wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2020 – 03:09 PM BST

PDB ID	:	6Y62
Title	:	Crystal structure of the envelope glycoprotein complex of Maporal virus in a prefusion conformation
Authors	:	Serris, A.; Rey, F.A.; Guardado-Calvo, P.
Deposited on	:	2020-02-26
Resolution	:	2.20 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 (i) symbol.

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

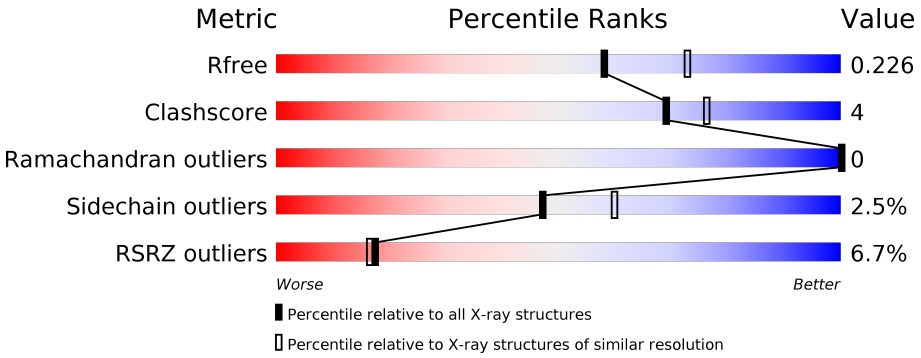
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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

