



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:35 PM BST

PDB ID : 6OSR
Title : Crystal structure of Influenza hemagglutinin from strain A/Melbourne/1/194
6(H1N1)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2019-05-02
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

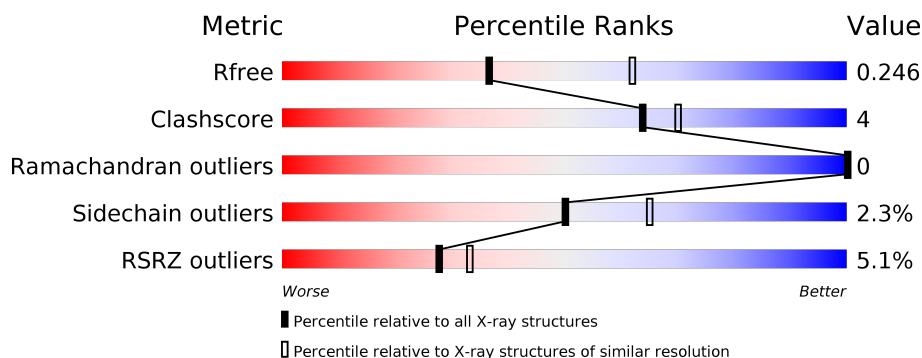
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	538	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>
1	B	538	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>11%</div> </div> </div>
1	C	538	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	D	538	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	E	538	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div> </div>
1	F	538	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	4	

