



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 8T1G / pdb_00008t1g
Title : The crystal structure of hemagglutinin from a h7n9 influenza virus
(a/shanghai/1/2013) in complex with antibody 1E11
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2023-06-02
Resolution : 3.50 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

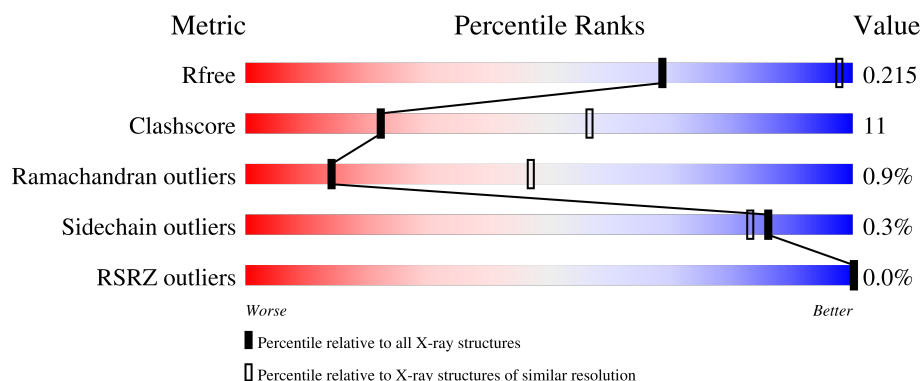
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



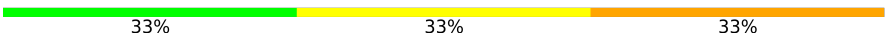
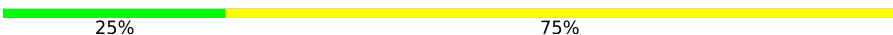
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	321	75% 25% .
1	C	321	76% 23% .
1	E	321	75% 24% .
2	B	210	65% 32% .
2	D	210	66% 31% ..

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Mol	Chain	Length	Quality of chain
2	F	210	 70%27%..
3	G	232	 76%22%..
3	H	232	 74%24%.
3	J	232	 72%27%.
4	I	219	 71%28%.
4	K	219	 76%24%
4	L	219	 74%24%..
5	M	3	 67%33%
5	O	3	 33%33%33%
5	Q	3	 67%33%
6	N	4	 25%75%
6	R	4	 50%50%
7	P	4	 75%25%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22809 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	1	0	0
			2436	1515	440	466	15			
1	C	319	Total	C	N	O	S	1	0	0
			2436	1515	440	466	15			
1	E	319	Total	C	N	O	S	1	0	0
			2436	1515	440	466	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1649	1022	288	332	7			
2	D	207	Total	C	N	O	S	0	0	0
			1672	1039	291	335	7			
2	F	205	Total	C	N	O	S	0	0	0
			1653	1024	289	333	7			

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	LEU	ILE	conflict	UNP A0A8E4VRS4
B	175	GLY	-	expression tag	UNP A0A8E4VRS4
B	176	SER	-	expression tag	UNP A0A8E4VRS4
B	177	GLY	-	expression tag	UNP A0A8E4VRS4
B	178	TYR	-	expression tag	UNP A0A8E4VRS4
B	179	ILE	-	expression tag	UNP A0A8E4VRS4
B	180	PRO	-	expression tag	UNP A0A8E4VRS4
B	181	GLU	-	expression tag	UNP A0A8E4VRS4
B	182	ALA	-	expression tag	UNP A0A8E4VRS4
B	183	PRO	-	expression tag	UNP A0A8E4VRS4
B	184	ARG	-	expression tag	UNP A0A8E4VRS4
B	185	ASP	-	expression tag	UNP A0A8E4VRS4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLY	-	expression tag	UNP A0A8E4VRS4
B	187	GLN	-	expression tag	UNP A0A8E4VRS4
B	188	ALA	-	expression tag	UNP A0A8E4VRS4
B	189	TYR	-	expression tag	UNP A0A8E4VRS4
B	190	VAL	-	expression tag	UNP A0A8E4VRS4
B	191	ARG	-	expression tag	UNP A0A8E4VRS4
B	192	LYS	-	expression tag	UNP A0A8E4VRS4
B	193	ASP	-	expression tag	UNP A0A8E4VRS4
B	194	GLY	-	expression tag	UNP A0A8E4VRS4
B	195	GLU	-	expression tag	UNP A0A8E4VRS4
B	196	TRP	-	expression tag	UNP A0A8E4VRS4
B	197	VAL	-	expression tag	UNP A0A8E4VRS4
B	198	LEU	-	expression tag	UNP A0A8E4VRS4
B	199	LEU	-	expression tag	UNP A0A8E4VRS4
B	200	SER	-	expression tag	UNP A0A8E4VRS4
B	201	THR	-	expression tag	UNP A0A8E4VRS4
B	202	PHE	-	expression tag	UNP A0A8E4VRS4
B	203	LEU	-	expression tag	UNP A0A8E4VRS4
B	204	SER	-	expression tag	UNP A0A8E4VRS4
B	205	GLY	-	expression tag	UNP A0A8E4VRS4
B	206	ARG	-	expression tag	UNP A0A8E4VRS4
B	207	LEU	-	expression tag	UNP A0A8E4VRS4
B	208	VAL	-	expression tag	UNP A0A8E4VRS4
B	209	PRO	-	expression tag	UNP A0A8E4VRS4
B	210	ARG	-	expression tag	UNP A0A8E4VRS4
D	55	LEU	ILE	conflict	UNP A0A8E4VRS4
D	175	GLY	-	expression tag	UNP A0A8E4VRS4
D	176	SER	-	expression tag	UNP A0A8E4VRS4
D	177	GLY	-	expression tag	UNP A0A8E4VRS4
D	178	TYR	-	expression tag	UNP A0A8E4VRS4
D	179	ILE	-	expression tag	UNP A0A8E4VRS4
D	180	PRO	-	expression tag	UNP A0A8E4VRS4
D	181	GLU	-	expression tag	UNP A0A8E4VRS4
D	182	ALA	-	expression tag	UNP A0A8E4VRS4
D	183	PRO	-	expression tag	UNP A0A8E4VRS4
D	184	ARG	-	expression tag	UNP A0A8E4VRS4
D	185	ASP	-	expression tag	UNP A0A8E4VRS4
D	186	GLY	-	expression tag	UNP A0A8E4VRS4
D	187	GLN	-	expression tag	UNP A0A8E4VRS4
D	188	ALA	-	expression tag	UNP A0A8E4VRS4
D	189	TYR	-	expression tag	UNP A0A8E4VRS4
D	190	VAL	-	expression tag	UNP A0A8E4VRS4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	191	ARG	-	expression tag	UNP A0A8E4VRS4
D	192	LYS	-	expression tag	UNP A0A8E4VRS4
D	193	ASP	-	expression tag	UNP A0A8E4VRS4
D	194	GLY	-	expression tag	UNP A0A8E4VRS4
D	195	GLU	-	expression tag	UNP A0A8E4VRS4
D	196	TRP	-	expression tag	UNP A0A8E4VRS4
D	197	VAL	-	expression tag	UNP A0A8E4VRS4
D	198	LEU	-	expression tag	UNP A0A8E4VRS4
D	199	LEU	-	expression tag	UNP A0A8E4VRS4
D	200	SER	-	expression tag	UNP A0A8E4VRS4
D	201	THR	-	expression tag	UNP A0A8E4VRS4
D	202	PHE	-	expression tag	UNP A0A8E4VRS4
D	203	LEU	-	expression tag	UNP A0A8E4VRS4
D	204	SER	-	expression tag	UNP A0A8E4VRS4
D	205	GLY	-	expression tag	UNP A0A8E4VRS4
D	206	ARG	-	expression tag	UNP A0A8E4VRS4
D	207	LEU	-	expression tag	UNP A0A8E4VRS4
D	208	VAL	-	expression tag	UNP A0A8E4VRS4
D	209	PRO	-	expression tag	UNP A0A8E4VRS4
D	210	ARG	-	expression tag	UNP A0A8E4VRS4
F	55	LEU	ILE	conflict	UNP A0A8E4VRS4
F	175	GLY	-	expression tag	UNP A0A8E4VRS4
F	176	SER	-	expression tag	UNP A0A8E4VRS4
F	177	GLY	-	expression tag	UNP A0A8E4VRS4
F	178	TYR	-	expression tag	UNP A0A8E4VRS4
F	179	ILE	-	expression tag	UNP A0A8E4VRS4
F	180	PRO	-	expression tag	UNP A0A8E4VRS4
F	181	GLU	-	expression tag	UNP A0A8E4VRS4
F	182	ALA	-	expression tag	UNP A0A8E4VRS4
F	183	PRO	-	expression tag	UNP A0A8E4VRS4
F	184	ARG	-	expression tag	UNP A0A8E4VRS4
F	185	ASP	-	expression tag	UNP A0A8E4VRS4
F	186	GLY	-	expression tag	UNP A0A8E4VRS4
F	187	GLN	-	expression tag	UNP A0A8E4VRS4
F	188	ALA	-	expression tag	UNP A0A8E4VRS4
F	189	TYR	-	expression tag	UNP A0A8E4VRS4
F	190	VAL	-	expression tag	UNP A0A8E4VRS4
F	191	ARG	-	expression tag	UNP A0A8E4VRS4
F	192	LYS	-	expression tag	UNP A0A8E4VRS4
F	193	ASP	-	expression tag	UNP A0A8E4VRS4
F	194	GLY	-	expression tag	UNP A0A8E4VRS4
F	195	GLU	-	expression tag	UNP A0A8E4VRS4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	TRP	-	expression tag	UNP A0A8E4VRS4
F	197	VAL	-	expression tag	UNP A0A8E4VRS4
F	198	LEU	-	expression tag	UNP A0A8E4VRS4
F	199	LEU	-	expression tag	UNP A0A8E4VRS4
F	200	SER	-	expression tag	UNP A0A8E4VRS4
F	201	THR	-	expression tag	UNP A0A8E4VRS4
F	202	PHE	-	expression tag	UNP A0A8E4VRS4
F	203	LEU	-	expression tag	UNP A0A8E4VRS4
F	204	SER	-	expression tag	UNP A0A8E4VRS4
F	205	GLY	-	expression tag	UNP A0A8E4VRS4
F	206	ARG	-	expression tag	UNP A0A8E4VRS4
F	207	LEU	-	expression tag	UNP A0A8E4VRS4
F	208	VAL	-	expression tag	UNP A0A8E4VRS4
F	209	PRO	-	expression tag	UNP A0A8E4VRS4
F	210	ARG	-	expression tag	UNP A0A8E4VRS4