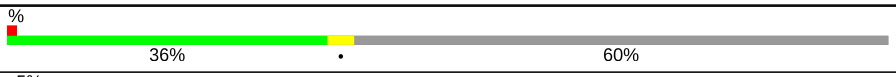
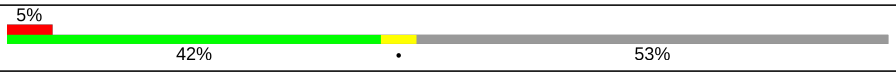
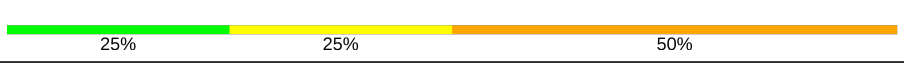
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	891	
1	B	891	
2	C	4	
2	D	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	D	3	-	-	-	X
2	MAN	D	4	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6270 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 Envelope polyprotein,Envelope polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2701	1709	447	523	22			
1	B	419	Total	C	N	O	S	0	0	0
			3194	1998	536	626	34			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	GLY	-	linker	UNP Q5MYC0
A	376	GLY	-	linker	UNP Q5MYC0
A	377	SER	-	linker	UNP Q5MYC0
A	378	GLY	-	linker	UNP Q5MYC0
A	379	LEU	-	linker	UNP Q5MYC0
A	380	VAL	-	linker	UNP Q5MYC0
A	381	PRO	-	linker	UNP Q5MYC0
A	382	ARG	-	linker	UNP Q5MYC0
A	383	GLY	-	linker	UNP Q5MYC0
A	384	SER	-	linker	UNP Q5MYC0
A	385	GLY	-	linker	UNP Q5MYC0
A	386	GLY	-	linker	UNP Q5MYC0
A	387	GLY	-	linker	UNP Q5MYC0
A	388	SER	-	linker	UNP Q5MYC0
A	389	GLY	-	linker	UNP Q5MYC0
A	390	GLY	-	linker	UNP Q5MYC0
A	391	GLY	-	linker	UNP Q5MYC0
A	392	SER	-	linker	UNP Q5MYC0
A	393	TRP	-	linker	UNP Q5MYC0
A	394	SER	-	linker	UNP Q5MYC0
A	395	HIS	-	linker	UNP Q5MYC0
A	396	PRO	-	linker	UNP Q5MYC0
A	397	GLN	-	linker	UNP Q5MYC0
A	398	PHE	-	linker	UNP Q5MYC0
A	399	GLU	-	linker	UNP Q5MYC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LYS	-	linker	UNP Q5MYC0
A	401	GLY	-	linker	UNP Q5MYC0
A	402	GLY	-	linker	UNP Q5MYC0
A	403	GLY	-	linker	UNP Q5MYC0
A	404	THR	-	linker	UNP Q5MYC0
A	405	GLY	-	linker	UNP Q5MYC0
A	406	GLY	-	linker	UNP Q5MYC0
A	407	GLY	-	linker	UNP Q5MYC0
A	408	THR	-	linker	UNP Q5MYC0
A	409	LEU	-	linker	UNP Q5MYC0
A	410	VAL	-	linker	UNP Q5MYC0
A	411	PRO	-	linker	UNP Q5MYC0
A	412	ARG	-	linker	UNP Q5MYC0
A	413	GLY	-	linker	UNP Q5MYC0
A	414	SER	-	linker	UNP Q5MYC0
A	415	GLY	-	linker	UNP Q5MYC0
A	416	THR	-	linker	UNP Q5MYC0
A	417	GLY	-	linker	UNP Q5MYC0
A	418	GLY	-	linker	UNP Q5MYC0
A	875	PRO	-	expression tag	UNP Q5MYC0
A	876	PHE	-	expression tag	UNP Q5MYC0
A	877	GLU	-	expression tag	UNP Q5MYC0
A	878	ASP	-	expression tag	UNP Q5MYC0
A	879	ASP	-	expression tag	UNP Q5MYC0
A	880	ASP	-	expression tag	UNP Q5MYC0
A	881	ASP	-	expression tag	UNP Q5MYC0
A	882	LYS	-	expression tag	UNP Q5MYC0
A	883	ALA	-	expression tag	UNP Q5MYC0
A	884	GLY	-	expression tag	UNP Q5MYC0
A	885	TRP	-	expression tag	UNP Q5MYC0
A	886	SER	-	expression tag	UNP Q5MYC0
A	887	HIS	-	expression tag	UNP Q5MYC0
A	888	PRO	-	expression tag	UNP Q5MYC0
A	889	GLN	-	expression tag	UNP Q5MYC0
A	890	PHE	-	expression tag	UNP Q5MYC0
A	891	GLU	-	expression tag	UNP Q5MYC0
A	892	LYS	-	expression tag	UNP Q5MYC0
A	893	GLY	-	expression tag	UNP Q5MYC0
A	894	GLY	-	expression tag	UNP Q5MYC0
A	895	GLY	-	expression tag	UNP Q5MYC0
A	896	SER	-	expression tag	UNP Q5MYC0
A	897	GLY	-	expression tag	UNP Q5MYC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	898	GLY	-	expression tag	UNP Q5MYC0
A	899	GLY	-	expression tag	UNP Q5MYC0
A	900	SER	-	expression tag	UNP Q5MYC0
A	901	GLY	-	expression tag	UNP Q5MYC0
A	902	GLY	-	expression tag	UNP Q5MYC0
A	903	GLY	-	expression tag	UNP Q5MYC0
A	904	SER	-	expression tag	UNP Q5MYC0
A	905	TRP	-	expression tag	UNP Q5MYC0
A	906	SER	-	expression tag	UNP Q5MYC0
A	907	HIS	-	expression tag	UNP Q5MYC0
A	908	PRO	-	expression tag	UNP Q5MYC0
A	909	GLN	-	expression tag	UNP Q5MYC0
A	910	PHE	-	expression tag	UNP Q5MYC0
A	911	GLU	-	expression tag	UNP Q5MYC0
A	912	LYS	-	expression tag	UNP Q5MYC0
B	608	GLY	-	linker	UNP Q5MYC0
B	609	GLY	-	linker	UNP Q5MYC0
B	610	SER	-	linker	UNP Q5MYC0
B	611	GLY	-	linker	UNP Q5MYC0
B	612	LEU	-	linker	UNP Q5MYC0
B	613	VAL	-	linker	UNP Q5MYC0
B	614	PRO	-	linker	UNP Q5MYC0
B	615	ARG	-	linker	UNP Q5MYC0
B	616	GLY	-	linker	UNP Q5MYC0
B	617	SER	-	linker	UNP Q5MYC0
B	618	GLY	-	linker	UNP Q5MYC0
B	619	GLY	-	linker	UNP Q5MYC0
B	620	GLY	-	linker	UNP Q5MYC0
B	621	SER	-	linker	UNP Q5MYC0
B	622	GLY	-	linker	UNP Q5MYC0
B	623	GLY	-	linker	UNP Q5MYC0
B	624	GLY	-	linker	UNP Q5MYC0
B	625	SER	-	linker	UNP Q5MYC0
B	626	TRP	-	linker	UNP Q5MYC0
B	627	SER	-	linker	UNP Q5MYC0
B	628	HIS	-	linker	UNP Q5MYC0
B	629	PRO	-	linker	UNP Q5MYC0
B	630	GLN	-	linker	UNP Q5MYC0
B	631	PHE	-	linker	UNP Q5MYC0
B	632	GLU	-	linker	UNP Q5MYC0
B	633	LYS	-	linker	UNP Q5MYC0
B	634	GLY	-	linker	UNP Q5MYC0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	635	GLY	-	linker	UNP Q5MYC0
B	636	GLY	-	linker	UNP Q5MYC0
B	637	THR	-	linker	UNP Q5MYC0
B	638	GLY	-	linker	UNP Q5MYC0
B	639	GLY	-	linker	UNP Q5MYC0
B	640	GLY	-	linker	UNP Q5MYC0
B	641	THR	-	linker	UNP Q5MYC0
B	642	LEU	-	linker	UNP Q5MYC0
B	643	VAL	-	linker	UNP Q5MYC0
B	644	PRO	-	linker	UNP Q5MYC0
B	645	ARG	-	linker	UNP Q5MYC0
B	646	GLY	-	linker	UNP Q5MYC0
B	647	SER	-	linker	UNP Q5MYC0
B	648	GLY	-	linker	UNP Q5MYC0
B	649	THR	-	linker	UNP Q5MYC0
B	650	GLY	-	linker	UNP Q5MYC0
B	651	GLY	-	linker	UNP Q5MYC0
B	1108	PRO	-	expression tag	UNP Q5MYC0
B	1109	PHE	-	expression tag	UNP Q5MYC0
B	1110	GLU	-	expression tag	UNP Q5MYC0
B	1111	ASP	-	expression tag	UNP Q5MYC0
B	1112	ASP	-	expression tag	UNP Q5MYC0
B	1113	ASP	-	expression tag	UNP Q5MYC0
B	1114	ASP	-	expression tag	UNP Q5MYC0
B	1115	LYS	-	expression tag	UNP Q5MYC0
B	1116	ALA	-	expression tag	UNP Q5MYC0
B	1117	GLY	-	expression tag	UNP Q5MYC0
B	1118	TRP	-	expression tag	UNP Q5MYC0
B	1119	SER	-	expression tag	UNP Q5MYC0
B	1120	HIS	-	expression tag	UNP Q5MYC0
B	1121	PRO	-	expression tag	UNP Q5MYC0
B	1122	GLN	-	expression tag	UNP Q5MYC0
B	1123	PHE	-	expression tag	UNP Q5MYC0
B	1124	GLU	-	expression tag	UNP Q5MYC0
B	1125	LYS	-	expression tag	UNP Q5MYC0
B	1126	GLY	-	expression tag	UNP Q5MYC0
B	1127	GLY	-	expression tag	UNP Q5MYC0
B	1128	GLY	-	expression tag	UNP Q5MYC0
B	1129	SER	-	expression tag	UNP Q5MYC0
B	1130	GLY	-	expression tag	UNP Q5MYC0
B	1131	GLY	-	expression tag	UNP Q5MYC0
B	1132	GLY	-	expression tag	UNP Q5MYC0