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
2	NAG	G	2	-	-	-	X
3	NAG	C	601	-	-	-	X
3	NAG	F	602	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23091 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	481	Total	C	N	O	S	0	0	0
			3695	2336	632	709	18			
1	B	477	Total	C	N	O	S	0	0	0
			3675	2318	632	707	18			
1	C	476	Total	C	N	O	S	0	0	0
			3650	2304	631	697	18			
1	D	483	Total	C	N	O	S	0	0	0
			3717	2349	639	711	18			
1	E	477	Total	C	N	O	S	0	0	0
			3706	2342	635	711	18			
1	F	476	Total	C	N	O	S	0	0	0
			3679	2327	631	703	18			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP C7S1Y2
A	2	SER	-	expression tag	UNP C7S1Y2
A	495	PHE	-	expression tag	UNP C7S1Y2
A	496	LEU	-	expression tag	UNP C7S1Y2
A	497	VAL	-	expression tag	UNP C7S1Y2
A	498	PRO	-	expression tag	UNP C7S1Y2
A	499	ARG	-	expression tag	UNP C7S1Y2
A	500	GLY	-	expression tag	UNP C7S1Y2
A	501	SER	-	expression tag	UNP C7S1Y2
A	502	PRO	-	expression tag	UNP C7S1Y2
A	503	GLY	-	expression tag	UNP C7S1Y2
A	504	SER	-	expression tag	UNP C7S1Y2
A	505	GLY	-	expression tag	UNP C7S1Y2
A	506	TYR	-	expression tag	UNP C7S1Y2
A	507	ILE	-	expression tag	UNP C7S1Y2
A	508	PRO	-	expression tag	UNP C7S1Y2
A	509	GLU	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	510	ALA	-	expression tag	UNP C7S1Y2
A	511	PRO	-	expression tag	UNP C7S1Y2
A	512	ARG	-	expression tag	UNP C7S1Y2
A	513	ASP	-	expression tag	UNP C7S1Y2
A	514	GLY	-	expression tag	UNP C7S1Y2
A	515	GLN	-	expression tag	UNP C7S1Y2
A	516	ALA	-	expression tag	UNP C7S1Y2
A	517	TYR	-	expression tag	UNP C7S1Y2
A	518	VAL	-	expression tag	UNP C7S1Y2
A	519	ARG	-	expression tag	UNP C7S1Y2
A	520	LYS	-	expression tag	UNP C7S1Y2
A	521	ASP	-	expression tag	UNP C7S1Y2
A	522	GLY	-	expression tag	UNP C7S1Y2
A	523	GLU	-	expression tag	UNP C7S1Y2
A	524	TRP	-	expression tag	UNP C7S1Y2
A	525	VAL	-	expression tag	UNP C7S1Y2
A	526	LEU	-	expression tag	UNP C7S1Y2
A	527	LEU	-	expression tag	UNP C7S1Y2
A	528	SER	-	expression tag	UNP C7S1Y2
A	529	THR	-	expression tag	UNP C7S1Y2
A	530	PHE	-	expression tag	UNP C7S1Y2
A	531	LEU	-	expression tag	UNP C7S1Y2
A	532	GLY	-	expression tag	UNP C7S1Y2
A	533	HIS	-	expression tag	UNP C7S1Y2
A	534	HIS	-	expression tag	UNP C7S1Y2
A	535	HIS	-	expression tag	UNP C7S1Y2
A	536	HIS	-	expression tag	UNP C7S1Y2
A	537	HIS	-	expression tag	UNP C7S1Y2
A	538	HIS	-	expression tag	UNP C7S1Y2
B	1	GLY	-	expression tag	UNP C7S1Y2
B	2	SER	-	expression tag	UNP C7S1Y2
B	495	PHE	-	expression tag	UNP C7S1Y2
B	496	LEU	-	expression tag	UNP C7S1Y2
B	497	VAL	-	expression tag	UNP C7S1Y2
B	498	PRO	-	expression tag	UNP C7S1Y2
B	499	ARG	-	expression tag	UNP C7S1Y2
B	500	GLY	-	expression tag	UNP C7S1Y2
B	501	SER	-	expression tag	UNP C7S1Y2
B	502	PRO	-	expression tag	UNP C7S1Y2
B	503	GLY	-	expression tag	UNP C7S1Y2
B	504	SER	-	expression tag	UNP C7S1Y2
B	505	GLY	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	506	TYR	-	expression tag	UNP C7S1Y2
B	507	ILE	-	expression tag	UNP C7S1Y2
B	508	PRO	-	expression tag	UNP C7S1Y2
B	509	GLU	-	expression tag	UNP C7S1Y2
B	510	ALA	-	expression tag	UNP C7S1Y2
B	511	PRO	-	expression tag	UNP C7S1Y2
B	512	ARG	-	expression tag	UNP C7S1Y2
B	513	ASP	-	expression tag	UNP C7S1Y2
B	514	GLY	-	expression tag	UNP C7S1Y2
B	515	GLN	-	expression tag	UNP C7S1Y2
B	516	ALA	-	expression tag	UNP C7S1Y2
B	517	TYR	-	expression tag	UNP C7S1Y2
B	518	VAL	-	expression tag	UNP C7S1Y2
B	519	ARG	-	expression tag	UNP C7S1Y2
B	520	LYS	-	expression tag	UNP C7S1Y2
B	521	ASP	-	expression tag	UNP C7S1Y2
B	522	GLY	-	expression tag	UNP C7S1Y2
B	523	GLU	-	expression tag	UNP C7S1Y2
B	524	TRP	-	expression tag	UNP C7S1Y2
B	525	VAL	-	expression tag	UNP C7S1Y2
B	526	LEU	-	expression tag	UNP C7S1Y2
B	527	LEU	-	expression tag	UNP C7S1Y2
B	528	SER	-	expression tag	UNP C7S1Y2
B	529	THR	-	expression tag	UNP C7S1Y2
B	530	PHE	-	expression tag	UNP C7S1Y2
B	531	LEU	-	expression tag	UNP C7S1Y2
B	532	GLY	-	expression tag	UNP C7S1Y2
B	533	HIS	-	expression tag	UNP C7S1Y2
B	534	HIS	-	expression tag	UNP C7S1Y2
B	535	HIS	-	expression tag	UNP C7S1Y2
B	536	HIS	-	expression tag	UNP C7S1Y2
B	537	HIS	-	expression tag	UNP C7S1Y2
B	538	HIS	-	expression tag	UNP C7S1Y2
C	1	GLY	-	expression tag	UNP C7S1Y2
C	2	SER	-	expression tag	UNP C7S1Y2
C	495	PHE	-	expression tag	UNP C7S1Y2
C	496	LEU	-	expression tag	UNP C7S1Y2
C	497	VAL	-	expression tag	UNP C7S1Y2
C	498	PRO	-	expression tag	UNP C7S1Y2
C	499	ARG	-	expression tag	UNP C7S1Y2
C	500	GLY	-	expression tag	UNP C7S1Y2
C	501	SER	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	502	PRO	-	expression tag	UNP C7S1Y2
C	503	GLY	-	expression tag	UNP C7S1Y2
C	504	SER	-	expression tag	UNP C7S1Y2
C	505	GLY	-	expression tag	UNP C7S1Y2
C	506	TYR	-	expression tag	UNP C7S1Y2
C	507	ILE	-	expression tag	UNP C7S1Y2
C	508	PRO	-	expression tag	UNP C7S1Y2
C	509	GLU	-	expression tag	UNP C7S1Y2
C	510	ALA	-	expression tag	UNP C7S1Y2
C	511	PRO	-	expression tag	UNP C7S1Y2
C	512	ARG	-	expression tag	UNP C7S1Y2
C	513	ASP	-	expression tag	UNP C7S1Y2
C	514	GLY	-	expression tag	UNP C7S1Y2
C	515	GLN	-	expression tag	UNP C7S1Y2
C	516	ALA	-	expression tag	UNP C7S1Y2
C	517	TYR	-	expression tag	UNP C7S1Y2
C	518	VAL	-	expression tag	UNP C7S1Y2
C	519	ARG	-	expression tag	UNP C7S1Y2
C	520	LYS	-	expression tag	UNP C7S1Y2
C	521	ASP	-	expression tag	UNP C7S1Y2
C	522	GLY	-	expression tag	UNP C7S1Y2
C	523	GLU	-	expression tag	UNP C7S1Y2
C	524	TRP	-	expression tag	UNP C7S1Y2
C	525	VAL	-	expression tag	UNP C7S1Y2
C	526	LEU	-	expression tag	UNP C7S1Y2
C	527	LEU	-	expression tag	UNP C7S1Y2
C	528	SER	-	expression tag	UNP C7S1Y2
C	529	THR	-	expression tag	UNP C7S1Y2
C	530	PHE	-	expression tag	UNP C7S1Y2
C	531	LEU	-	expression tag	UNP C7S1Y2
C	532	GLY	-	expression tag	UNP C7S1Y2
C	533	HIS	-	expression tag	UNP C7S1Y2
C	534	HIS	-	expression tag	UNP C7S1Y2
C	535	HIS	-	expression tag	UNP C7S1Y2
C	536	HIS	-	expression tag	UNP C7S1Y2
C	537	HIS	-	expression tag	UNP C7S1Y2
C	538	HIS	-	expression tag	UNP C7S1Y2
D	1	GLY	-	expression tag	UNP C7S1Y2
D	2	SER	-	expression tag	UNP C7S1Y2
D	495	PHE	-	expression tag	UNP C7S1Y2
D	496	LEU	-	expression tag	UNP C7S1Y2
D	497	VAL	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	498	PRO	-	expression tag	UNP C7S1Y2
D	499	ARG	-	expression tag	UNP C7S1Y2
D	500	GLY	-	expression tag	UNP C7S1Y2
D	501	SER	-	expression tag	UNP C7S1Y2
D	502	PRO	-	expression tag	UNP C7S1Y2
D	503	GLY	-	expression tag	UNP C7S1Y2
D	504	SER	-	expression tag	UNP C7S1Y2
D	505	GLY	-	expression tag	UNP C7S1Y2
D	506	TYR	-	expression tag	UNP C7S1Y2
D	507	ILE	-	expression tag	UNP C7S1Y2
D	508	PRO	-	expression tag	UNP C7S1Y2
D	509	GLU	-	expression tag	UNP C7S1Y2
D	510	ALA	-	expression tag	UNP C7S1Y2
D	511	PRO	-	expression tag	UNP C7S1Y2
D	512	ARG	-	expression tag	UNP C7S1Y2
D	513	ASP	-	expression tag	UNP C7S1Y2
D	514	GLY	-	expression tag	UNP C7S1Y2
D	515	GLN	-	expression tag	UNP C7S1Y2
D	516	ALA	-	expression tag	UNP C7S1Y2
D	517	TYR	-	expression tag	UNP C7S1Y2
D	518	VAL	-	expression tag	UNP C7S1Y2
D	519	ARG	-	expression tag	UNP C7S1Y2
D	520	LYS	-	expression tag	UNP C7S1Y2
D	521	ASP	-	expression tag	UNP C7S1Y2
D	522	GLY	-	expression tag	UNP C7S1Y2
D	523	GLU	-	expression tag	UNP C7S1Y2
D	524	TRP	-	expression tag	UNP C7S1Y2
D	525	VAL	-	expression tag	UNP C7S1Y2
D	526	LEU	-	expression tag	UNP C7S1Y2
D	527	LEU	-	expression tag	UNP C7S1Y2
D	528	SER	-	expression tag	UNP C7S1Y2
D	529	THR	-	expression tag	UNP C7S1Y2
D	530	PHE	-	expression tag	UNP C7S1Y2
D	531	LEU	-	expression tag	UNP C7S1Y2
D	532	GLY	-	expression tag	UNP C7S1Y2
D	533	HIS	-	expression tag	UNP C7S1Y2
D	534	HIS	-	expression tag	UNP C7S1Y2
D	535	HIS	-	expression tag	UNP C7S1Y2
D	536	HIS	-	expression tag	UNP C7S1Y2
D	537	HIS	-	expression tag	UNP C7S1Y2
D	538	HIS	-	expression tag	UNP C7S1Y2
E	1	GLY	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	SER	-	expression tag	UNP C7S1Y2
E	495	PHE	-	expression tag	UNP C7S1Y2
E	496	LEU	-	expression tag	UNP C7S1Y2
E	497	VAL	-	expression tag	UNP C7S1Y2
E	498	PRO	-	expression tag	UNP C7S1Y2
E	499	ARG	-	expression tag	UNP C7S1Y2
E	500	GLY	-	expression tag	UNP C7S1Y2
E	501	SER	-	expression tag	UNP C7S1Y2
E	502	PRO	-	expression tag	UNP C7S1Y2
E	503	GLY	-	expression tag	UNP C7S1Y2
E	504	SER	-	expression tag	UNP C7S1Y2
E	505	GLY	-	expression tag	UNP C7S1Y2
E	506	TYR	-	expression tag	UNP C7S1Y2
E	507	ILE	-	expression tag	UNP C7S1Y2
E	508	PRO	-	expression tag	UNP C7S1Y2
E	509	GLU	-	expression tag	UNP C7S1Y2
E	510	ALA	-	expression tag	UNP C7S1Y2
E	511	PRO	-	expression tag	UNP C7S1Y2
E	512	ARG	-	expression tag	UNP C7S1Y2
E	513	ASP	-	expression tag	UNP C7S1Y2
E	514	GLY	-	expression tag	UNP C7S1Y2
E	515	GLN	-	expression tag	UNP C7S1Y2
E	516	ALA	-	expression tag	UNP C7S1Y2
E	517	TYR	-	expression tag	UNP C7S1Y2
E	518	VAL	-	expression tag	UNP C7S1Y2
E	519	ARG	-	expression tag	UNP C7S1Y2
E	520	LYS	-	expression tag	UNP C7S1Y2
E	521	ASP	-	expression tag	UNP C7S1Y2
E	522	GLY	-	expression tag	UNP C7S1Y2
E	523	GLU	-	expression tag	UNP C7S1Y2
E	524	TRP	-	expression tag	UNP C7S1Y2
E	525	VAL	-	expression tag	UNP C7S1Y2
E	526	LEU	-	expression tag	UNP C7S1Y2
E	527	LEU	-	expression tag	UNP C7S1Y2
E	528	SER	-	expression tag	UNP C7S1Y2
E	529	THR	-	expression tag	UNP C7S1Y2
E	530	PHE	-	expression tag	UNP C7S1Y2
E	531	LEU	-	expression tag	UNP C7S1Y2
E	532	GLY	-	expression tag	UNP C7S1Y2
E	533	HIS	-	expression tag	UNP C7S1Y2
E	534	HIS	-	expression tag	UNP C7S1Y2
E	535	HIS	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	536	HIS	-	expression tag	UNP C7S1Y2
E	537	HIS	-	expression tag	UNP C7S1Y2
E	538	HIS	-	expression tag	UNP C7S1Y2
F	1	GLY	-	expression tag	UNP C7S1Y2
F	2	SER	-	expression tag	UNP C7S1Y2
F	495	PHE	-	expression tag	UNP C7S1Y2
F	496	LEU	-	expression tag	UNP C7S1Y2
F	497	VAL	-	expression tag	UNP C7S1Y2
F	498	PRO	-	expression tag	UNP C7S1Y2
F	499	ARG	-	expression tag	UNP C7S1Y2
F	500	GLY	-	expression tag	UNP C7S1Y2
F	501	SER	-	expression tag	UNP C7S1Y2
F	502	PRO	-	expression tag	UNP C7S1Y2
F	503	GLY	-	expression tag	UNP C7S1Y2
F	504	SER	-	expression tag	UNP C7S1Y2
F	505	GLY	-	expression tag	UNP C7S1Y2
F	506	TYR	-	expression tag	UNP C7S1Y2
F	507	ILE	-	expression tag	UNP C7S1Y2
F	508	PRO	-	expression tag	UNP C7S1Y2
F	509	GLU	-	expression tag	UNP C7S1Y2
F	510	ALA	-	expression tag	UNP C7S1Y2
F	511	PRO	-	expression tag	UNP C7S1Y2
F	512	ARG	-	expression tag	UNP C7S1Y2
F	513	ASP	-	expression tag	UNP C7S1Y2
F	514	GLY	-	expression tag	UNP C7S1Y2
F	515	GLN	-	expression tag	UNP C7S1Y2
F	516	ALA	-	expression tag	UNP C7S1Y2
F	517	TYR	-	expression tag	UNP C7S1Y2
F	518	VAL	-	expression tag	UNP C7S1Y2
F	519	ARG	-	expression tag	UNP C7S1Y2
F	520	LYS	-	expression tag	UNP C7S1Y2
F	521	ASP	-	expression tag	UNP C7S1Y2
F	522	GLY	-	expression tag	UNP C7S1Y2
F	523	GLU	-	expression tag	UNP C7S1Y2
F	524	TRP	-	expression tag	UNP C7S1Y2
F	525	VAL	-	expression tag	UNP C7S1Y2
F	526	LEU	-	expression tag	UNP C7S1Y2
F	527	LEU	-	expression tag	UNP C7S1Y2
F	528	SER	-	expression tag	UNP C7S1Y2
F	529	THR	-	expression tag	UNP C7S1Y2
F	530	PHE	-	expression tag	UNP C7S1Y2
F	531	LEU	-	expression tag	UNP C7S1Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	532	GLY	-	expression tag	UNP C7S1Y2
F	533	HIS	-	expression tag	UNP C7S1Y2
F	534	HIS	-	expression tag	UNP C7S1Y2
F	535	HIS	-	expression tag	UNP C7S1Y2
F	536	HIS	-	expression tag	UNP C7S1Y2
F	537	HIS	-	expression tag	UNP C7S1Y2
F	538	HIS	-	expression tag	UNP C7S1Y2

