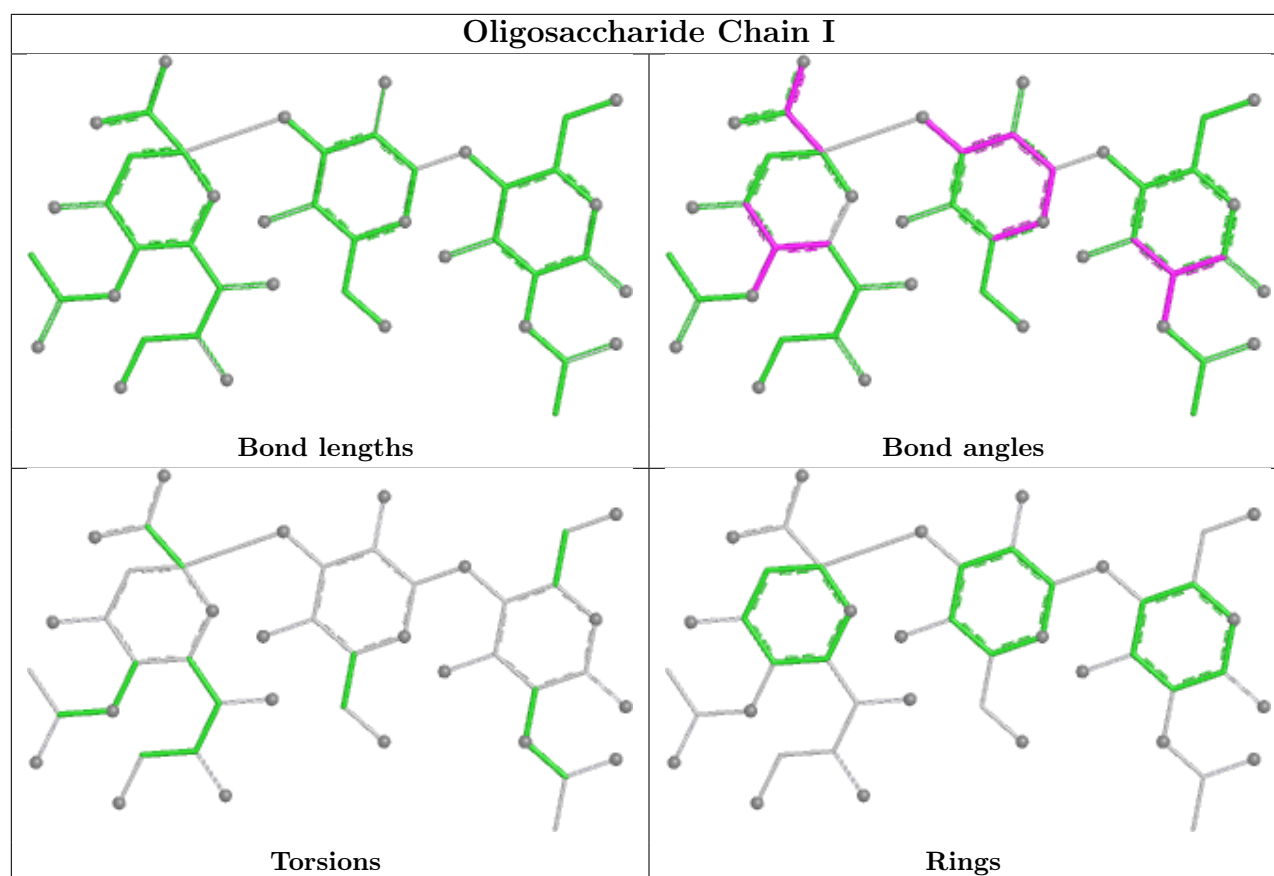
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G



Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	NAG	A	1023	1	14,14,15	0.74	1 (7%)	17,19,21	2.58	6 (35%)
4	NAG	C	1023	1	14,14,15	0.69	0	17,19,21	2.31	5 (29%)
4	NAG	E	1011	1	14,14,15	0.50	0	17,19,21	1.14	1 (5%)
4	NAG	E	1023	1	14,14,15	0.69	0	17,19,21	2.05	4 (23%)
4	NAG	A	1011	1	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
4	NAG	C	1011	1	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
4	NAG	E	1164	1	14,14,15	0.42	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1164	1	14,14,15	0.49	0	17,19,21	1.21	2 (11%)
5	PO4	A	1325	-	4,4,4	0.94	0	6,6,6	0.57	0
4	NAG	A	1164	1	14,14,15	0.45	0	17,19,21	1.02	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
4	NAG	A	1023	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	C	1023	1	-	3/6/23/26	0/1/1/1
4	NAG	E	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1023	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1011	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1164	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1164	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1164	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1023	NAG	C1-C2	2.22	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1023	NAG	C2-N2-C7	7.03	132.33	122.90
4	A	1023	NAG	C2-N2-C7	6.91	132.17	122.90