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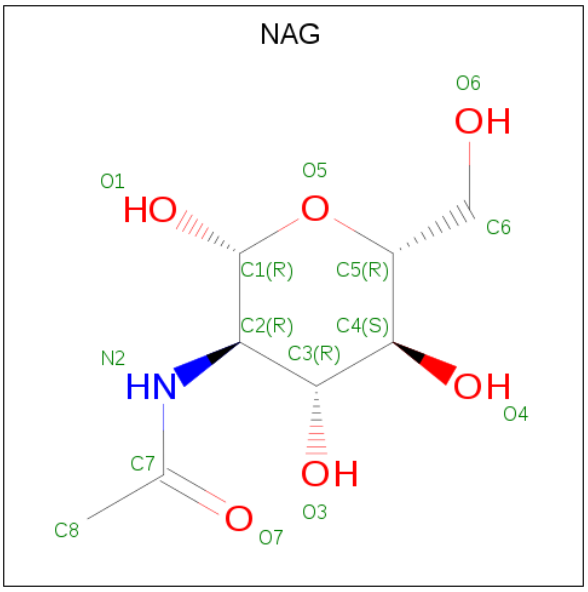
Chain	Residue	Modelled	Actual	Comment	Reference
B	1133	SER	-	expression tag	UNP Q5MYC0
B	1134	GLY	-	expression tag	UNP Q5MYC0
B	1135	GLY	-	expression tag	UNP Q5MYC0
B	1136	GLY	-	expression tag	UNP Q5MYC0
B	1137	SER	-	expression tag	UNP Q5MYC0
B	1138	TRP	-	expression tag	UNP Q5MYC0
B	1139	SER	-	expression tag	UNP Q5MYC0
B	1140	HIS	-	expression tag	UNP Q5MYC0
B	1141	PRO	-	expression tag	UNP Q5MYC0
B	1142	GLN	-	expression tag	UNP Q5MYC0
B	1143	PHE	-	expression tag	UNP Q5MYC0
B	1144	GLU	-	expression tag	UNP Q5MYC0
B	1145	LYS	-	expression tag	UNP Q5MYC0

- Molecule 2 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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	D	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: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is water.

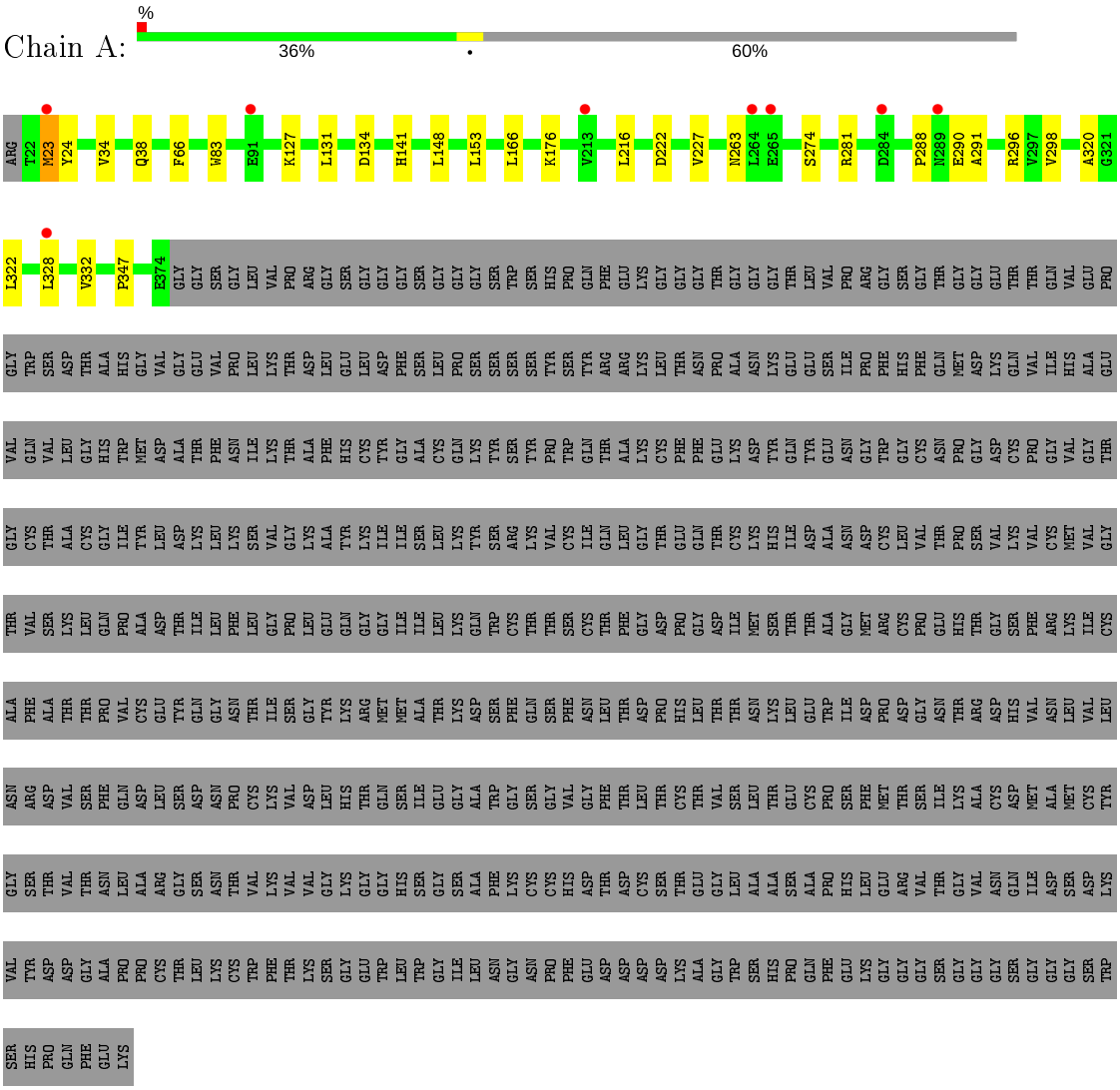
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	175	Total O 175 175	0	0
4	B	86	Total O 86 86	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