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranoside-(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
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0
6	F	1	Total Na 1 1	0	0
6	E	1	Total Na 1 1	0	0

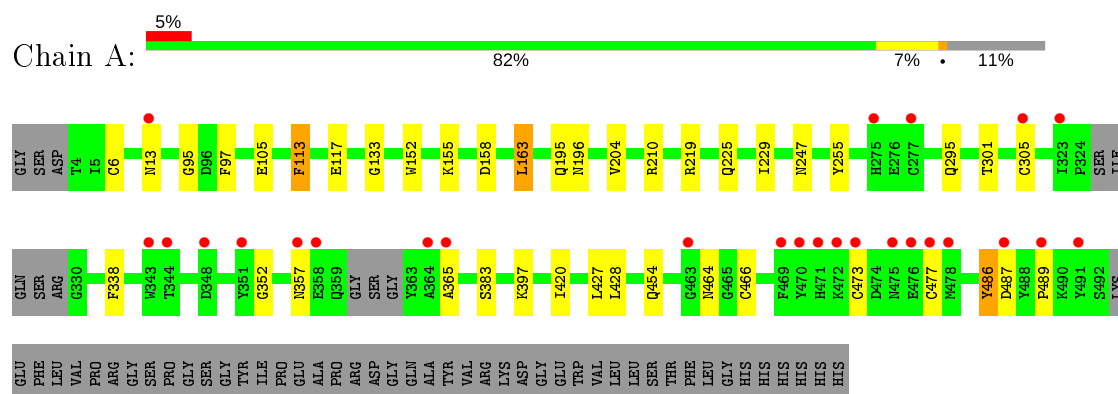
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	100	Total O 101 101	0	1
7	B	84	Total O 84 84	0	0
7	C	112	Total O 112 112	0	0
7	D	131	Total O 131 131	0	0
7	E	94	Total O 95 95	0	1
7	F	123	Total O 123 123	0	0

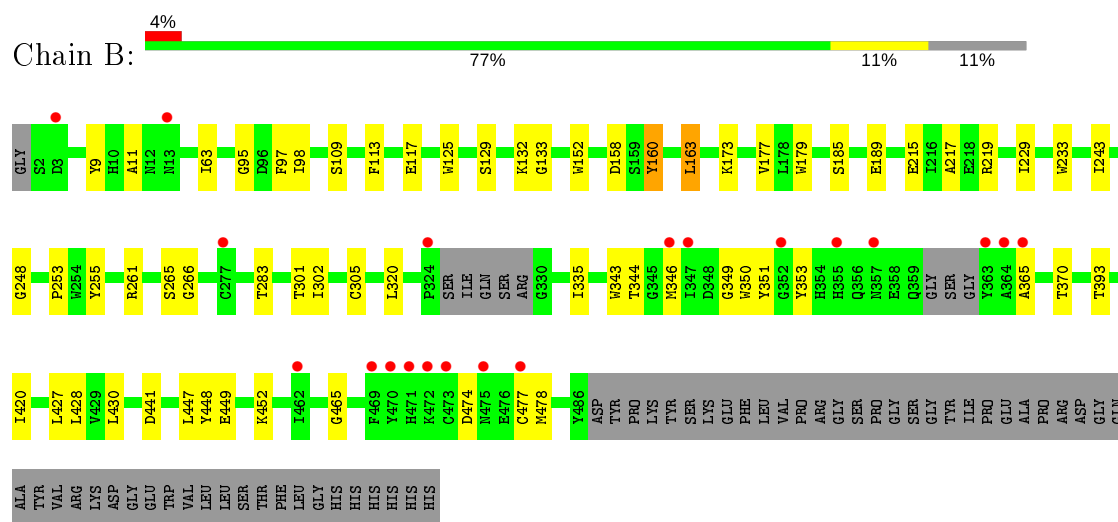
3 Residue-property plots

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.