4	E	1023	NAG	C2-N2-C7	5.92	130.83	122.90
4	A	1023	NAG	C1-O5-C5	4.09	117.67	112.19
4	A	1011	NAG	C1-O5-C5	3.87	117.37	112.19
4	A	1023	NAG	O5-C1-C2	-3.86	105.33	111.29
4	E	1011	NAG	C1-O5-C5	3.77	117.24	112.19
4	C	1023	NAG	C8-C7-N2	3.60	122.08	116.12
4	E	1023	NAG	C8-C7-N2	3.51	121.94	116.12
4	C	1164	NAG	C1-O5-C5	3.47	116.84	112.19
4	A	1023	NAG	C8-C7-N2	3.45	121.85	116.12
4	C	1023	NAG	C1-O5-C5	3.41	116.76	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1023	NAG	C1-C2-N2	3.33	115.69	110.43
4	A	1164	NAG	C1-O5-C5	3.23	116.51	112.19
4	E	1164	NAG	C1-O5-C5	2.85	116.00	112.19
4	C	1011	NAG	C1-O5-C5	2.79	115.92	112.19
4	E	1023	NAG	C4-C3-C2	2.63	114.87	111.02
4	E	1023	NAG	O7-C7-C8	-2.51	117.59	122.05
4	C	1023	NAG	O7-C7-C8	-2.39	117.80	122.05
4	A	1023	NAG	O7-C7-C8	-2.37	117.84	122.05
4	C	1023	NAG	C1-C2-N2	2.22	113.93	110.43
4	C	1164	NAG	C3-C4-C5	-2.05	106.51	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1023	NAG	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1023	NAG	C3-C2-N2-C7
4	C	1023	NAG	C3-C2-N2-C7
4	E	1023	NAG	O5-C5-C6-O6
4	C	1011	NAG	O5-C5-C6-O6
4	E	1023	NAG	C4-C5-C6-O6
4	A	1011	NAG	C8-C7-N2-C2
4	A	1011	NAG	O7-C7-N2-C2
4	A	1023	NAG	C8-C7-N2-C2
4	A	1023	NAG	O7-C7-N2-C2
4	C	1023	NAG	C8-C7-N2-C2
4	C	1023	NAG	O7-C7-N2-C2
4	E	1023	NAG	C8-C7-N2-C2
4	E	1023	NAG	O7-C7-N2-C2
4	A	1023	NAG	O5-C5-C6-O6
4	C	1011	NAG	C4-C5-C6-O6
4	C	1164	NAG	C4-C5-C6-O6
4	C	1164	NAG	O5-C5-C6-O6
4	E	1023	NAG	C3-C2-N2-C7