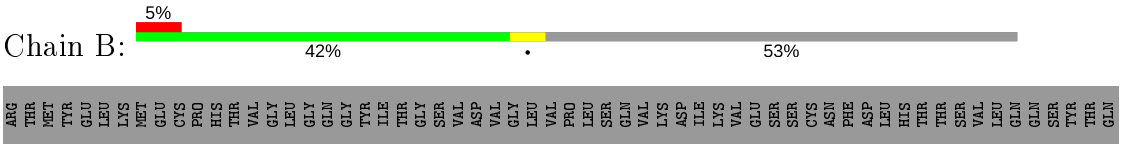
- Molecule 1: Envelope polyprotein,Envelope polyprotein

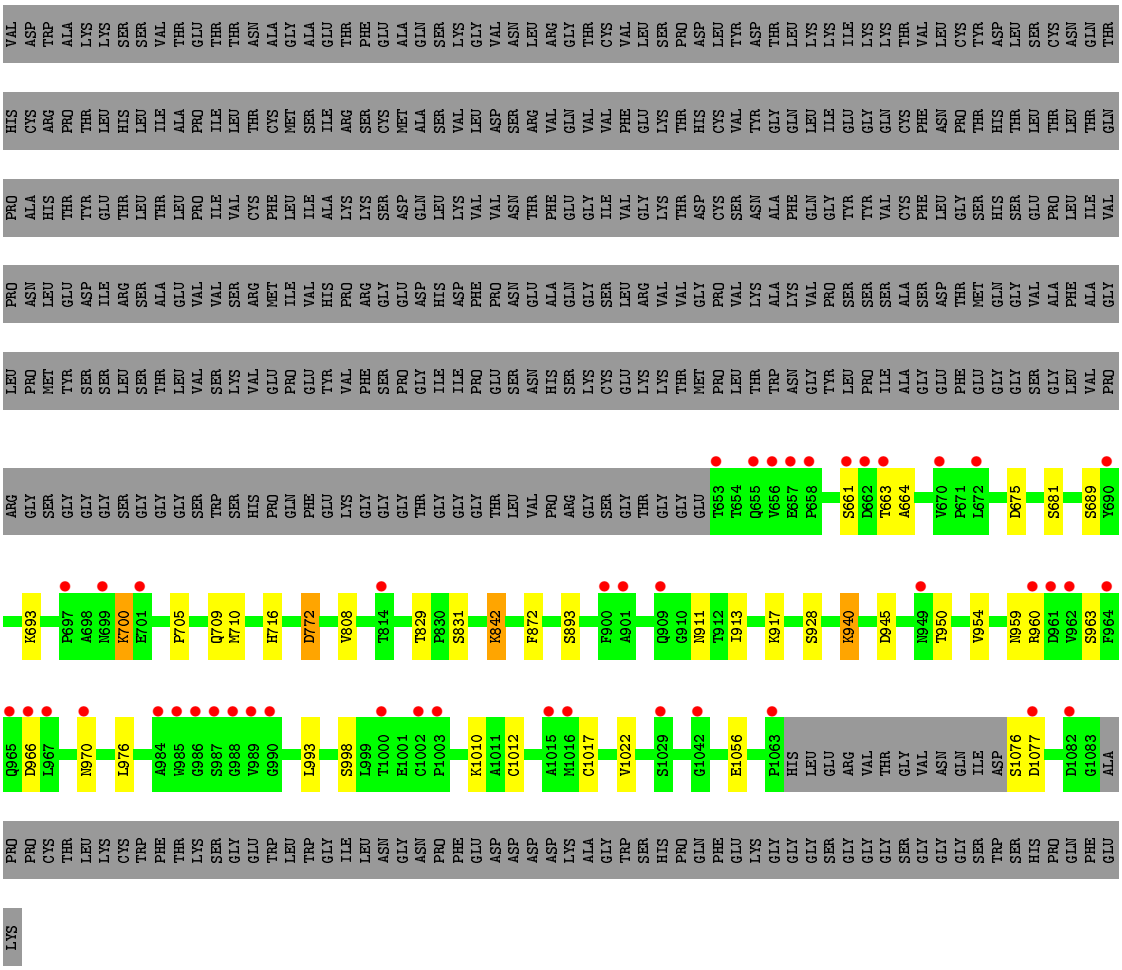
Chain A:



- Molecule 1: Envelope polyprotein,Envelope polyprotein

Chain B:





• 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

Chain C:

• 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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.33Å 65.01Å 144.76Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	35.14 – 2.20 35.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.14-2.20) 99.3 (35.14-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14rc3_3199	Depositor
R, R_{free}	0.194 , 0.226 0.195 , 0.226	Depositor DCC
R_{free} test set	2815 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6270	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.26	0/2759	0.48	0/3752
1	B	0.27	0/3268	0.49	0/4432
All	All	0.26	0/6027	0.48	0/8184

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

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	2701	0	2678	17	0
1	B	3194	0	3050	27	0
2	C	50	0	43	0	0
2	D	50	0	43	2	0
3	B	14	0	13	1	0
4	A	175	0	0	0	0
4	B	86	0	0	0	0
All	All	6270	0	5827	44	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.