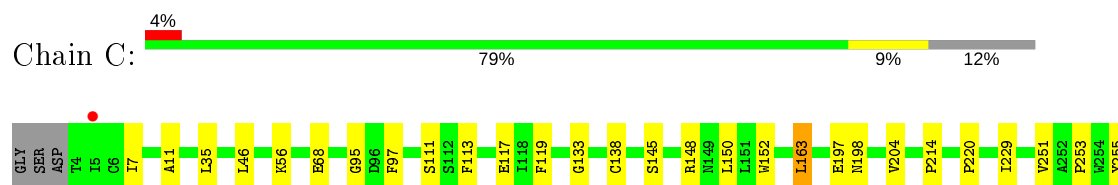
• Molecule 1: Hemagglutinin

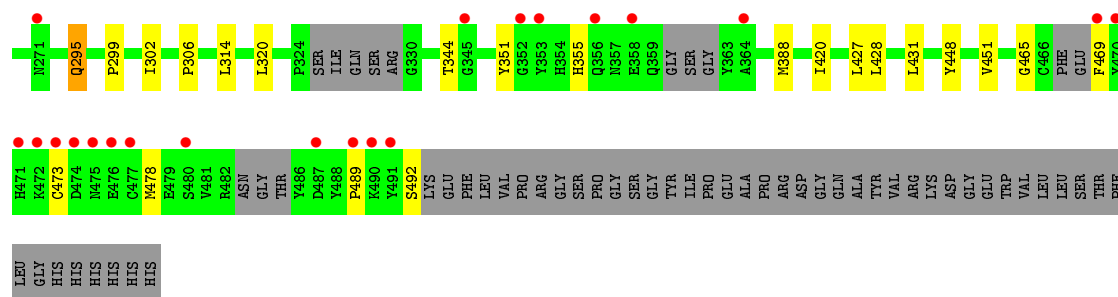


• Molecule 1: Hemagglutinin

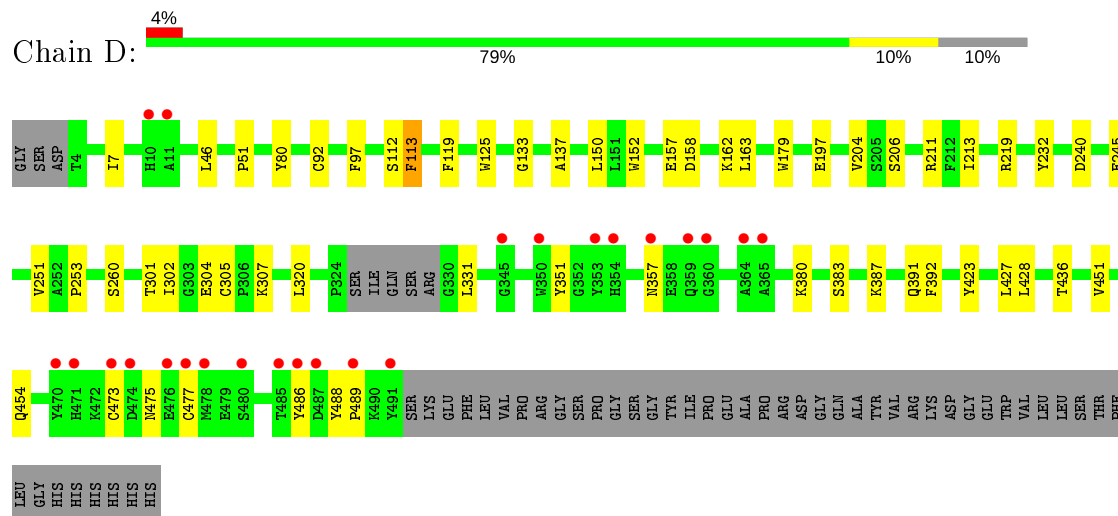


• Molecule 1: Hemagglutinin

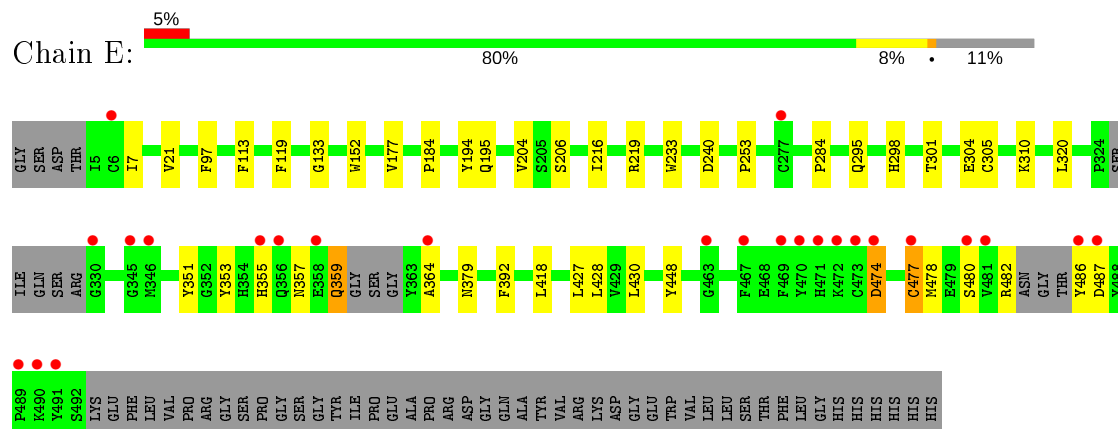




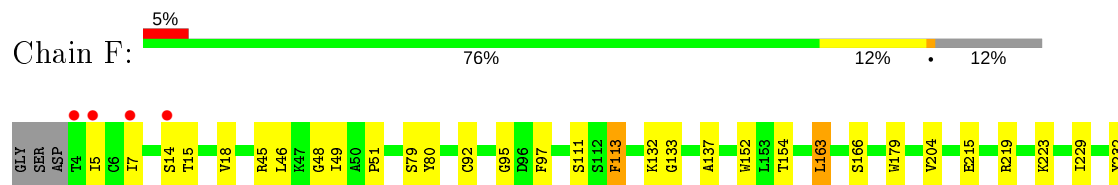
• Molecule 1: Hemagglutinin

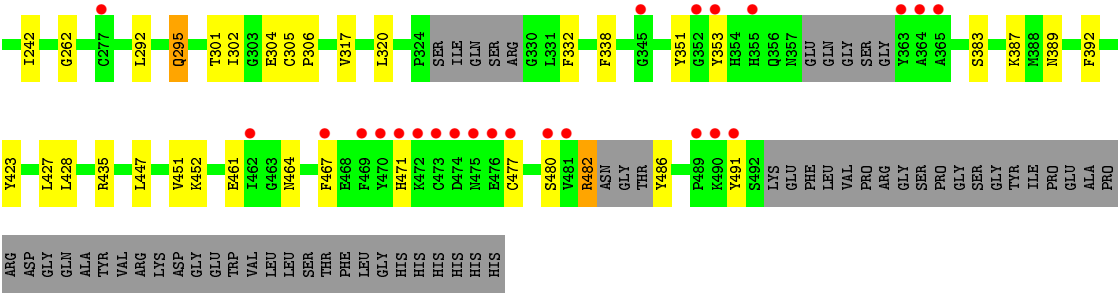


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





● Molecule 2: 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.10 Å 113.97 Å 246.38 Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	48.74 – 2.55 48.74 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.74-2.55) 99.9 (48.74-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.54 Å)	Xtriage
Refinement program	PHENIX dev_3409	Depositor
R, R_{free}	0.191 , 0.246 0.191 , 0.246	Depositor DCC
R_{free} test set	1955 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23091	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NA, K, EDO, MAN

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	0.45	0/3784	0.60	0/5151
1	B	0.47	0/3761	0.59	0/5115
1	C	0.43	0/3734	0.60	0/5077
1	D	0.45	0/3808	0.62	0/5179
1	E	0.42	0/3794	0.60	0/5154
1	F	0.41	0/3766	0.61	0/5119
All	All	0.44	0/22647	0.60	0/30795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3695	0	3430	26	0
1	B	3675	0	3445	37	0
1	C	3650	0	3420	29	0
1	D	3717	0	3469	37	0
1	E	3706	0	3491	30	0
1	F	3679	0	3466	46	0
2	G	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	56	0	52	1	0
3	B	42	0	39	1	0
3	C	42	0	39	0	0
3	D	14	0	13	0	0
3	E	28	0	26	0	0
3	F	42	0	39	0	0
4	A	8	0	12	0	0
4	C	8	0	12	2	0
4	D	16	0	24	2	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	101	0	0	1	0
7	B	84	0	0	1	0
7	C	112	0	0	1	0
7	D	131	0	0	0	0
7	E	95	0	0	0	0
7	F	123	0	0	0	0
All	All	23091	0	21038	183	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 4.