4	A	1023	NAG	C4-C5-C6-O6
4	A	1011	NAG	C4-C5-C6-O6
4	E	1164	NAG	C4-C5-C6-O6
4	E	1164	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1023	NAG	1	0
4	C	1023	NAG	1	0
4	E	1023	NAG	2	0
4	E	1164	NAG	2	0
4	A	1164	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 ⓘ

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	324/327 (99%)	-0.16	3 (0%) 81 82	27, 42, 57, 84	0
1	C	322/327 (98%)	-0.27	2 (0%) 85 86	24, 35, 60, 114	0
1	E	322/327 (98%)	-0.17	7 (2%) 62 64	25, 37, 71, 122	0
2	B	163/166 (98%)	0.46	13 (7%) 18 20	23, 51, 80, 99	0
2	D	163/166 (98%)	1.30	52 (31%) 1 1	25, 74, 147, 156	0
2	F	163/166 (98%)	1.30	42 (25%) 1 2	23, 80, 145, 171	0
All	All	1457/1479 (98%)	0.21	119 (8%) 17 19	23, 41, 126, 171	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	134	GLY	5.1
2	D	136	GLY	4.9
2	D	7	ALA	4.8
2	D	5	ALA	4.4
1	E	273	CYS	4.4
2	F	5	ALA	4.3
1	E	320	PRO	4.2
2	D	138	PHE	4.1
2	B	7	ALA	4.0
2	D	9	PHE	3.9
2	B	163	SER	3.9
1	C	320	PRO	3.9
2	D	2	LEU	3.8
2	D	6	ILE	3.8
2	F	29	GLU	3.7
2	D	162	TYR	3.7
2	F	7	ALA	3.7
2	B	9	PHE	3.7
2	F	3	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	6	ILE	3.7
2	F	124	LEU	3.7
2	F	141	TYR	3.7
2	F	160	PRO	3.7
2	F	163	SER	3.6
2	F	56	ILE	3.6
2	D	133	LEU	3.5
1	A	273	CYS	3.5
2	F	152	VAL	3.5
2	D	3	PHE	3.4
2	D	135	ASN	3.3
2	D	141	TYR	3.3
2	D	153	ARG	3.3
2	F	157	TYR	3.3
2	F	18	VAL	3.3
2	F	159	TYR	3.3
2	F	33	GLY	3.2
2	D	155	GLY	3.2
2	D	137	CYS	3.2