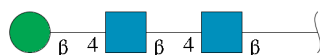
- Molecule 3 is a protein called 1E11 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	229	Total	C	N	O	S	0	0	0
			1702	1077	278	342	5			
3	H	229	Total	C	N	O	S	0	0	0
			1702	1077	278	342	5			
3	J	230	Total	C	N	O	S	0	0	0
			1708	1080	279	343	6			

- Molecule 4 is a protein called 1E11 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	217	Total	C	N	O	S	0	0	0
			1682	1052	294	330	6			
4	K	219	Total	C	N	O	S	0	0	0
			1697	1060	296	334	7			
4	L	217	Total	C	N	O	S	0	0	0
			1682	1052	294	330	6			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

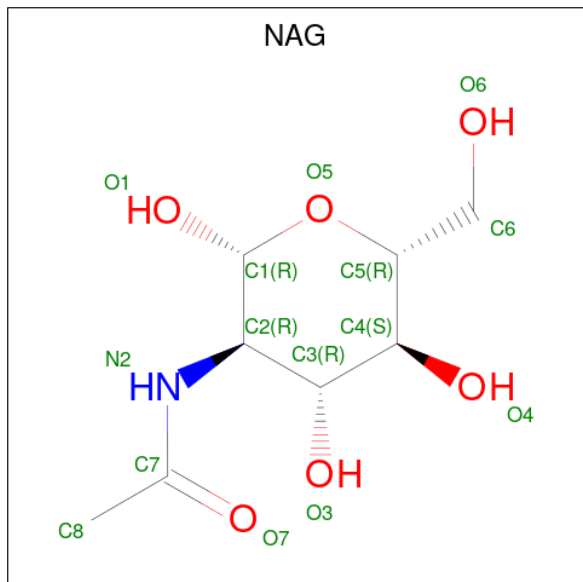


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

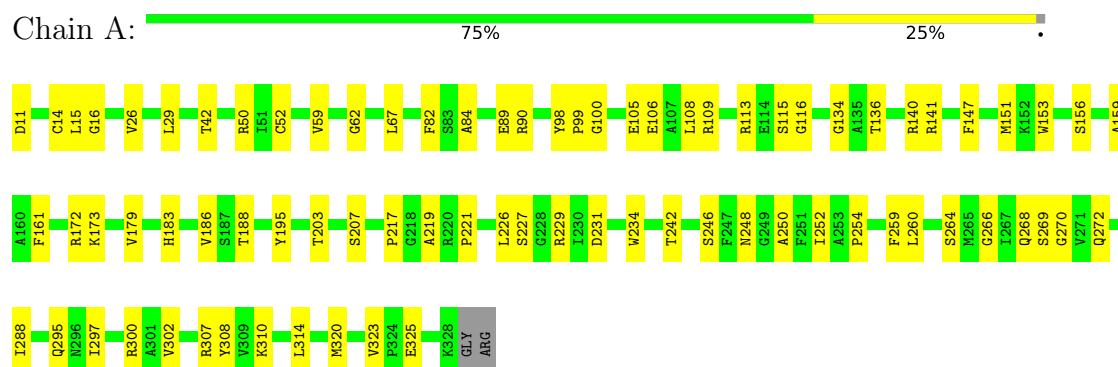


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		

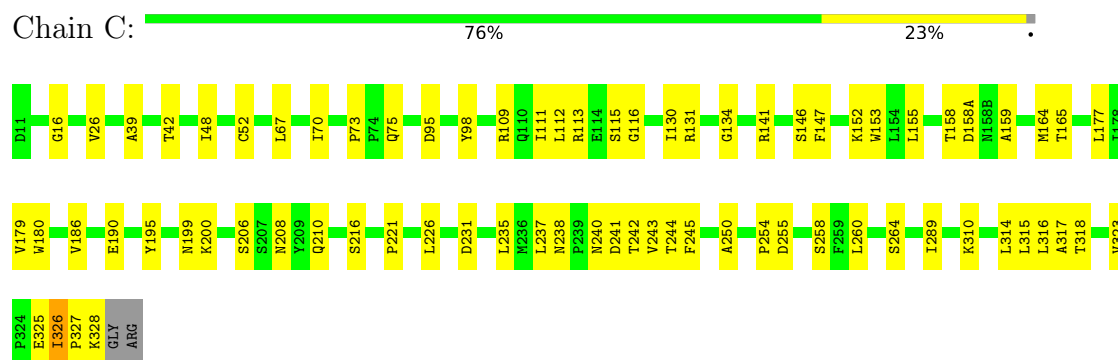
3 Residue-property plots

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.