All (183) 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:163:LEU:HA	4:C:604:EDO:H22	1.58	0.84
1:A:155:LYS:HD2	1:A:195:GLN:HG2	1.66	0.76
1:A:427:LEU:HD21	1:C:428:LEU:HD13	1.67	0.76
1:D:219:ARG:HG2	1:F:204:VAL:HG11	1.67	0.75
1:D:204:VAL:HG11	1:E:219:ARG:HG2	1.69	0.74
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.70	0.74
1:D:133:GLY:HA3	1:D:152:TRP:HB3	1.69	0.73
1:E:133:GLY:HA3	1:E:152:TRP:HB3	1.72	0.69
1:C:163:LEU:C	1:C:163:LEU:HD12	2.14	0.68
1:E:428:LEU:HD13	1:F:427:LEU:HD21	1.74	0.68
1:A:487:ASP:OD1	1:A:489:PRO:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LEU:HD12	1:F:163:LEU:C	2.15	0.67
1:D:380:LYS:HG3	1:E:21:VAL:HG22	1.75	0.66
1:D:427:LEU:HD21	1:F:428:LEU:HD13	1.78	0.66
1:D:307:LYS:NZ	1:D:391:GLN:OE1	2.23	0.66
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.77	0.66
1:D:428:LEU:HD13	1:E:427:LEU:HD21	1.78	0.65
1:F:480:SER:OG	1:F:486:TYR:HA	1.96	0.65
1:A:163:LEU:C	1:A:163:LEU:HD12	2.18	0.64
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.80	0.64
1:F:304:GLU:HG2	1:F:392:PHE:HE1	1.61	0.64
1:B:179:TRP:HB3	1:B:253:PRO:HD3	1.80	0.62
1:E:474:ASP:OD1	1:E:474:ASP:N	2.30	0.62
1:E:364:ALA:HB3	1:E:482:ARG:HH22	1.64	0.62
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.80	0.62
1:E:204:VAL:HG11	1:F:219:ARG:HG2	1.82	0.61
1:F:18:VAL:HG21	1:F:317:VAL:CG2	2.31	0.61
1:F:304:GLU:HG2	1:F:392:PHE:CE1	2.36	0.61
1:B:163:LEU:HD12	1:B:163:LEU:C	2.22	0.60
1:F:482:ARG:NH1	1:F:482:ARG:HG3	2.16	0.60
1:D:331:LEU:HD13	1:F:332:PHE:HZ	1.66	0.59
1:C:111:SER:HA	7:C:750:HOH:O	2.01	0.59
1:F:295:GLN:HG2	1:F:306:PRO:HG2	1.85	0.59
1:A:428:LEU:HD13	1:B:427:LEU:HD21	1.83	0.58
1:E:480:SER:OG	1:E:486:TYR:HA	2.04	0.58
1:F:482:ARG:HH11	1:F:482:ARG:CG	2.17	0.58
1:A:210:ARG:NH1	7:A:701:HOH:O	2.34	0.57
1:E:301:THR:HB	1:E:305:CYS:SG	2.44	0.57
1:B:302:ILE:HD13	1:B:393:THR:HG23	1.87	0.57
1:F:133:GLY:HA3	1:F:152:TRP:HB3	1.87	0.56
1:A:95:GLY:HA3	1:A:229:ILE:O	2.05	0.56
1:A:155:LYS:HE2	1:A:158:ASP:HA	1.87	0.56
3:B:602:NAG:H83	3:B:602:NAG:H3	1.88	0.56
1:D:7:ILE:HD11	1:D:451:VAL:HG21	1.87	0.55
1:A:219:ARG:HG2	1:C:204:VAL:HG21	1.89	0.55
1:F:353:TYR:CE1	1:F:482:ARG:HD3	2.42	0.55
1:F:383:SER:O	1:F:387:LYS:HG2	2.07	0.55
1:D:125:TRP:HA	4:D:604:EDO:H12	1.89	0.55
1:D:357:ASN:ND2	1:D:475:ASN:OD1	2.40	0.54
1:A:383:SER:HB3	1:B:430:LEU:HD21	1.89	0.54
1:D:331:LEU:HD13	1:F:332:PHE:CZ	2.42	0.54
1:A:163:LEU:O	1:A:163:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:VAL:HG11	1:E:219:ARG:CG	2.36	0.54
1:E:304:GLU:HG2	1:E:392:PHE:HE1	1.72	0.53
1:B:335:ILE:N	1:B:441:ASP:OD1	2.37	0.53
1:F:92:CYS:HB2	1:F:137:ALA:O	2.09	0.53
1:F:111:SER:HB3	1:F:262:GLY:HA3	1.92	0.52
1:D:301:THR:HB	1:D:305:CYS:SG	2.50	0.52
1:F:452:LYS:NZ	1:F:461:GLU:OE2	2.23	0.52
1:B:185:SER:OG	1:B:189:GLU:OE1	2.27	0.52
1:F:132:LYS:HE3	1:F:154:THR:OG1	2.09	0.52
1:C:299:PRO:HB2	4:C:605:EDO:H12	1.92	0.51
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.45	0.51
1:B:343:TRP:HE3	1:B:346:MET:HE2	1.76	0.51
1:B:215:GLU:O	1:B:219:ARG:NH2	2.39	0.51
1:A:301:THR:HB	1:A:305:CYS:SG	2.51	0.51
1:D:219:ARG:CG	1:F:204:VAL:HG11	2.39	0.51
1:B:283:THR:HG22	1:B:301:THR:HG22	1.92	0.50
1:C:163:LEU:HD12	1:C:163:LEU:O	2.10	0.50
1:F:7:ILE:HD11	1:F:451:VAL:HG21	1.93	0.50
1:A:486:TYR:CD2	1:A:486:TYR:C	2.85	0.50
1:B:428:LEU:HD13	1:C:427:LEU:HD21	1.94	0.49
1:B:420:ILE:HG21	1:C:420:ILE:HD13	1.94	0.49
1:D:206:SER:HB2	1:D:240:ASP:OD2	2.13	0.49
1:E:355:HIS:HB2	1:E:478:MET:SD	2.52	0.49
1:F:215:GLU:O	1:F:219:ARG:NH2	2.46	0.49
1:C:489:PRO:HA	1:C:492:SER:HB2	1.95	0.49
1:D:46:LEU:HD22	1:D:302:ILE:HG22	1.95	0.48
1:F:482:ARG:HH11	1:F:482:ARG:HG3	1.76	0.48
1:B:350:TRP:HB2	1:B:370:THR:HG23	1.95	0.48
1:E:482:ARG:H	1:E:482:ARG:HD2	1.79	0.48
1:B:117:GLU:HG3	1:B:255:TYR:CZ	2.48	0.48
1:B:109:SER:OG	1:B:261:ARG:NH1	2.46	0.48
1:B:125:TRP:HZ3	1:B:163:LEU:HD13	1.79	0.48
1:C:35:LEU:HB2	1:C:314:LEU:HB2	1.94	0.48
1:D:157:GLU:O	1:D:158:ASP:HB2	2.14	0.48
1:D:51:PRO:HB3	1:D:80:TYR:CZ	2.49	0.47
1:E:184:PRO:HG2	1:E:216:ILE:HG13	1.96	0.47
1:F:301:THR:HB	1:F:305:CYS:SG	2.54	0.47
1:B:95:GLY:HA3	1:B:229:ILE:O	2.15	0.47
1:C:7:ILE:HD11	1:C:451:VAL:HG21	1.96	0.47
1:E:284:PRO:HG2	1:E:298:HIS:CE1	2.49	0.47
1:E:204:VAL:HG11	1:F:219:ARG:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:SER:O	1:D:387:LYS:HG2	2.14	0.47
1:D:304:GLU:HG2	1:D:392:PHE:CE1	2.50	0.47
1:D:380:LYS:NZ	1:D:436:THR:OG1	2.37	0.47
1:A:352:GLY:HA3	1:A:365:ALA:HA	1.96	0.47
1:A:420:ILE:HG21	1:B:420:ILE:HD13	1.96	0.46
1:B:243:ILE:HD12	1:C:220:PRO:HD3	1.97	0.46
1:F:423:TYR:CZ	1:F:427:LEU:HD22	2.50	0.46
1:D:211:ARG:NH2	1:D:213:ILE:HD11	2.30	0.46
1:D:383:SER:HB3	1:E:430:LEU:HD21	1.98	0.46
1:C:355:HIS:HB2	1:C:478:MET:SD	2.55	0.46
1:B:129:SER:OG	1:B:132:LYS:HG3	2.15	0.46
1:C:119:PHE:CE2	1:C:253:PRO:HG2	2.51	0.46
1:C:388:MET:HE3	1:C:388:MET:HB3	1.74	0.46
1:A:163:LEU:C	1:A:163:LEU:CD1	2.84	0.45
1:D:119:PHE:CE2	1:D:253:PRO:HG2	2.50	0.45
1:F:179:TRP:CE2	1:F:232:TYR:HB2	2.51	0.45
1:A:6:CYS:HA	1:A:466:CYS:HA	1.98	0.45
1:C:95:GLY:HA3	1:C:229:ILE:O	2.16	0.45
1:D:423:TYR:CZ	1:D:427:LEU:HD22	2.51	0.45
1:E:7:ILE:HD13	1:E:448:TYR:HA	1.98	0.45
1:F:5:ILE:HG22	1:F:467:PHE:HB2	1.98	0.45
1:F:353:TYR:OH	1:F:447:LEU:HD11	2.17	0.45
1:F:292:LEU:O	1:F:306:PRO:HB3	2.16	0.45
1:A:13:ASN:HD22	3:A:601:NAG:C7	2.28	0.45
1:F:163:LEU:CD1	1:F:163:LEU:C	2.85	0.45
1:F:471:HIS:CD2	1:F:491:TYR:HD2	2.34	0.45
1:F:51:PRO:HB3	1:F:80:TYR:CZ	2.52	0.45
1:D:51:PRO:HB3	1:D:80:TYR:CE1	2.52	0.45
1:B:11:ALA:O	1:B:344:THR:HA	2.17	0.44
1:C:56:LYS:HE2	1:C:68:GLU:HB3	1.99	0.44
1:A:113:PHE:HD1	1:A:113:PHE:O	1.98	0.44
1:D:150:LEU:HB3	1:D:251:VAL:HG12	1.98	0.44
1:E:304:GLU:HG2	1:E:392:PHE:CE1	2.53	0.44
1:B:474:ASP:O	1:B:478:MET:HG2	2.17	0.44
1:F:166:SER:HA	1:F:242:ILE:O	2.18	0.44
1:C:46:LEU:HD13	1:C:302:ILE:HG22	2.00	0.44
1:D:179:TRP:CE2	1:D:232:TYR:HB2	2.52	0.44
1:E:310:LYS:HG3	1:E:418:LEU:HD21	2.00	0.44
1:D:163:LEU:O	1:D:245:GLU:HA	2.18	0.43
1:C:119:PHE:HE2	1:C:253:PRO:HG2	1.82	0.43
1:E:194:TYR:O	1:E:195:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:TYR:CG	1:E:487:ASP:N	2.86	0.43
1:F:46:LEU:HD22	1:F:302:ILE:HG22	2.00	0.43
1:D:454:GLN:O	1:D:486:TYR:HD2	2.01	0.43
1:A:196:ASN:ND2	1:A:247:ASN:O	2.42	0.43
1:F:18:VAL:HG21	1:F:317:VAL:HG22	1.99	0.43
1:A:204:VAL:HG21	1:B:219:ARG:HG2	2.00	0.43
1:A:155:LYS:CD	1:A:195:GLN:HG2	2.43	0.43
1:B:117:GLU:HG3	1:B:255:TYR:CE2	2.54	0.43
1:B:63:ILE:HD12	1:B:63:ILE:HA	1.81	0.43
1:E:177:VAL:O	1:E:233:TRP:HA	2.18	0.43
1:F:338:PHE:O	1:F:464:ASN:HA	2.19	0.43
1:B:217:ALA:O	1:B:219:ARG:HG3	2.19	0.42
1:D:112:SER:OG	1:D:260:SER:HB2	2.19	0.42
1:F:49:ILE:HB	1:F:79:SER:HB3	2.01	0.42
1:C:448:TYR:CE2	1:C:465:GLY:HA2	2.54	0.42
1:A:105:GLU:OE2	1:A:397:LYS:NZ	2.53	0.42
1:F:477:CYS:O	1:F:480:SER:HB3	2.19	0.42
1:B:177:VAL:O	1:B:233:TRP:HA	2.20	0.42
1:A:338:PHE:O	1:A:464:ASN:HA	2.20	0.42
1:B:265:SER:OG	1:B:266:GLY:N	2.52	0.42
1:E:353:TYR:HB2	1:E:482:ARG:NH2	2.35	0.42
1:D:488:TYR:N	1:D:489:PRO:HD2	2.35	0.42
1:F:92:CYS:O	1:F:223:LYS:HD3	2.19	0.42
1:B:160:TYR:CZ	1:B:248:GLY:HA2	2.55	0.42
1:C:117:GLU:HG3	1:C:255:TYR:CZ	2.54	0.42
1:D:92:CYS:HB2	1:D:137:ALA:O	2.20	0.42
1:F:45:ARG:HD3	1:F:48:GLY:O	2.20	0.42
1:E:477:CYS:O	1:E:480:SER:HB3	2.20	0.42
1:C:197:GLU:HG3	1:C:198:ASN:OD1	2.20	0.41
1:C:150:LEU:HB3	1:C:251:VAL:HG12	2.02	0.41
1:F:5:ILE:HA	1:F:5:ILE:HD12	1.94	0.41
1:B:98:ILE:HD11	7:B:735:HOH:O	2.20	0.41
1:F:95:GLY:HA3	1:F:229:ILE:O	2.20	0.41
1:B:301:THR:HB	1:B:305:CYS:SG	2.60	0.41
1:F:113:PHE:CD1	1:F:113:PHE:C	2.94	0.41
1:B:449:GLU:OE2	1:B:452:LYS:HD3	2.21	0.41
1:C:11:ALA:O	1:C:344:THR:HA	2.20	0.41
1:A:117:GLU:HG3	1:A:255:TYR:CZ	2.55	0.41
1:C:431:LEU:HA	1:C:431:LEU:HD23	1.89	0.41
1:B:349:GLY:HA3	1:B:365:ALA:HB1	2.02	0.41
1:B:9:TYR:HB2	1:B:320:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LYS:HG3	1:E:21:VAL:CG2	2.49	0.40
1:E:119:PHE:CE2	1:E:253:PRO:HG2	2.56	0.40
1:E:206:SER:HB2	1:E:240:ASP:OD2	2.21	0.40
1:E:357:ASN:ND2	1:E:359:GLN:HG3	2.35	0.40
1:D:197:GLU:O	4:D:602:EDO:H21	2.22	0.40
1:D:113:PHE:CD1	1:D:113:PHE:C	2.94	0.40
1:B:353:TYR:OH	1:B:447:LEU:HD11	2.22	0.40
1:C:138:CYS:O	1:C:145:SER:HB3	2.22	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	475/538 (88%)	462 (97%)	13 (3%)	0	100	100
1	B	471/538 (88%)	453 (96%)	18 (4%)	0	100	100
1	C	466/538 (87%)	452 (97%)	14 (3%)	0	100	100
1	D	479/538 (89%)	463 (97%)	16 (3%)	0	100	100
1	E	469/538 (87%)	456 (97%)	13 (3%)	0	100	100
1	F	468/538 (87%)	454 (97%)	14 (3%)	0	100	100
All	All	2828/3228 (88%)	2740 (97%)	88 (3%)	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	387/467 (83%)	377 (97%)	10 (3%)	46	61
1	B	391/467 (84%)	383 (98%)	8 (2%)	55	70
1	C	386/467 (83%)	376 (97%)	10 (3%)	46	61
1	D	390/467 (84%)	383 (98%)	7 (2%)	59	74
1	E	397/467 (85%)	388 (98%)	9 (2%)	50	65
1	F	392/467 (84%)	381 (97%)	11 (3%)	43	58
All	All	2343/2802 (84%)	2288 (98%)	55 (2%)	50	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	PHE
1	A	113	PHE
1	A	163	LEU
1	A	225	GLN
1	A	295	GLN
1	A	357	ASN
1	A	454	GLN
1	A	473	CYS
1	A	477	CYS
1	A	486	TYR
1	B	97	PHE
1	B	113	PHE
1	B	158	ASP
1	B	160	TYR
1	B	163	LEU
1	B	173	LYS
1	B	351	TYR
1	B	477	CYS
1	C	97	PHE
1	C	113	PHE
1	C	148	ARG
1	C	163	LEU
1	C	214	PRO
1	C	295	GLN
1	C	320	LEU
1	C	351	TYR
1	C	469	PHE