The worst 5 of 44 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:B:829:THR:HG22	1:B:831:SER:H	1.41	0.86
1:B:689:SER:OG	1:B:709:GLN:NE2	2.23	0.72
1:A:38:GLN:OE1	1:A:127:LYS:NZ	2.29	0.65
1:A:290:GLU:N	1:A:290:GLU:OE2	2.27	0.62
1:B:716:HIS:HB3	1:B:940:LYS:NZ	2.15	0.60

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	350/891 (39%)	335 (96%)	15 (4%)	0	100	100
1	B	415/891 (47%)	392 (94%)	23 (6%)	0	100	100
All	All	765/1782 (43%)	727 (95%)	38 (5%)	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	314/757 (42%)	307 (98%)	7 (2%)	52	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	359/757 (47%)	349 (97%)	10 (3%)	43 56
All	All	673/1514 (44%)	656 (98%)	17 (2%)	47 60

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	661	SER
1	B	681	SER
1	B	940	LYS
1	A	296	ARG
1	B	976	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	709	GLN
1	B	816	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

8 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	C	1	1,2	14,14,15	0.29	0	17,19,21	0.80	0
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.55	0
2	BMA	C	3	2	11,11,12	0.57	0	15,15,17	1.02	1 (6%)
2	MAN	C	4	2	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.68	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	0.59	0
2	BMA	D	3	2	11,11,12	0.90	1 (9%)	15,15,17	0.90	1 (6%)
2	MAN	D	4	2	11,11,12	1.43	1 (9%)	15,15,17	1.52	3 (20%)

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	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	1/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	C1-C2	3.84	1.61	1.52
2	D	3	BMA	C1-C2	2.19	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	MAN	C1-O5-C5	3.76	117.29	112.19
2	C	4	MAN	C1-O5-C5	3.71	117.21	112.19
2	D	4	MAN	C1-C2-C3	3.33	113.76	109.67
2	D	4	MAN	O2-C2-C3	-2.35	105.43	110.14
2	D	3	BMA	O3-C3-C2	2.28	114.36	109.99

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	BMA	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6

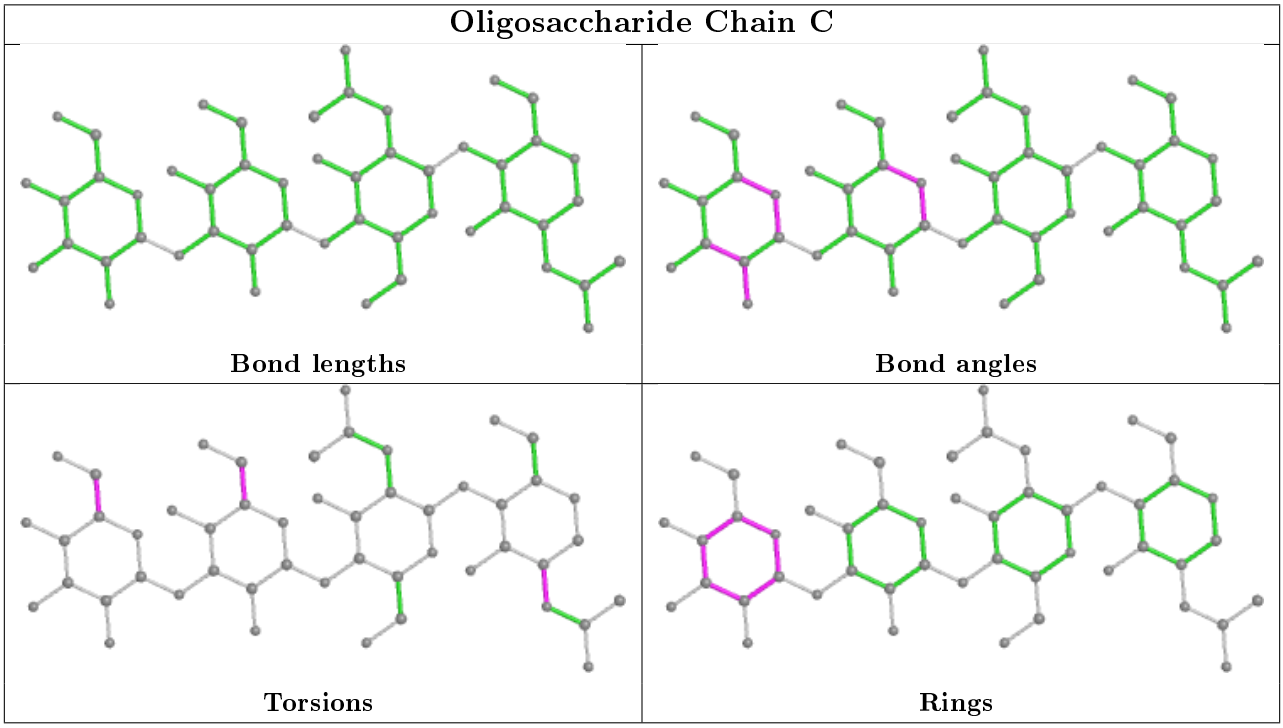
All (1) ring outliers are listed below:

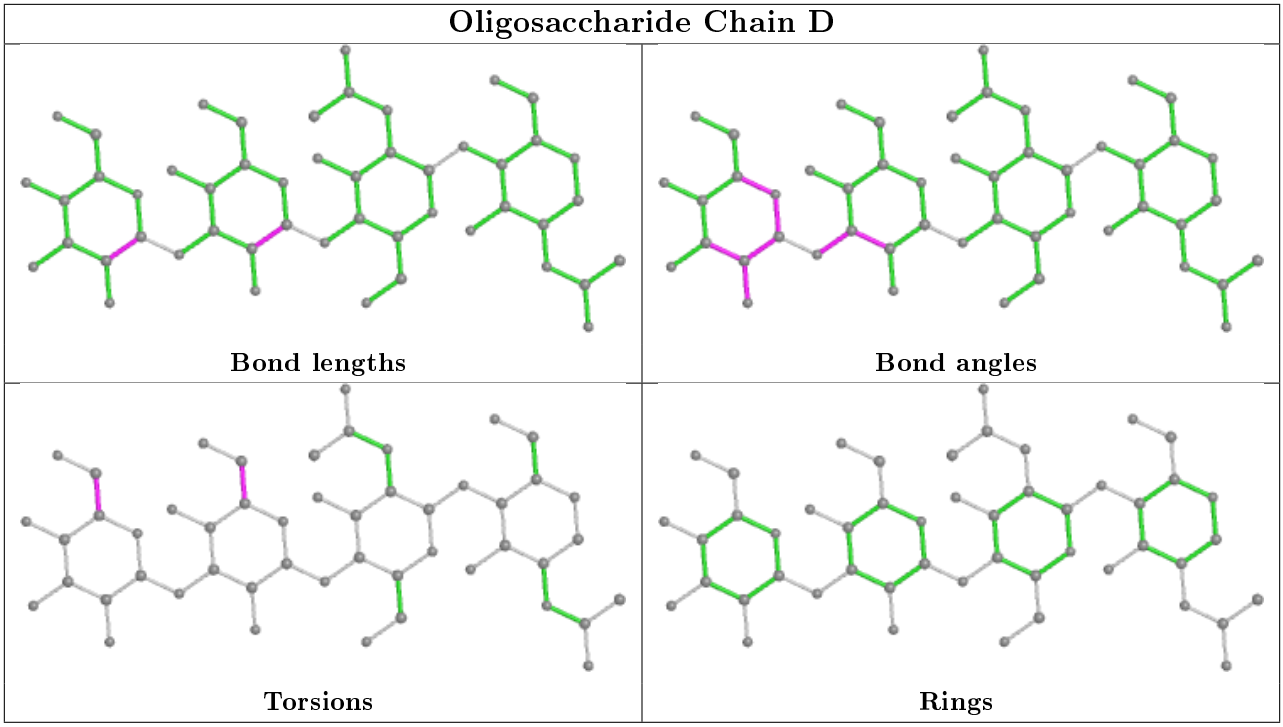
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	BMA	1	0
2	D	4	MAN	1	0
2	D	1	NAG	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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1201	1	14,14,15	0.63	1 (7%)	17,19,21	0.66	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1201	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	NAG	C1-C2	2.05	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1201	NAG	C1-O5-C5	2.05	114.98	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1201	NAG	O5-C5-C6-O6
3	B	1201	NAG	C4-C5-C6-O6

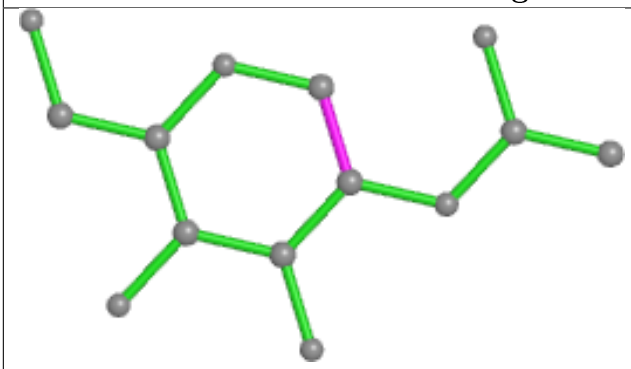
There are no ring outliers.

1 monomer is involved in 1 short contact:

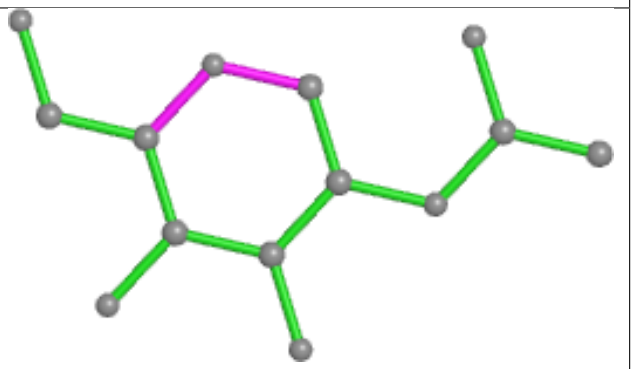
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1201	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