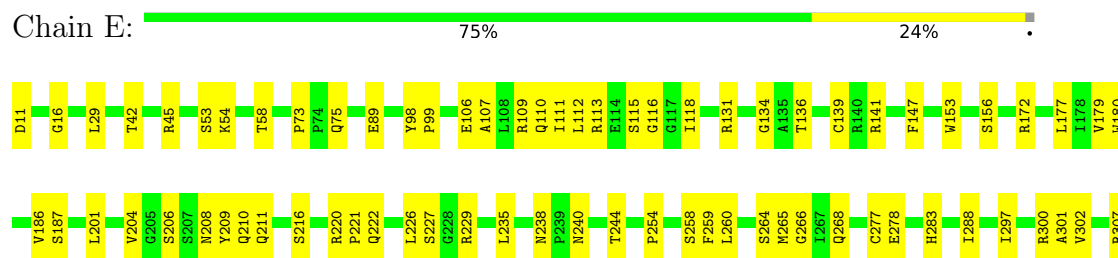
• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1



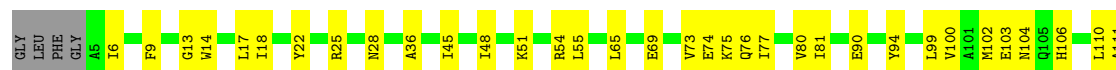
• Molecule 1: Hemagglutinin HA1





• Molecule 2: Hemagglutinin HA2

Chain B: 65% 32%



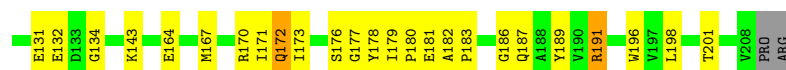
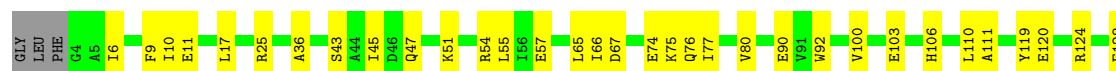
• Molecule 2: Hemagglutinin HA2

Chain D: 66% 31%



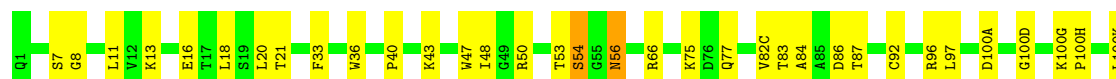
• Molecule 2: Hemagglutinin HA2

Chain F: 70% 27%



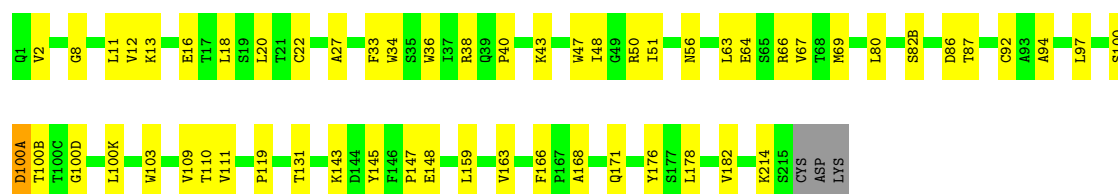
• Molecule 3: 1E11 Fab Heavy chain

Chain G: 76% 22%



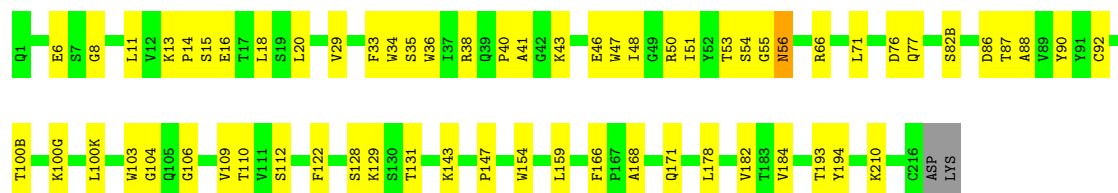
• Molecule 3: 1E11 Fab Heavy chain

Chain H: 74% 24%



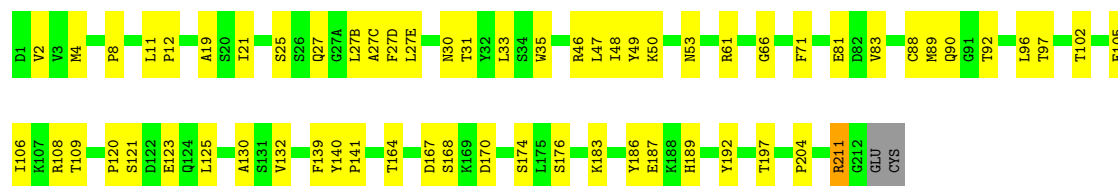
• Molecule 3: 1E11 Fab Heavy chain

Chain J: 72% 27% .



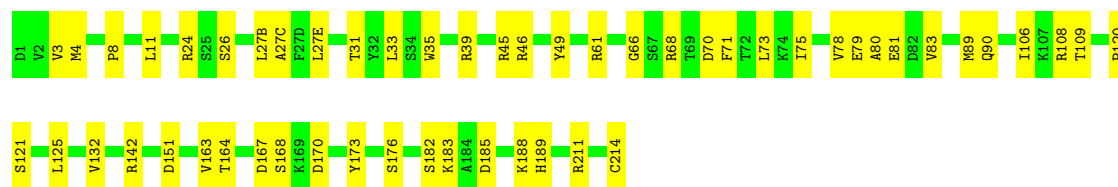
• Molecule 4: 1E11 Fab Light chain

Chain I: 71% 28% .



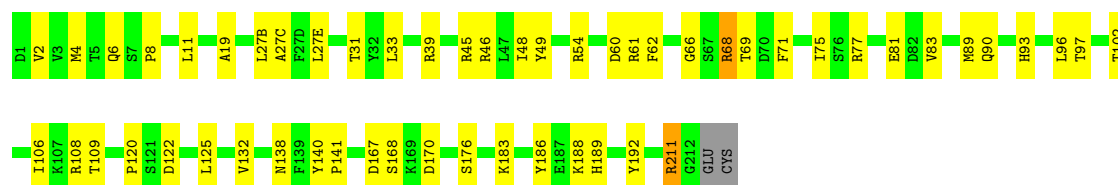
• Molecule 4: 1E11 Fab Light chain

Chain K: 76% 24%



• Molecule 4: 1E11 Fab Light chain

Chain L: 74% 24% ..



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 33% 33%

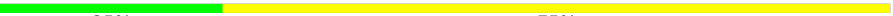


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%



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

Chain N:  25% 75%



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

Chain R:  50% 50%



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	303.28Å 303.28Å 153.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.77 – 3.50 45.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.77-3.50) 98.5 (45.77-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.215 0.182 , 0.215	Depositor DCC
R_{free} test set	1979 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 110.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22809	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: NAG, BMA, MAN, CA

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	0.13	0/2483	0.33	0/3356
1	C	0.14	0/2483	0.33	0/3356
1	E	0.14	0/2483	0.34	0/3356
2	B	0.14	0/1679	0.32	0/2266
2	D	0.15	0/1703	0.37	0/2298
2	F	0.15	0/1683	0.35	0/2271
3	G	0.15	0/1745	0.37	0/2386
3	H	0.16	0/1745	0.38	0/2386
3	J	0.15	0/1751	0.38	0/2394
4	I	0.15	0/1719	0.38	0/2331
4	K	0.15	0/1734	0.36	0/2351
4	L	0.16	0/1719	0.35	0/2331
All	All	0.15	0/22927	0.35	0/31082

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	191	ARG	Sidechain
3	J	77	GLN	Peptide

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	2436	0	2400	60	0
1	C	2436	0	2400	53	0
1	E	2436	0	2400	53	0
2	B	1649	0	1544	58	0
2	D	1672	0	1567	60	0
2	F	1653	0	1547	55	0
3	G	1702	0	1680	36	1
3	H	1702	0	1680	33	0
3	J	1708	0	1684	36	0
4	I	1682	0	1648	43	0
4	K	1697	0	1658	37	1
4	L	1682	0	1648	39	1
5	M	39	0	34	0	0
5	O	39	0	34	1	0
5	Q	39	0	34	0	0
6	N	50	0	43	0	0
6	R	50	0	43	1	0
7	P	50	0	43	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
9	A	14	0	13	1	0
9	B	14	0	13	0	0
9	C	14	0	13	0	0
9	D	14	0	13	0	0
9	E	14	0	13	0	0
9	F	14	0	13	0	0
All	All	22809	0	22165	476	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 476 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)
4:K:4:MET:HE2	4:K:90:GLN:HB3	1.50	0.91
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.56	0.88
3:G:209:LYS:NZ	4:I:123:GLU:OE2	2.08	0.85
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.14	0.81
1:E:216:SER:O	1:E:220:ARG:NH1	2.14	0.80

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:79:GLU:OE1	4:K:108:ARG:NH1[7_554]	2.17	0.03
3:G:183:THR:OG1	4:L:60:ASP:OD2[3_454]	2.18	0.02