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Mol	Chain	Res	Type
1	C	473	CYS
1	D	97	PHE
1	D	113	PHE
1	D	162	LYS
1	D	320	LEU
1	D	351	TYR
1	D	473	CYS
1	D	477	CYS
1	E	97	PHE
1	E	113	PHE
1	E	295	GLN
1	E	320	LEU
1	E	351	TYR
1	E	359	GLN
1	E	379	ASN
1	E	474	ASP
1	E	477	CYS
1	F	14	SER
1	F	15	THR
1	F	97	PHE
1	F	113	PHE
1	F	163	LEU
1	F	295	GLN
1	F	320	LEU
1	F	351	TYR
1	F	389	ASN
1	F	435	ARG
1	F	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	1	1,2	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	0.47	0
2	BMA	G	3	2	11,11,12	0.88	0	15,15,17	0.95	1 (6%)
2	MAN	G	4	2	11,11,12	1.08	1 (9%)	15,15,17	1.29	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
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	MAN	O5-C1	-2.07	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	MAN	C1-O5-C5	3.14	116.44	112.19
2	G	4	MAN	O2-C2-C3	-2.79	104.54	110.14
2	G	3	BMA	O2-C2-C3	-2.13	105.86	110.14

There are no chirality outliers.

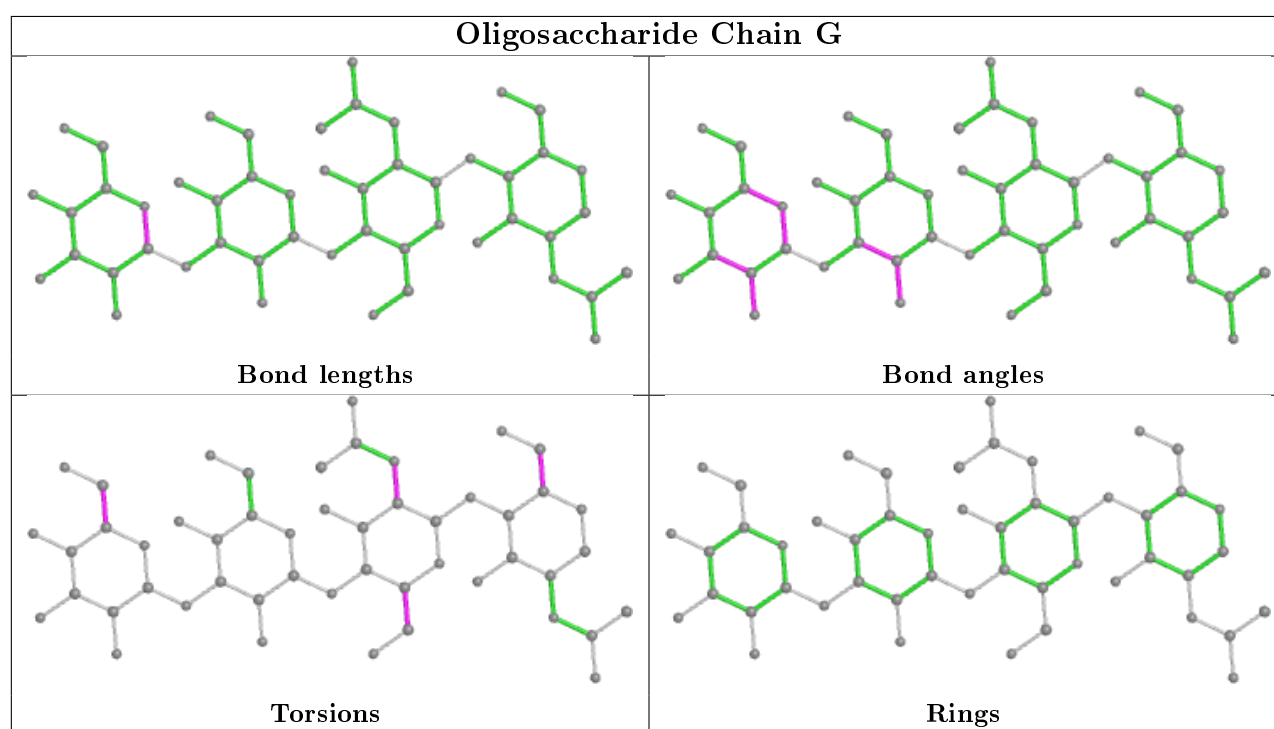
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	G	4	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 5 are monoatomic - leaving 27 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
3	NAG	A	602	1	14,14,15	0.47	0	17,19,21	0.40	0
4	EDO	A	605	-	3,3,3	0.55	0	2,2,2	0.31	0
3	NAG	F	602	1	14,14,15	0.72	1 (7%)	17,19,21	0.49	0
3	NAG	C	603	1	14,14,15	0.56	0	17,19,21	0.47	0
4	EDO	F	603	-	3,3,3	0.48	0	2,2,2	0.28	0
3	NAG	F	601	1	14,14,15	0.41	0	17,19,21	0.38	0
4	EDO	D	602	-	3,3,3	0.39	0	2,2,2	0.40	0
3	NAG	C	602	1	14,14,15	0.43	0	17,19,21	0.47	0
3	NAG	F	604	1	14,14,15	0.68	0	17,19,21	1.70	4 (23%)
4	EDO	E	604	-	3,3,3	0.48	0	2,2,2	0.25	0
4	EDO	C	604	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	D	603	-	3,3,3	0.38	0	2,2,2	0.57	0
3	NAG	A	601	1	14,14,15	0.49	0	17,19,21	0.75	1 (5%)
3	NAG	D	601	1	14,14,15	0.35	0	17,19,21	0.40	0
4	EDO	D	605	-	3,3,3	0.50	0	2,2,2	0.22	0
4	EDO	D	604	-	3,3,3	0.60	0	2,2,2	0.39	0
4	EDO	E	603	-	3,3,3	0.57	0	2,2,2	0.20	0
3	NAG	A	603	1	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
3	NAG	A	604	1	14,14,15	0.45	0	17,19,21	0.61	0
3	NAG	B	601	1	14,14,15	0.44	0	17,19,21	0.38	0
3	NAG	C	601	1	14,14,15	0.37	0	17,19,21	0.45	0
4	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.61	0
3	NAG	B	602	1	14,14,15	0.64	1 (7%)	17,19,21	1.25	1 (5%)
3	NAG	E	602	1	14,14,15	0.31	0	17,19,21	0.45	0
3	NAG	B	607	1	14,14,15	0.61	0	17,19,21	0.64	1 (5%)
4	EDO	C	605	-	3,3,3	0.46	0	2,2,2	0.36	0
3	NAG	E	601	1	14,14,15	0.56	0	17,19,21	0.48	0