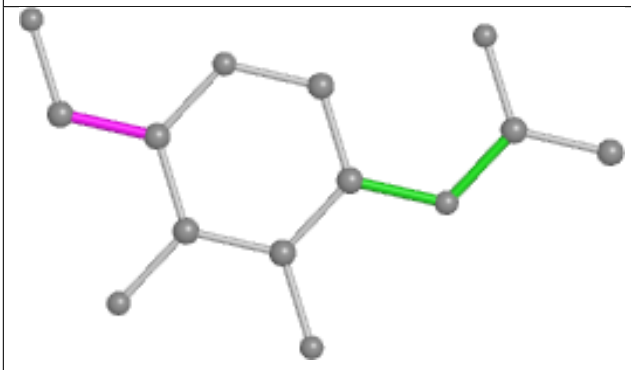
Ligand NAG B 1201



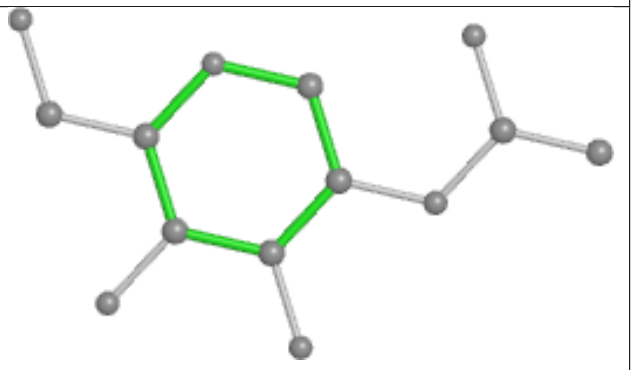
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	352/891 (39%)	0.20	8 (2%) 60 58	33, 47, 76, 126	0
1	B	419/891 (47%)	0.52	44 (10%) 6 5	31, 59, 106, 123	0
All	All	771/1782 (43%)	0.38	52 (6%) 17 16	31, 53, 99, 126	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	653	THR	8.8
1	B	989	VAL	6.8
1	B	986	GLY	6.4
1	B	656	VAL	5.3
1	B	987	SER	4.7

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.33	0.51	117,120,122,122	0
2	MAN	D	4	11/12	0.49	0.47	115,118,121,122	0
2	MAN	C	4	11/12	0.71	0.32	59,85,92,94	0
2	NAG	D	2	14/15	0.79	0.32	88,100,110,112	0
2	BMA	C	3	11/12	0.82	0.22	80,85,90,93	0

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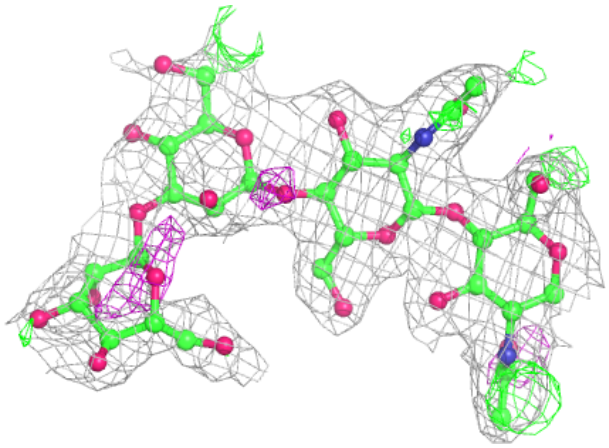
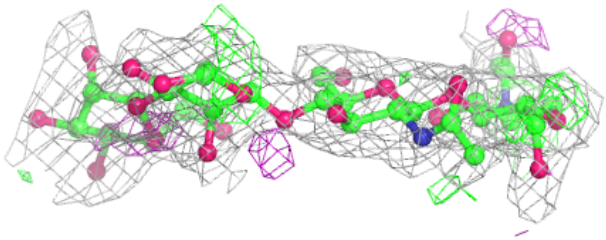
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	1	14/15	0.86	0.16	51,67,78,86	0
2	NAG	C	2	14/15	0.90	0.13	45,54,61,73	0
2	NAG	C	1	14/15	0.91	0.15	31,41,56,71	0

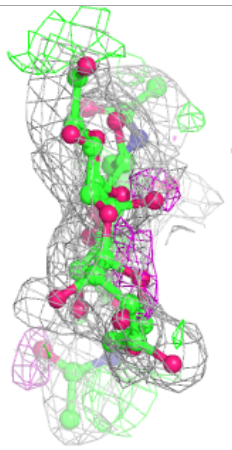
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