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	317/321 (99%)	293 (92%)	23 (7%)	1 (0%)	36 67
1	C	317/321 (99%)	299 (94%)	16 (5%)	2 (1%)	21 54
1	E	317/321 (99%)	300 (95%)	16 (5%)	1 (0%)	36 67
2	B	202/210 (96%)	189 (94%)	12 (6%)	1 (0%)	24 57
2	D	205/210 (98%)	184 (90%)	16 (8%)	5 (2%)	4 29
2	F	203/210 (97%)	189 (93%)	11 (5%)	3 (2%)	8 37
3	G	227/232 (98%)	210 (92%)	15 (7%)	2 (1%)	14 47
3	H	227/232 (98%)	212 (93%)	12 (5%)	3 (1%)	9 39
3	J	228/232 (98%)	210 (92%)	15 (7%)	3 (1%)	9 39
4	I	215/219 (98%)	204 (95%)	9 (4%)	2 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
4	L	215/219 (98%)	208 (97%)	4 (2%)	3 (1%)	9	38
All	All	2890/2946 (98%)	2701 (94%)	163 (6%)	26 (1%)	14	47

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	327	PRO
2	F	11	GLU
2	F	172	GLN
3	J	56	ASN
1	C	52	CYS

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	268/269 (100%)	268 (100%)	0	100	100
1	C	268/269 (100%)	267 (100%)	1 (0%)	84	81
1	E	268/269 (100%)	266 (99%)	2 (1%)	76	78
2	B	174/178 (98%)	173 (99%)	1 (1%)	78	79
2	D	176/178 (99%)	176 (100%)	0	100	100
2	F	174/178 (98%)	174 (100%)	0	100	100
3	G	195/198 (98%)	194 (100%)	1 (0%)	81	80
3	H	195/198 (98%)	193 (99%)	2 (1%)	68	75
3	J	196/198 (99%)	195 (100%)	1 (0%)	81	80
4	I	191/193 (99%)	191 (100%)	0	100	100
4	K	193/193 (100%)	193 (100%)	0	100	100
4	L	191/193 (99%)	191 (100%)	0	100	100
All	All	2489/2514 (99%)	2481 (100%)	8 (0%)	86	83

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	92	CYS
3	H	92	CYS
3	G	92	CYS
1	E	277	CYS
3	H	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	159	HIS
4	I	124	GLN
4	L	137	ASN
4	I	38	GLN
3	J	39	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 ⓘ

21 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	$\# Z > 2$
5	NAG	M	1	5,1	14,14,15	0.42	0	17,19,21	0.52	0
5	NAG	M	2	5	14,14,15	0.28	0	17,19,21	0.68	0
5	BMA	M	3	5	11,11,12	0.65	0	15,15,17	1.29	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	1	6,2	14,14,15	0.21	0	17,19,21	0.73	1 (5%)
6	NAG	N	2	6	14,14,15	0.33	0	17,19,21	0.41	0
6	BMA	N	3	6	11,11,12	1.53	3 (27%)	15,15,17	1.09	1 (6%)
6	MAN	N	4	6	11,11,12	1.46	3 (27%)	15,15,17	1.67	3 (20%)
5	NAG	O	1	5,1	14,14,15	0.56	0	17,19,21	0.56	0
5	NAG	O	2	5	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
5	BMA	O	3	5	11,11,12	1.61	3 (27%)	15,15,17	1.86	4 (26%)
7	NAG	P	1	7,2	14,14,15	0.29	0	17,19,21	0.52	0
7	NAG	P	2	7	14,14,15	0.27	0	17,19,21	0.37	0
7	BMA	P	3	7	11,11,12	0.86	0	15,15,17	0.88	0
7	MAN	P	4	7	11,11,12	0.97	1 (9%)	15,15,17	0.93	0
5	NAG	Q	1	5,1	14,14,15	0.53	0	17,19,21	0.51	0
5	NAG	Q	2	5	14,14,15	0.22	0	17,19,21	0.62	0
5	BMA	Q	3	5	11,11,12	0.84	1 (9%)	15,15,17	1.00	0
6	NAG	R	1	6,2	14,14,15	0.48	0	17,19,21	0.60	0
6	NAG	R	2	6	14,14,15	0.33	0	17,19,21	0.39	0
6	BMA	R	3	6	11,11,12	1.40	1 (9%)	15,15,17	1.27	3 (20%)
6	MAN	R	4	6	11,11,12	1.08	1 (9%)	15,15,17	1.35	2 (13%)

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	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	4/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
7	NAG	P	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	0/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	0/2/19/22	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	4	MAN	C1-C2	3.56	1.60	1.52
5	O	3	BMA	C1-C2	3.21	1.59	1.52
6	N	3	BMA	C1-C2	3.14	1.59	1.52
6	R	3	BMA	C1-C2	2.95	1.59	1.52
6	R	4	MAN	C1-C2	2.74	1.58	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	4	MAN	C1-O5-C5	5.23	119.19	112.19
5	O	3	BMA	C1-O5-C5	4.35	118.02	112.19
6	R	4	MAN	C1-O5-C5	3.99	117.53	112.19
5	M	3	BMA	C1-O5-C5	3.30	116.61	112.19
5	O	2	NAG	C1-O5-C5	2.67	115.76	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

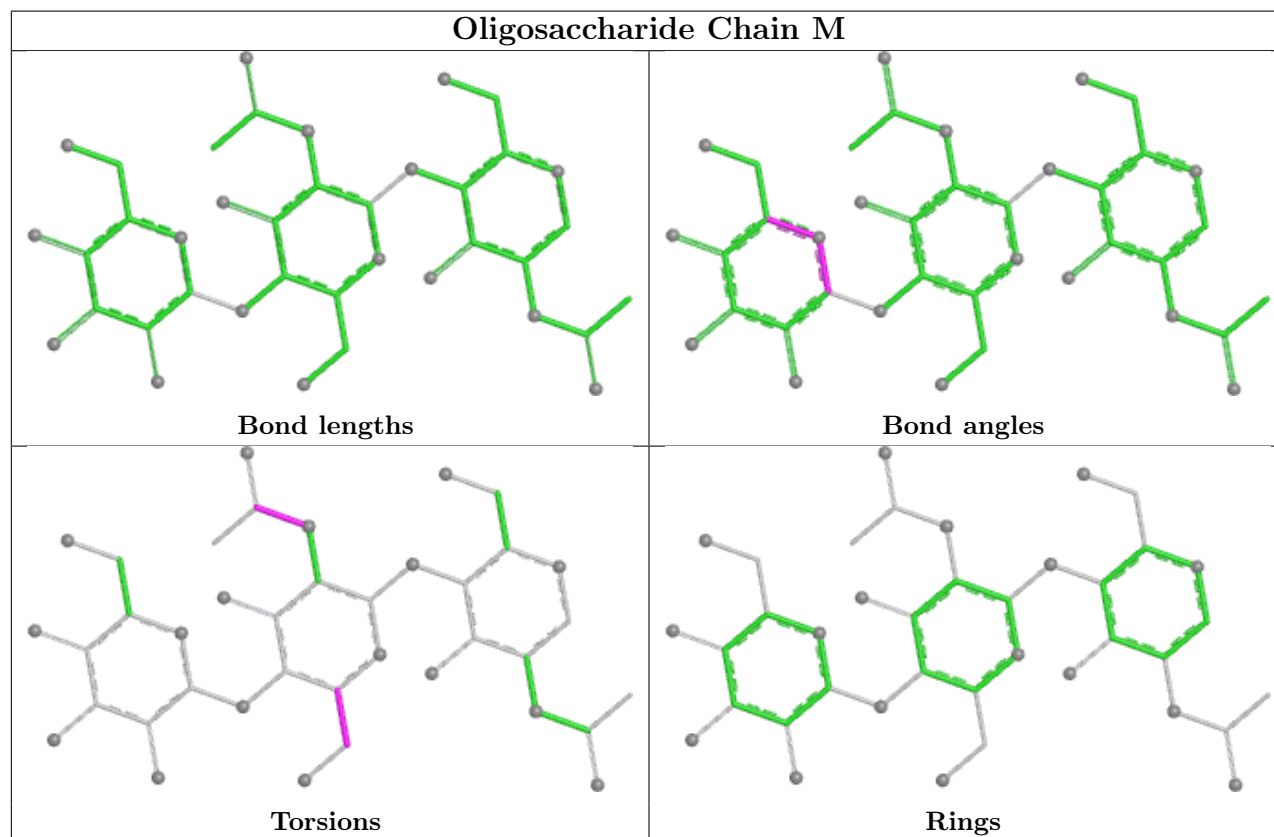
Mol	Chain	Res	Type	Atoms
7	P	1	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6