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	A	602	1	-	2/6/23/26	0/1/1/1
4	EDO	A	605	-	-	0/1/1/1	-
3	NAG	F	602	1	-	2/6/23/26	0/1/1/1
3	NAG	C	603	1	-	0/6/23/26	0/1/1/1
4	EDO	F	603	-	-	1/1/1/1	-
3	NAG	F	601	1	-	2/6/23/26	0/1/1/1
4	EDO	D	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	602	1	-	2/6/23/26	0/1/1/1
3	NAG	F	604	1	-	5/6/23/26	0/1/1/1
4	EDO	E	604	-	-	0/1/1/1	-
4	EDO	C	604	-	-	0/1/1/1	-
4	EDO	D	603	-	-	1/1/1/1	-
3	NAG	A	601	1	-	1/6/23/26	0/1/1/1
3	NAG	D	601	1	-	1/6/23/26	0/1/1/1
4	EDO	D	605	-	-	0/1/1/1	-
4	EDO	D	604	-	-	1/1/1/1	-
4	EDO	E	603	-	-	0/1/1/1	-
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	4/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	EDO	A	606	-	-	1/1/1/1	-
3	NAG	B	602	1	-	4/6/23/26	0/1/1/1
3	NAG	E	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	607	1	-	2/6/23/26	0/1/1/1
4	EDO	C	605	-	-	1/1/1/1	-
3	NAG	E	601	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	NAG	C1-C2	2.50	1.56	1.52
3	B	602	NAG	C1-C2	2.04	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C2-N2-C7	4.25	128.96	122.90
3	F	604	NAG	O5-C1-C2	-3.46	105.82	111.29
3	F	604	NAG	C1-O5-C5	3.26	116.61	112.19
3	F	604	NAG	O5-C5-C6	3.05	111.99	107.20
3	A	603	NAG	C3-C4-C5	2.56	114.80	110.24
3	A	601	NAG	C1-O5-C5	2.51	115.59	112.19
3	B	607	NAG	C1-O5-C5	2.27	115.27	112.19
3	F	604	NAG	C2-N2-C7	2.07	125.85	122.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	NAG	C4-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
3	F	604	NAG	C8-C7-N2-C2
3	F	604	NAG	O7-C7-N2-C2
3	B	607	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	A	604	NAG	O5-C5-C6-O6
3	C	602	NAG	C4-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
3	F	602	NAG	O5-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	F	604	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	C	601	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	F	604	NAG	C4-C5-C6-O6
3	B	607	NAG	O5-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	B	601	NAG	C1-C2-N2-C7
3	A	602	NAG	O5-C5-C6-O6
4	F	603	EDO	O1-C1-C2-O2
3	A	604	NAG	C4-C5-C6-O6
4	D	604	EDO	O1-C1-C2-O2
4	C	605	EDO	O1-C1-C2-O2
3	B	602	NAG	C4-C5-C6-O6
4	D	603	EDO	O1-C1-C2-O2
3	F	604	NAG	C3-C2-N2-C7
3	B	601	NAG	C3-C2-N2-C7
3	C	601	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	B	602	NAG	C3-C2-N2-C7
3	D	601	NAG	O5-C5-C6-O6
4	D	602	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	EDO	1	0
4	C	604	EDO	1	0
3	A	601	NAG	1	0
4	D	604	EDO	1	0
3	B	602	NAG	1	0
4	C	605	EDO	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	481/538 (89%)	0.18	26 (5%)	25	30	24, 47, 111, 147	0
1	B	477/538 (88%)	0.14	20 (4%)	36	42	27, 52, 99, 125	0
1	C	476/538 (88%)	0.20	22 (4%)	32	39	24, 48, 110, 190	0
1	D	483/538 (89%)	0.14	24 (4%)	28	34	25, 43, 109, 130	0
1	E	477/538 (88%)	0.16	25 (5%)	27	32	24, 49, 107, 135	0
1	F	476/538 (88%)	0.20	28 (5%)	22	26	24, 50, 115, 157	0
All	All	2870/3228 (88%)	0.17	145 (5%)	28	33	24, 49, 110, 190	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	473	CYS	6.1
1	F	473	CYS	5.8
1	B	364	ALA	5.7
1	C	473	CYS	5.7
1	C	477	CYS	5.3
1	A	364	ALA	5.1
1	E	470	TYR	5.0
1	C	470	TYR	4.9
1	D	477	CYS	4.9
1	D	473	CYS	4.7
1	F	491	TYR	4.6
1	F	364	ALA	4.5
1	C	490	LYS	4.5
1	A	472	LYS	4.5
1	D	365	ALA	4.4
1	F	470	TYR	4.4
1	C	364	ALA	4.2
1	C	352	GLY	4.1
1	F	352	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	467	PHE	4.0
1	A	463	GLY	4.0
1	A	489	PRO	3.9
1	D	491	TYR	3.9
1	E	477	CYS	3.9
1	F	353	TYR	3.8
1	F	5	ILE	3.8
1	F	277	CYS	3.8
1	C	472	LYS	3.8
1	F	355	HIS	3.8
1	C	353	TYR	3.8
1	C	475	ASN	3.8
1	C	491	TYR	3.7
1	C	469	PHE	3.7
1	B	355	HIS	3.6
1	C	487	ASP	3.6
1	D	486	TYR	3.6
1	A	365	ALA	3.5
1	A	491	TYR	3.4
1	B	462	ILE	3.4
1	E	471	HIS	3.4
1	A	477	CYS	3.4
1	B	473	CYS	3.4
1	A	476	GLU	3.3
1	F	474	ASP	3.3
1	C	474	ASP	3.3
1	F	345	GLY	3.3
1	E	489	PRO	3.3
1	B	470	TYR	3.2
1	B	352	GLY	3.2
1	E	491	TYR	3.2
1	D	489	PRO	3.2
1	F	467	PHE	3.2
1	A	348	ASP	3.2
1	C	471	HIS	3.2
1	F	365	ALA	3.2
1	C	476	GLU	3.1
1	F	7	ILE	3.1
1	F	472	LYS	3.1
1	F	489	PRO	3.1
1	D	485	THR	3.1
1	F	475	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	477	CYS	3.1
1	A	13	ASN	3.1
1	A	473	CYS	3.1
1	B	346	MET	3.1
1	F	363	TYR	3.1
1	A	344	THR	3.1
1	A	277	CYS	3.0
1	A	471	HIS	3.0
1	B	477	CYS	3.0
1	E	486	TYR	3.0
1	D	353	TYR	3.0
1	A	343	TRP	3.0
1	E	472	LYS	2.9
1	D	480	SER	2.9
1	E	355	HIS	2.9
1	C	489	PRO	2.9
1	A	469	PHE	2.8
1	A	358	GLU	2.8
1	E	480	SER	2.8
1	B	3	ASP	2.8
1	D	350	TRP	2.7
1	E	463	GLY	2.7
1	F	469	PHE	2.7
1	B	363	TYR	2.7
1	F	480	SER	2.7
1	B	475	ASN	2.7
1	D	360	GLY	2.7
1	D	476	GLU	2.6
1	F	471	HIS	2.6
1	C	358	GLU	2.6
1	A	323	ILE	2.6
1	E	481	VAL	2.6
1	B	471	HIS	2.6
1	E	356	GLN	2.6
1	C	345	GLY	2.6
1	A	478	MET	2.5
1	D	354	HIS	2.5
1	C	356	GLN	2.5
1	D	474	ASP	2.5
1	E	487	ASP	2.5
1	F	14	SER	2.5
1	E	358	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	13	ASN	2.5
1	F	490	LYS	2.4
1	A	487	ASP	2.4
1	E	345	GLY	2.4
1	C	480	SER	2.4
1	A	351	TYR	2.4
1	B	357	ASN	2.4
1	D	471	HIS	2.4
1	D	11	ALA	2.4
1	F	476	GLU	2.4
1	A	357	ASN	2.3
1	D	357	ASN	2.3
1	E	277	CYS	2.3
1	E	469	PHE	2.3
1	D	487	ASP	2.3
1	D	359	GLN	2.3
1	D	10	HIS	2.3
1	B	347	ILE	2.2
1	A	470	TYR	2.2
1	A	275	HIS	2.2
1	F	481	VAL	2.2
1	B	324	PRO	2.2
1	E	474	ASP	2.2
1	B	277	CYS	2.2
1	F	4	THR	2.2
1	D	470	TYR	2.2
1	E	364	ALA	2.2
1	D	345	GLY	2.2
1	F	462	ILE	2.1
1	C	5	ILE	2.1
1	D	478	MET	2.1
1	D	364	ALA	2.1
1	E	330	GLY	2.1
1	B	365	ALA	2.1
1	A	305	CYS	2.1
1	B	472	LYS	2.0
1	E	6	CYS	2.0
1	E	346	MET	2.0
1	A	475	ASN	2.0
1	E	490	LYS	2.0
1	C	271	ASN	2.0
1	B	469	PHE	2.0