2	B	56	ILE	3.2
2	F	31	GLY	3.2
2	F	58	LYS	3.1
2	D	140	PHE	3.1
2	F	140	PHE	3.1
2	F	2	LEU	3.1
2	D	163	SER	3.1
2	B	2	LEU	3.1
2	F	9	PHE	3.0
2	F	126	LEU	3.0
2	B	3	PHE	3.0
2	D	126	LEU	3.0
2	F	162	TYR	3.0
2	D	124	LEU	2.9
2	D	156	THR	2.9
2	D	142	HIS	2.8
2	D	1	GLY	2.8
1	A	322	ARG	2.8
2	D	33	GLY	2.7
2	F	27	SER	2.7
2	D	160	PRO	2.7
2	D	38	LYS	2.7
1	E	5	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	156	THR	2.7
2	B	8	GLY	2.7
2	F	137	CYS	2.7
2	D	152	VAL	2.7
2	D	4	GLY	2.7
2	F	61	THR	2.6
2	B	6	ILE	2.6
2	D	8	GLY	2.6
2	F	34	TYR	2.6
2	D	31	GLY	2.6
2	D	61	THR	2.6
2	B	160	PRO	2.6
2	F	14	TRP	2.6
1	C	0	PRO	2.6
2	F	138	PHE	2.6
2	B	1	GLY	2.5
2	D	36	ALA	2.5
2	D	144	CYS	2.5
2	F	16	GLY	2.5
2	F	26	HIS	2.5
2	D	149	MET	2.5
1	E	9	ALA	2.5
1	E	0	PRO	2.5
2	F	25	HIS	2.5
2	D	148	CYS	2.4
2	B	159	TYR	2.4
1	E	3	ILE	2.4
2	D	11	GLU	2.4
2	B	61	THR	2.4
2	B	156	THR	2.4
2	D	159	TYR	2.3
2	D	131	LYS	2.3
2	D	29	GLU	2.3
2	D	62	GLN	2.3
2	F	38	LYS	2.3
2	F	133	LEU	2.3
2	F	127	ARG	2.3
2	D	132	GLU	2.3
2	D	56	ILE	2.3
2	D	125	GLN	2.2
2	D	10	ILE	2.2
1	E	316	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	18	VAL	2.2
2	F	19	ASP	2.2
2	F	128	ASP	2.2
2	F	143	ARG	2.2
2	F	10	ILE	2.2
2	F	55	ILE	2.2
2	F	158	ASP	2.1
2	D	157	TYR	2.1
2	D	154	ASN	2.1
2	D	139	GLU	2.1
2	F	4	GLY	2.1
2	D	40	SER	2.0
2	D	143	ARG	2.0
2	D	39	GLU	2.0
2	D	35	ALA	2.0
1	A	84	ASN	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](#)