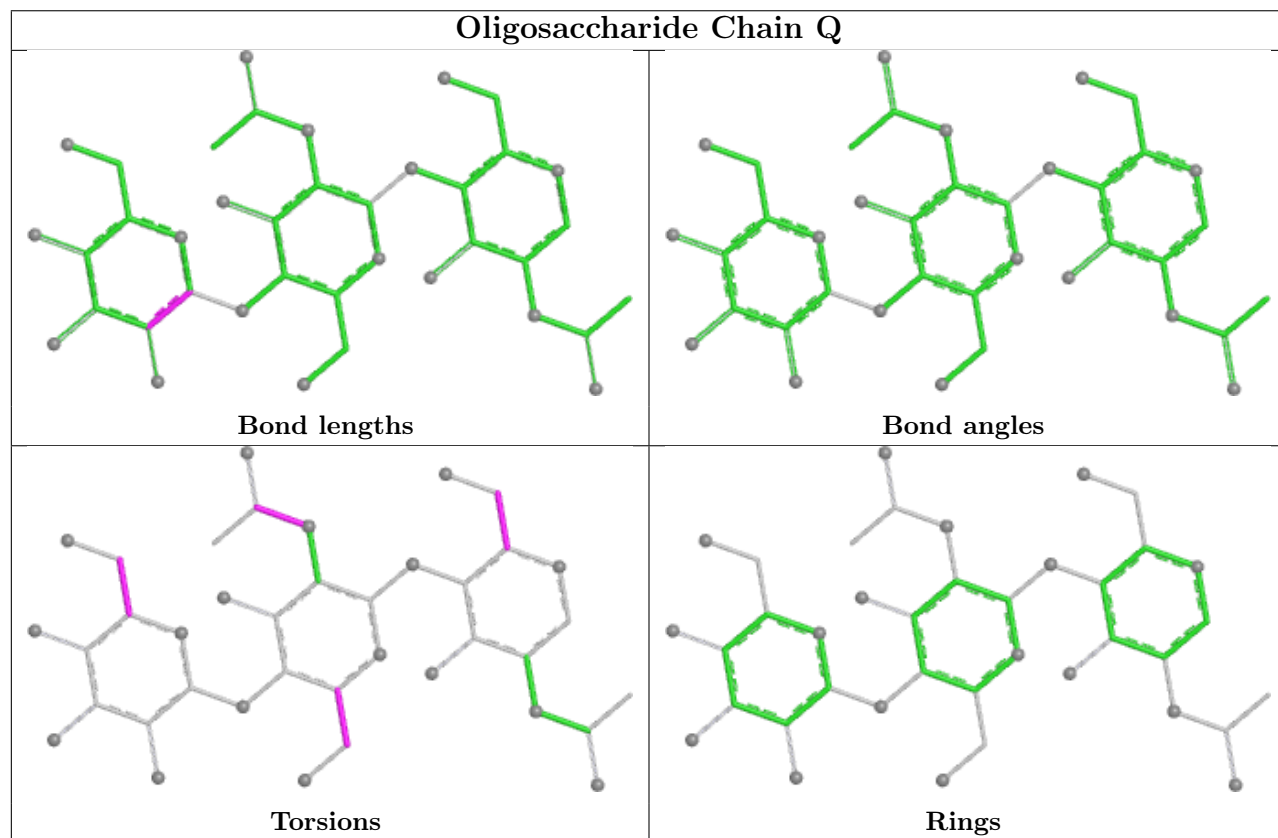
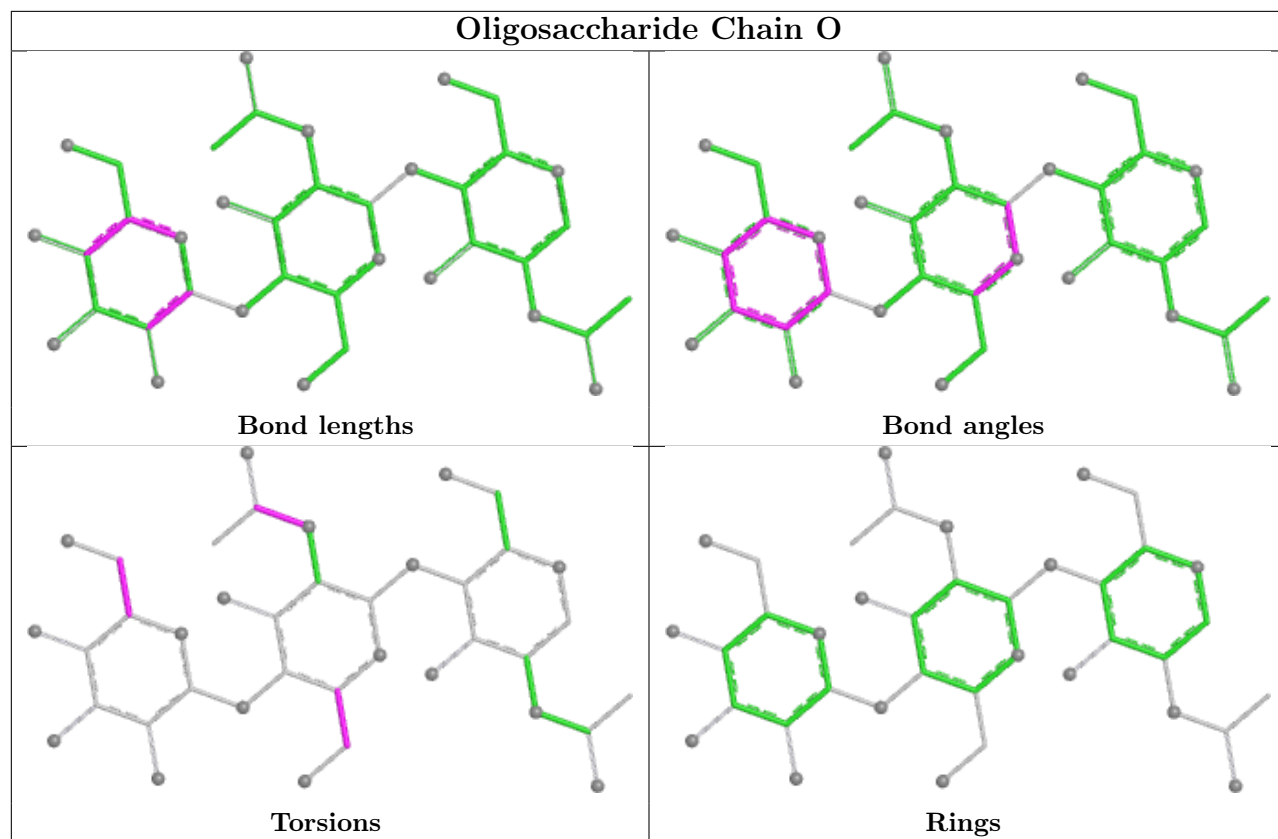
There are no ring outliers.