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

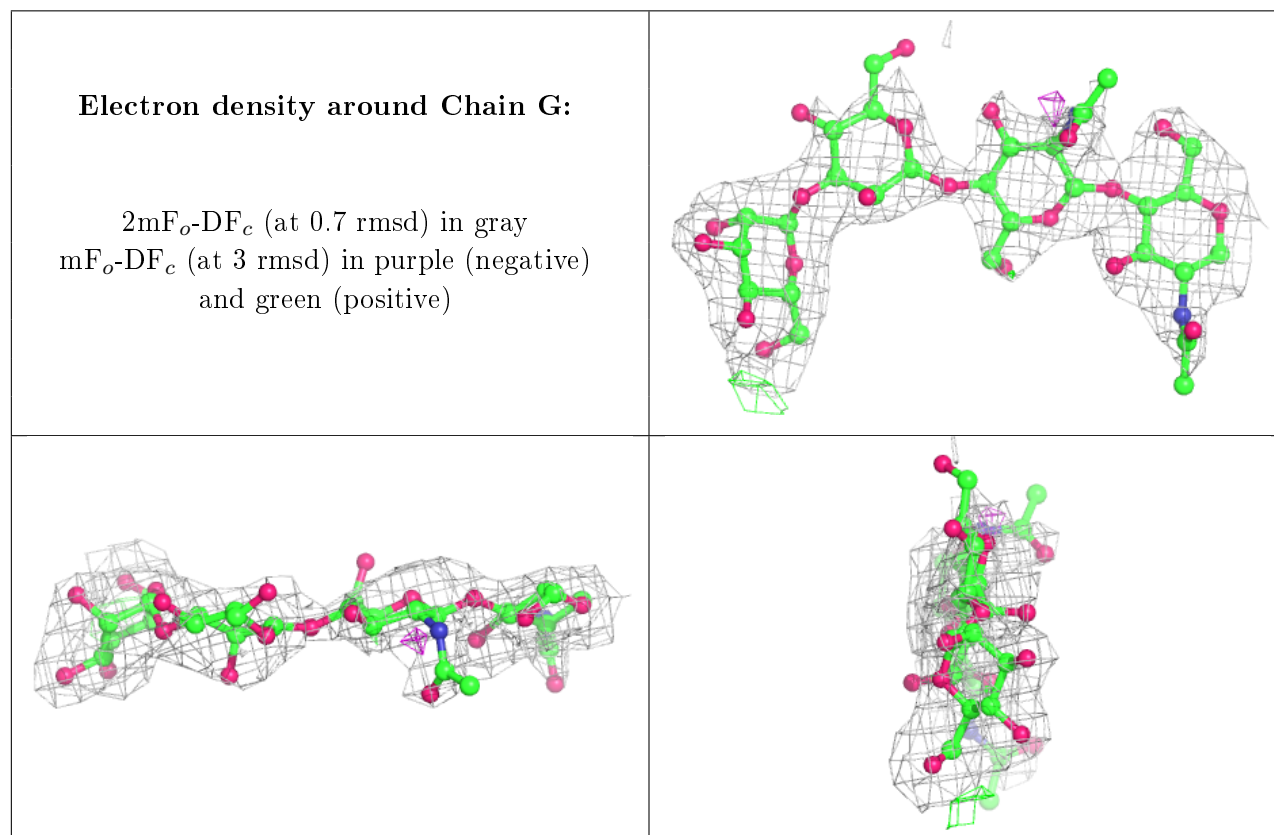
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	NAG	G	2	14/15	0.80	0.49	94,108,114,115	0
2	NAG	G	1	14/15	0.89	0.38	66,86,95,105	0
2	BMA	G	3	11/12	0.89	0.28	72,94,103,104	0
2	MAN	G	4	11/12	0.94	0.13	37,54,63,64	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.



6.4 Ligands ⓘ

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	A	603	14/15	0.48	0.38	91,106,115,116	0
3	NAG	F	602	14/15	0.61	0.43	78,102,111,115	0
3	NAG	B	602	14/15	0.63	0.28	80,94,109,112	0
3	NAG	E	601	14/15	0.66	0.38	91,104,114,119	0
3	NAG	A	601	14/15	0.67	0.35	77,92,97,99	0
3	NAG	A	602	14/15	0.68	0.33	87,101,107,108	0
3	NAG	B	601	14/15	0.68	0.37	81,97,107,111	0
3	NAG	F	601	14/15	0.70	0.36	74,91,99,99	0
3	NAG	C	601	14/15	0.71	0.42	86,108,121,122	0
3	NAG	C	602	14/15	0.76	0.17	78,94,97,99	0
3	NAG	F	604	14/15	0.77	0.31	89,102,111,113	0
3	NAG	D	601	14/15	0.77	0.36	74,92,109,113	0
3	NAG	B	607	14/15	0.79	0.34	74,96,99,102	0
3	NAG	A	604	14/15	0.80	0.46	79,94,108,117	0
4	EDO	D	604	4/4	0.80	0.32	58,60,64,70	0
3	NAG	C	603	14/15	0.86	0.28	75,94,98,102	0
3	NAG	E	602	14/15	0.86	0.38	75,90,101,103	0
4	EDO	A	605	4/4	0.88	0.21	51,61,66,67	0
4	EDO	E	603	4/4	0.88	0.23	43,44,46,54	0
4	EDO	D	603	4/4	0.90	0.23	59,59,60,67	0
6	NA	F	605	1/1	0.90	0.35	40,40,40,40	0
6	NA	C	606	1/1	0.91	0.34	44,44,44,44	0
4	EDO	C	604	4/4	0.92	0.17	55,57,58,59	0
4	EDO	D	605	4/4	0.94	0.23	58,59,61,62	0
4	EDO	F	603	4/4	0.94	0.19	50,51,52,52	0
4	EDO	C	605	4/4	0.95	0.20	53,55,56,64	0
4	EDO	E	604	4/4	0.95	0.22	56,56,59,60	0
4	EDO	A	606	4/4	0.96	0.20	43,46,52,57	0
6	NA	E	605	1/1	0.96	0.38	47,47,47,47	0
4	EDO	D	602	4/4	0.96	0.14	45,47,48,57	0
5	K	D	606	1/1	0.97	0.18	61,61,61,61	0
5	K	A	607	1/1	0.97	0.25	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.