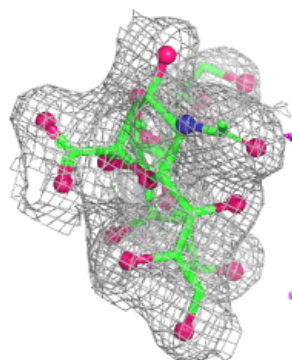
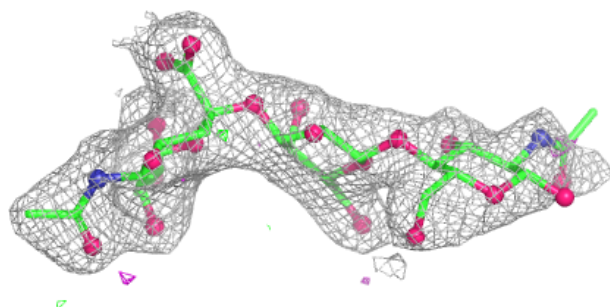
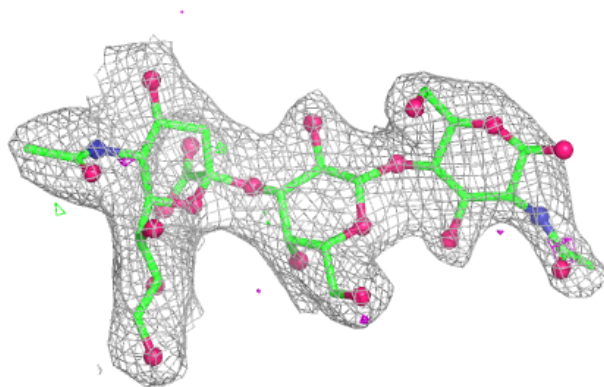
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	I	1	15/15	0.82	0.14	52,60,66,67	0
3	NAG	H	1	15/15	0.87	0.11	48,58,67,67	0
3	NAG	G	1	15/15	0.87	0.13	59,68,76,77	0
3	GAL	I	2	11/12	0.92	0.08	38,43,45,47	0
3	GAL	G	2	11/12	0.93	0.08	44,47,51,53	0
3	SIA	G	3	20/21	0.94	0.08	34,39,43,44	0
3	SIA	H	3	20/21	0.94	0.07	27,31,33,35	0
3	GAL	H	2	11/12	0.97	0.05	35,37,41,42	0
3	SIA	I	3	20/21	0.97	0.06	29,31,36,36	0

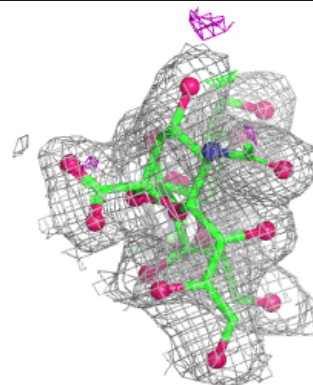
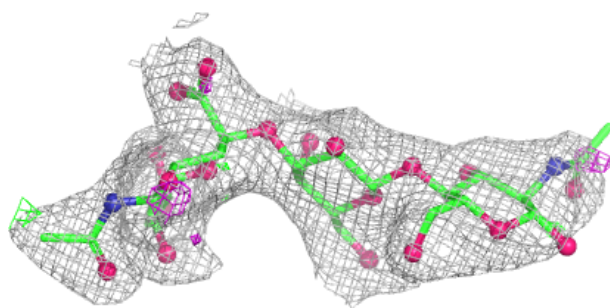
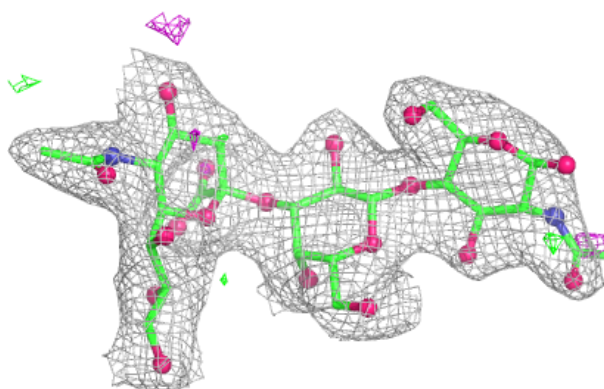
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

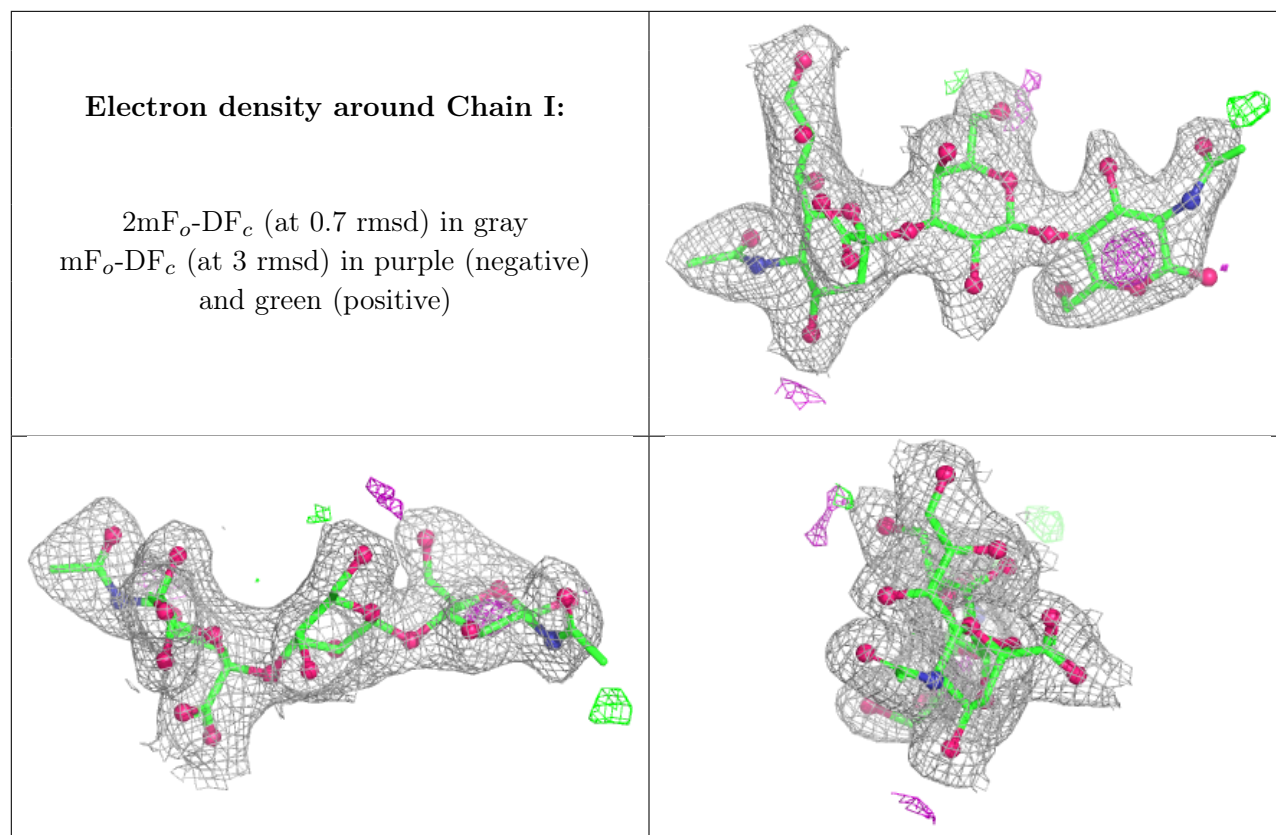
Electron density around Chain G:

$2mF_o-DF_c$ (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)





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($\text{\AA}^2$)	Q<0.9
4	NAG	C	1023	14/15	0.59	0.16	65,78,87,90	0
4	NAG	A	1023	14/15	0.67	0.15	50,61,65,68	0
4	NAG	E	1023	14/15	0.68	0.14	60,70,76,76	0
5	PO4	A	1325	5/5	0.79	0.18	79,82,86,87	0
4	NAG	E	1011	14/15	0.80	0.14	55,64,68,70	0
4	NAG	C	1011	14/15	0.87	0.10	47,54,58,59	0
4	NAG	A	1164	14/15	0.89	0.09	35,40,46,47	0
4	NAG	E	1164	14/15	0.90	0.09	33,38,41,44	0
4	NAG	C	1164	14/15	0.90	0.09	33,39,45,51	0
4	NAG	A	1011	14/15	0.93	0.08	33,40,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.