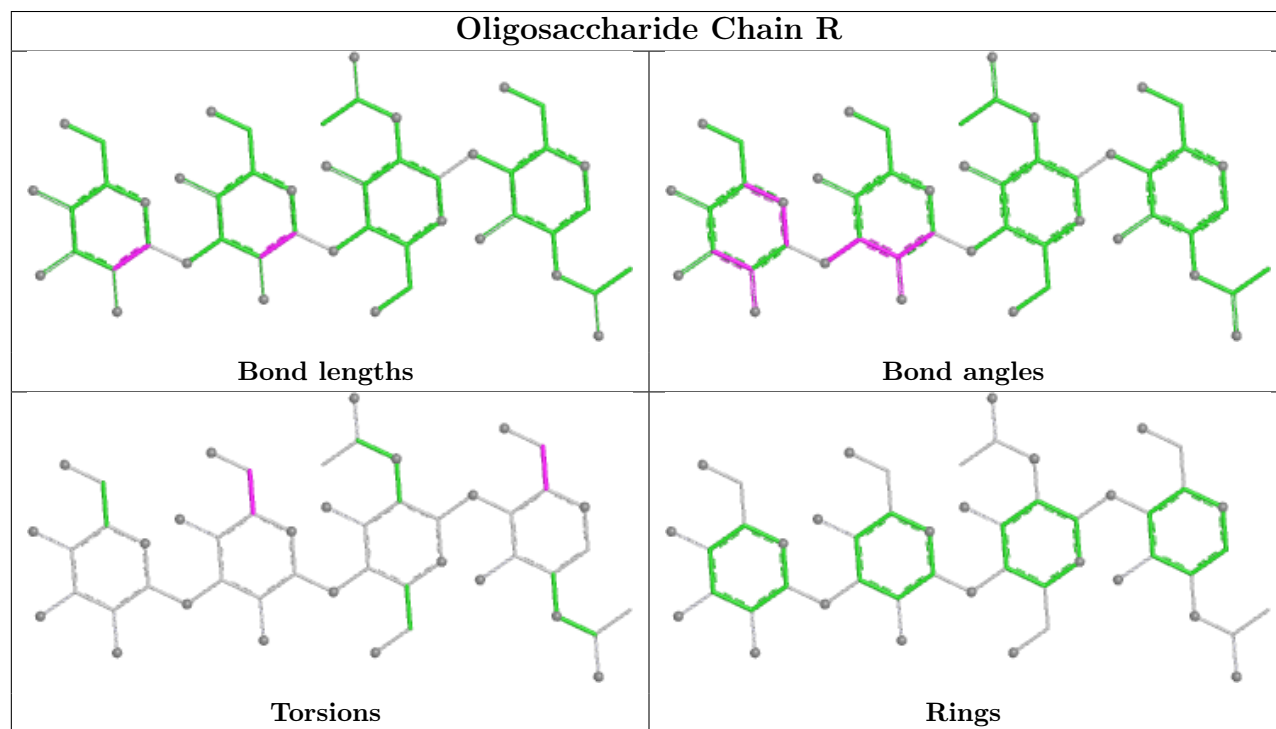
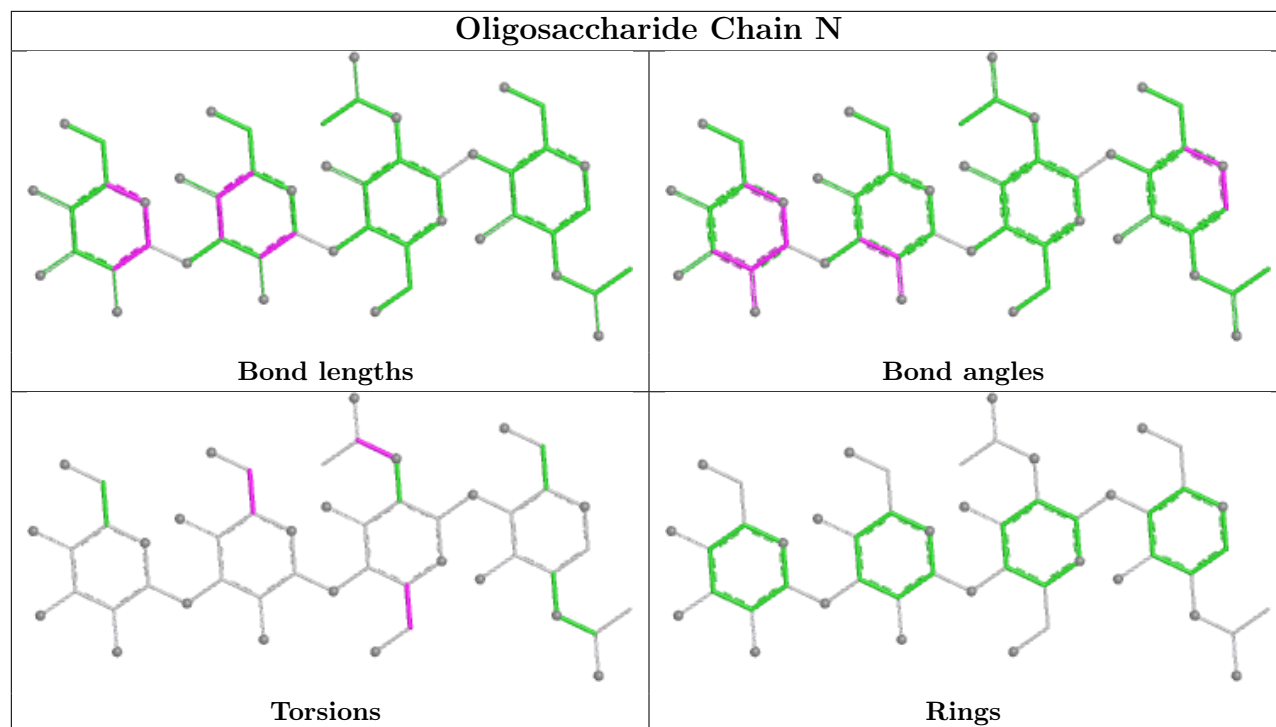
3 monomers are involved in 2 short contacts:

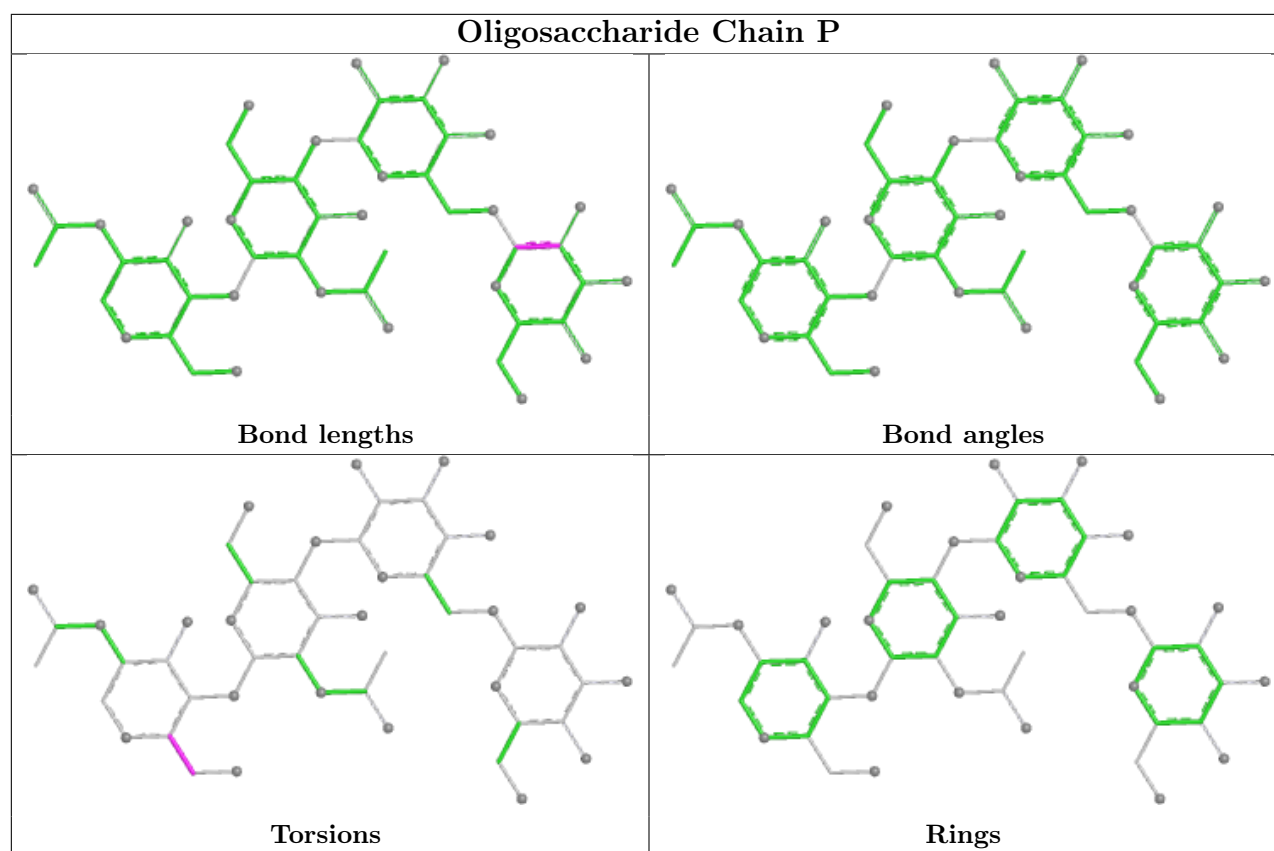
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	3	BMA	1	0
6	R	4	MAN	1	0
5	O	3	BMA	1	0