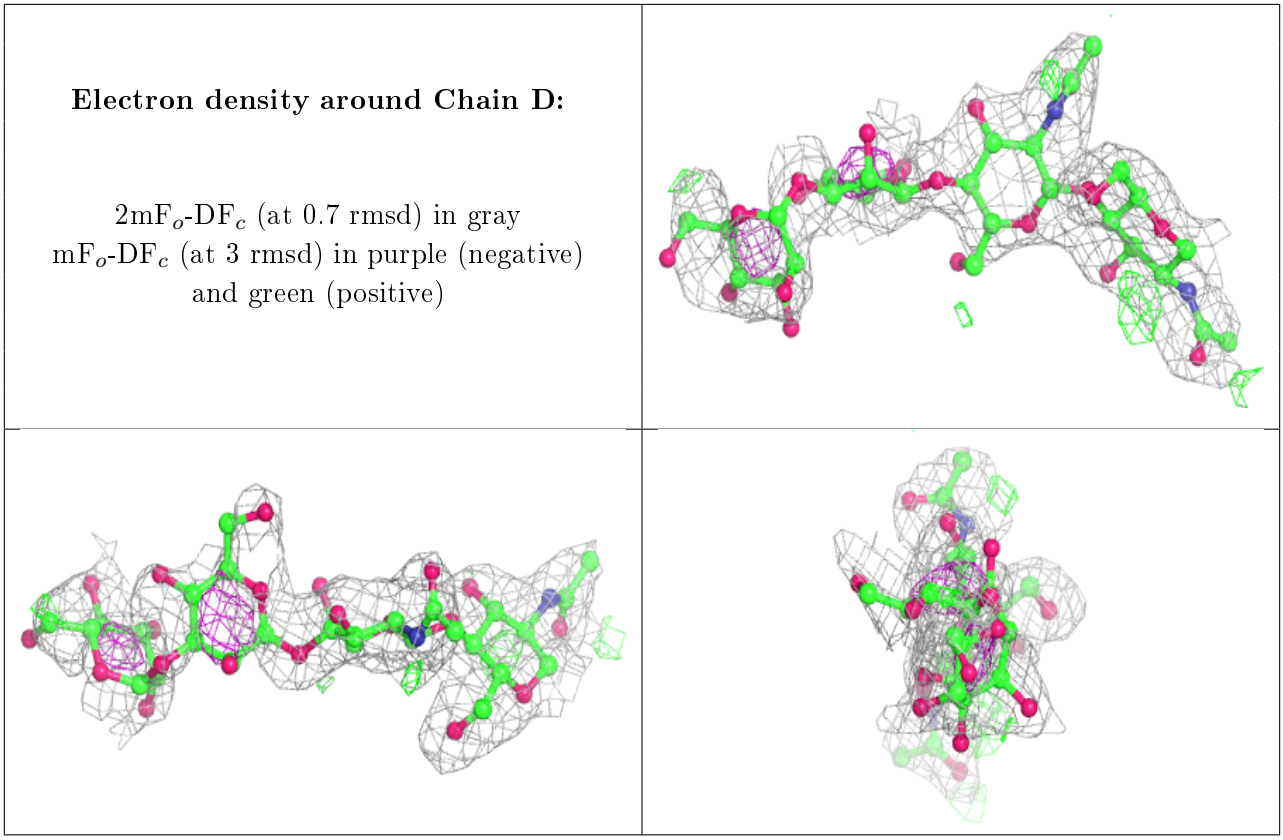






Electron density around Chain D:

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



6.4 Ligands

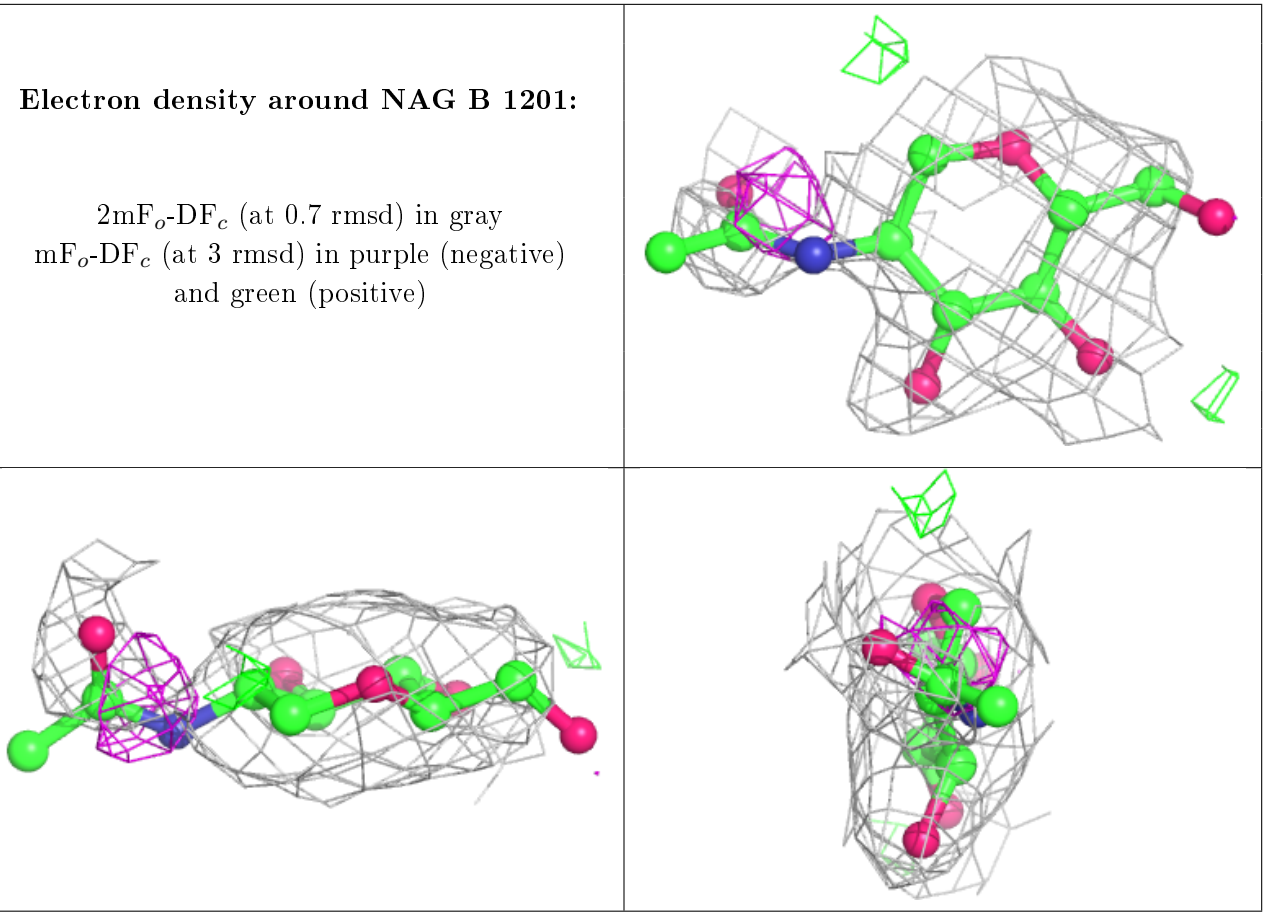
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	1201	14/15	0.82	0.36	66,90,96,100	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG B 1201:

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



6.5 Other polymers

There are no such residues in this entry.