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









5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
9	NAG	B	301	2	14,14,15	0.42	0	17,19,21	0.60	1 (5%)
9	NAG	A	402	1	14,14,15	0.29	0	17,19,21	0.49	0
9	NAG	F	301	2	14,14,15	0.44	0	17,19,21	0.49	0
9	NAG	D	301	2	14,14,15	0.26	0	17,19,21	0.60	0
9	NAG	E	402	1	14,14,15	0.40	0	17,19,21	0.47	0
9	NAG	C	402	1	14,14,15	0.62	0	17,19,21	0.61	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
9	NAG	B	301	2	-	0/6/23/26	0/1/1/1
9	NAG	A	402	1	-	0/6/23/26	0/1/1/1
9	NAG	F	301	2	-	0/6/23/26	0/1/1/1
9	NAG	D	301	2	-	3/6/23/26	0/1/1/1
9	NAG	E	402	1	-	2/6/23/26	0/1/1/1
9	NAG	C	402	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	402	NAG	C1-O5-C5	2.03	114.91	112.19
9	B	301	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	301	NAG	C8-C7-N2-C2
9	D	301	NAG	O7-C7-N2-C2
9	E	402	NAG	O5-C5-C6-O6
9	D	301	NAG	O5-C5-C6-O6
9	E	402	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	402	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(Å²)	Q<0.9	
1	A	319/321 (99%)	-0.52	0	100	100	80, 117, 150, 192	1 (0%)
1	C	319/321 (99%)	-0.48	0	100	100	81, 115, 154, 205	1 (0%)
1	E	319/321 (99%)	-0.47	0	100	100	85, 118, 153, 195	1 (0%)
2	B	204/210 (97%)	-0.38	0	100	100	82, 121, 170, 194	0
2	D	207/210 (98%)	-0.38	1 (0%)	87	68	83, 114, 167, 223	0
2	F	205/210 (97%)	-0.38	0	100	100	82, 117, 168, 201	0
3	G	229/232 (98%)	-0.36	0	100	100	90, 121, 155, 200	0
3	H	229/232 (98%)	-0.42	0	100	100	80, 109, 149, 196	0
3	J	230/232 (99%)	-0.40	0	100	100	90, 121, 165, 223	0
4	I	217/219 (99%)	-0.44	0	100	100	85, 107, 157, 178	0
4	K	219/219 (100%)	-0.44	0	100	100	88, 109, 167, 208	0
4	L	217/219 (99%)	-0.49	0	100	100	84, 105, 145, 166	0
All	All	2914/2946 (98%)	-0.44	1 (0%)	100	100	80, 115, 161, 223	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	LEU	2.5

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

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

6.3 Carbohydrates

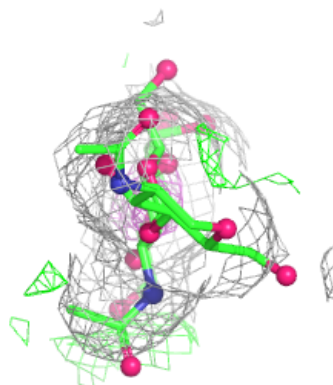
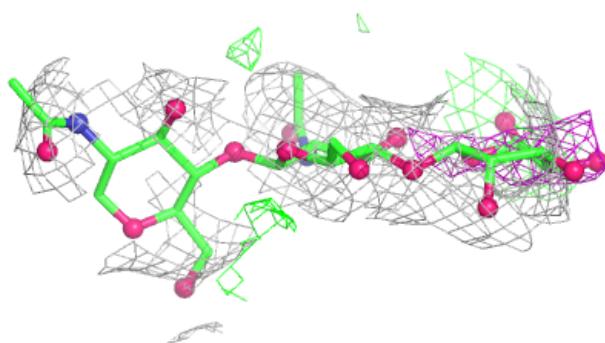
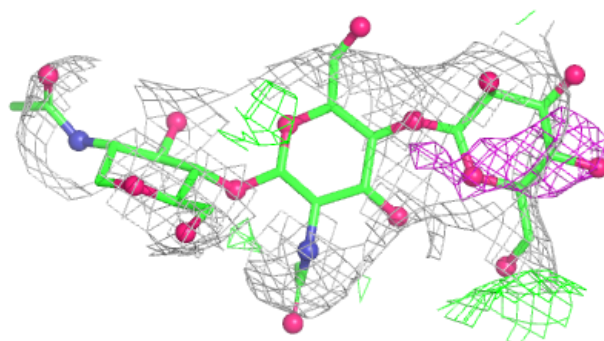
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	P	4	11/12	0.33	0.11	169,186,193,195	0
6	BMA	R	3	11/12	0.39	0.11	153,165,174,177	0
5	BMA	M	3	11/12	0.44	0.15	139,172,183,186	0
7	BMA	P	3	11/12	0.46	0.11	170,176,184,187	0
5	BMA	O	3	11/12	0.54	0.13	146,165,171,173	0
6	MAN	R	4	11/12	0.56	0.10	153,168,173,174	0
6	MAN	N	4	11/12	0.60	0.10	153,166,183,187	0
6	BMA	N	3	11/12	0.61	0.10	141,161,177,177	0
5	NAG	O	2	14/15	0.69	0.12	138,147,166,172	0
5	NAG	M	2	14/15	0.70	0.12	138,151,167,168	0
5	BMA	Q	3	11/12	0.71	0.12	151,168,173,173	0
5	NAG	Q	2	14/15	0.83	0.09	131,142,154,163	0
7	NAG	P	1	14/15	0.87	0.10	102,114,123,125	0
6	NAG	N	1	14/15	0.87	0.10	111,120,131,135	0
6	NAG	R	2	14/15	0.87	0.09	121,145,156,162	0
6	NAG	N	2	14/15	0.89	0.10	119,136,160,164	0
6	NAG	R	1	14/15	0.90	0.09	106,115,127,132	0
5	NAG	M	1	14/15	0.91	0.08	114,125,139,141	0
7	NAG	P	2	14/15	0.91	0.09	120,138,152,161	0
5	NAG	O	1	14/15	0.92	0.09	107,116,131,137	0
5	NAG	Q	1	14/15	0.96	0.06	104,111,119,128	0

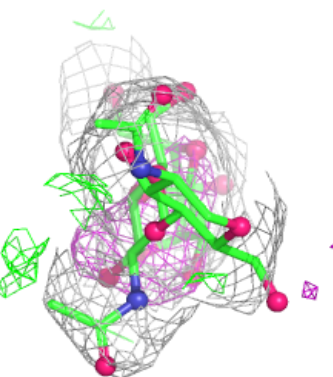
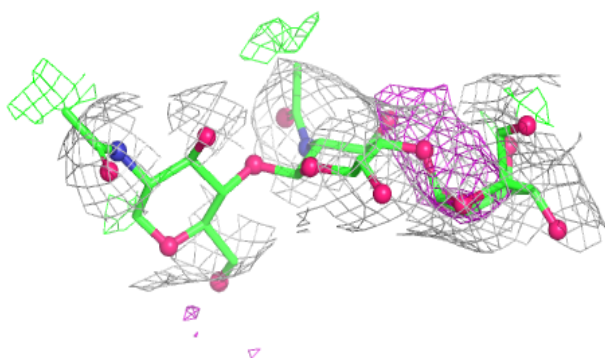
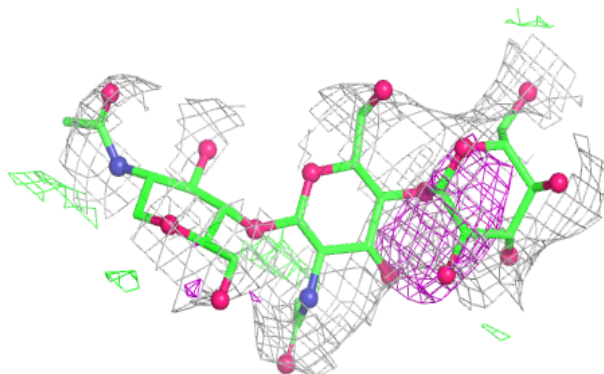
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

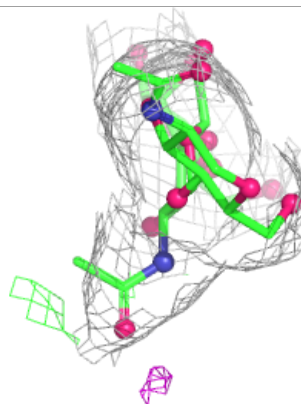
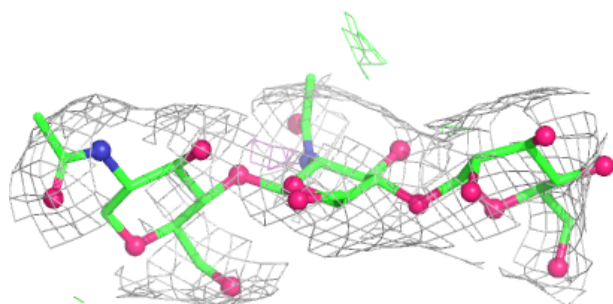
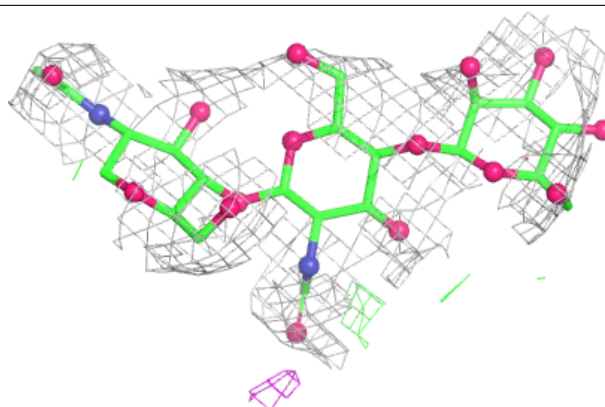
**Electron density around Chain O:**

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

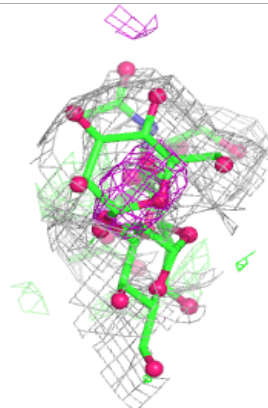
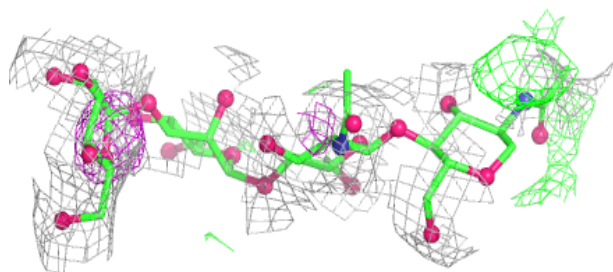
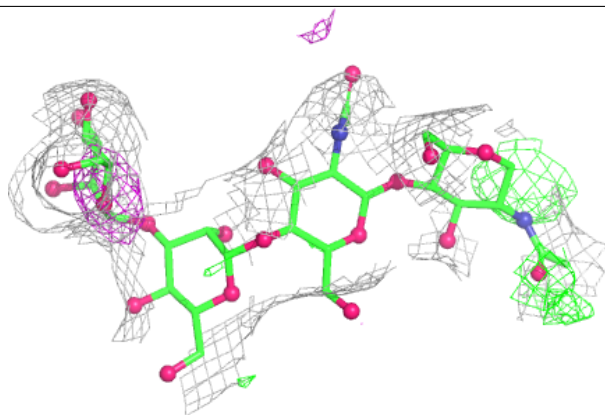


Electron density around Chain Q:

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

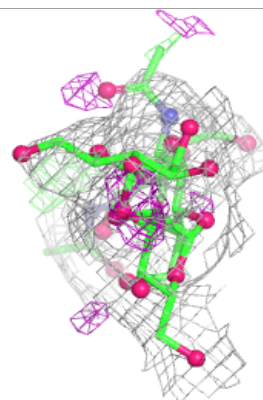
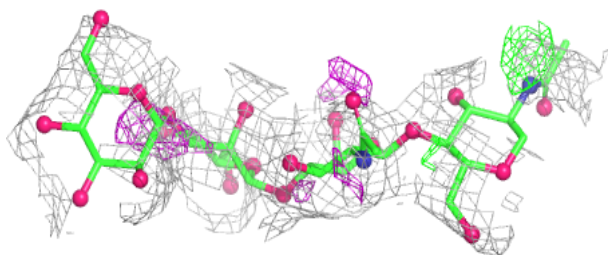
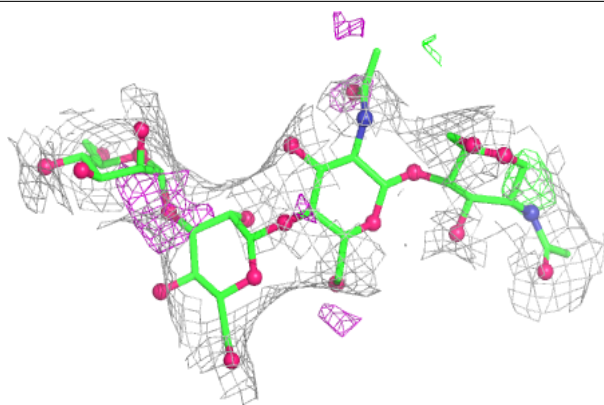
**Electron density around Chain N:**

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

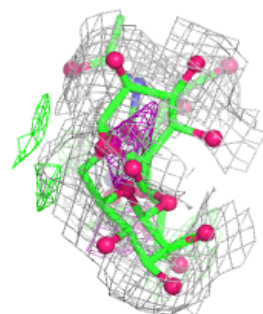
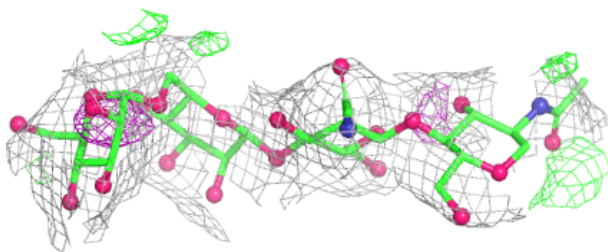
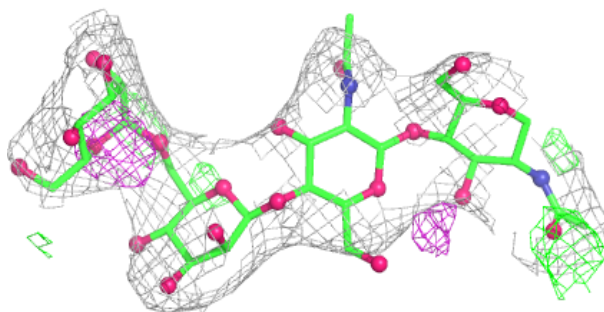


Electron density around Chain R:

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

**Electron density around Chain P:**

$2mF_o-DF_c$ (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
9	NAG	A	402	14/15	0.44	0.14	158,182,190,192	0
9	NAG	C	402	14/15	0.45	0.12	164,173,177,178	0
8	CA	C	401	1/1	0.59	0.18	170,170,170,170	0
8	CA	A	401	1/1	0.70	0.09	164,164,164,164	0
9	NAG	E	402	14/15	0.73	0.09	172,184,188,191	0
9	NAG	D	301	14/15	0.75	0.12	138,151,175,181	0
8	CA	E	401	1/1	0.81	0.05	162,162,162,162	0
9	NAG	F	301	14/15	0.86	0.08	144,150,158,161	0
9	NAG	B	301	14/15	0.90	0.07	135,143,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.