WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 08:12 am GMT

PDB ID	:	6EGT
Title	:	Structure of RVFV envelope protein Gc in postfusion conformation in complex with MES
Authors	:	Guardado-Calvo, P.; Rey, F.A.
Deposited on	:	2017-09-12
Resolution	:	2.50 Å(reported)

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

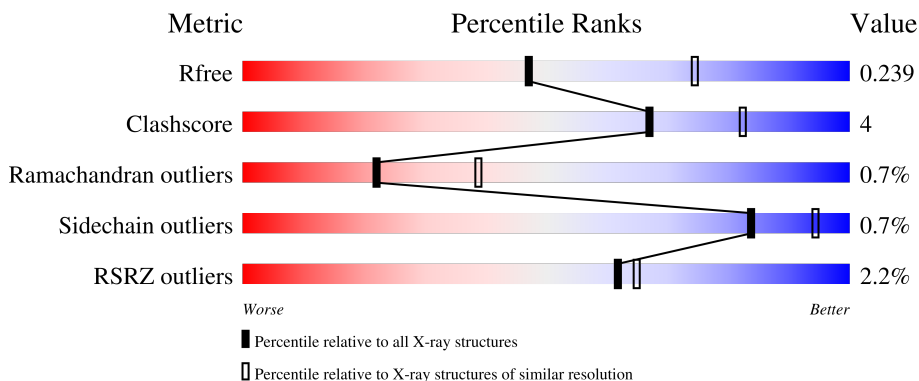|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		4
Ramachandran outliers		0.7%
Sidechain outliers		0.7%
RSRZ outliers		2.2%

Worse　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	531	2% — 76% · 7% · 16%
1	B	531	3% — 76% · 7% · 16%
1	C	531	% — 76% · 7% · 16%
2	D	2	50% · 50%

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
3	NAG	C	1303	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10583 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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	1	0
			3387	2097	585	676	29			
1	B	445	Total	C	N	O	S	0	0	0
			3378	2092	583	674	29			
1	C	444	Total	C	N	O	S	0	0	0
			3371	2087	582	673	29			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	821	HIS	TRP	engineered mutation	UNP A2T087
A	1159	ASP	-	expression tag	UNP A2T087
A	1160	PRO	-	expression tag	UNP A2T087
A	1161	THR	-	expression tag	UNP A2T087
A	1162	GLY	-	expression tag	UNP A2T087
A	1163	ASP	-	expression tag	UNP A2T087
A	1164	TYR	-	expression tag	UNP A2T087
A	1165	LYS	-	expression tag	UNP A2T087
A	1166	ASP	-	expression tag	UNP A2T087
A	1167	ASP	-	expression tag	UNP A2T087
A	1168	ASP	-	expression tag	UNP A2T087
A	1169	ASP	-	expression tag	UNP A2T087
A	1170	ALA	-	expression tag	UNP A2T087
A	1171	GLY	-	expression tag	UNP A2T087
A	1172	PRO	-	expression tag	UNP A2T087
A	1173	GLY	-	expression tag	UNP A2T087
A	1174	TRP	-	expression tag	UNP A2T087
A	1175	SER	-	expression tag	UNP A2T087
A	1176	HIS	-	expression tag	UNP A2T087
A	1177	PRO	-	expression tag	UNP A2T087
A	1178	GLN	-	expression tag	UNP A2T087
A	1179	PHE	-	expression tag	UNP A2T087
A	1180	GLU	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1181	LYS	-	expression tag	UNP A2T087
A	1182	GLY	-	expression tag	UNP A2T087
A	1183	GLY	-	expression tag	UNP A2T087
A	1184	GLY	-	expression tag	UNP A2T087
A	1185	SER	-	expression tag	UNP A2T087
A	1186	GLY	-	expression tag	UNP A2T087
A	1187	GLY	-	expression tag	UNP A2T087
A	1188	GLY	-	expression tag	UNP A2T087
A	1189	SER	-	expression tag	UNP A2T087
A	1190	GLY	-	expression tag	UNP A2T087
A	1191	GLY	-	expression tag	UNP A2T087
A	1192	GLY	-	expression tag	UNP A2T087
A	1193	SER	-	expression tag	UNP A2T087
A	1194	TRP	-	expression tag	UNP A2T087
A	1195	SER	-	expression tag	UNP A2T087
A	1196	HIS	-	expression tag	UNP A2T087
A	1197	PRO	-	expression tag	UNP A2T087
A	1198	GLN	-	expression tag	UNP A2T087
A	1199	PHE	-	expression tag	UNP A2T087
A	1200	GLU	-	expression tag	UNP A2T087
A	1201	LYS	-	expression tag	UNP A2T087
A	1202	GLY	-	expression tag	UNP A2T087
A	1203	GLY	-	expression tag	UNP A2T087
A	1204	GLY	-	expression tag	UNP A2T087
A	1205	SER	-	expression tag	UNP A2T087
A	1206	GLY	-	expression tag	UNP A2T087
A	1207	GLY	-	expression tag	UNP A2T087
A	1208	GLY	-	expression tag	UNP A2T087
A	1209	SER	-	expression tag	UNP A2T087
A	1210	GLY	-	expression tag	UNP A2T087
A	1211	GLY	-	expression tag	UNP A2T087
A	1212	GLY	-	expression tag	UNP A2T087
A	1213	SER	-	expression tag	UNP A2T087
A	1214	TRP	-	expression tag	UNP A2T087
A	1215	SER	-	expression tag	UNP A2T087
A	1216	HIS	-	expression tag	UNP A2T087
A	1217	PRO	-	expression tag	UNP A2T087
A	1218	GLN	-	expression tag	UNP A2T087
A	1219	PHE	-	expression tag	UNP A2T087
A	1220	GLU	-	expression tag	UNP A2T087
A	1221	LYS	-	expression tag	UNP A2T087
B	821	HIS	TRP	engineered mutation	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1159	ASP	-	expression tag	UNP A2T087
B	1160	PRO	-	expression tag	UNP A2T087
B	1161	THR	-	expression tag	UNP A2T087
B	1162	GLY	-	expression tag	UNP A2T087
B	1163	ASP	-	expression tag	UNP A2T087
B	1164	TYR	-	expression tag	UNP A2T087
B	1165	LYS	-	expression tag	UNP A2T087
B	1166	ASP	-	expression tag	UNP A2T087
B	1167	ASP	-	expression tag	UNP A2T087
B	1168	ASP	-	expression tag	UNP A2T087
B	1169	ASP	-	expression tag	UNP A2T087
B	1170	ALA	-	expression tag	UNP A2T087
B	1171	GLY	-	expression tag	UNP A2T087
B	1172	PRO	-	expression tag	UNP A2T087
B	1173	GLY	-	expression tag	UNP A2T087
B	1174	TRP	-	expression tag	UNP A2T087
B	1175	SER	-	expression tag	UNP A2T087
B	1176	HIS	-	expression tag	UNP A2T087
B	1177	PRO	-	expression tag	UNP A2T087
B	1178	GLN	-	expression tag	UNP A2T087
B	1179	PHE	-	expression tag	UNP A2T087
B	1180	GLU	-	expression tag	UNP A2T087
B	1181	LYS	-	expression tag	UNP A2T087
B	1182	GLY	-	expression tag	UNP A2T087
B	1183	GLY	-	expression tag	UNP A2T087
B	1184	GLY	-	expression tag	UNP A2T087
B	1185	SER	-	expression tag	UNP A2T087
B	1186	GLY	-	expression tag	UNP A2T087
B	1187	GLY	-	expression tag	UNP A2T087
B	1188	GLY	-	expression tag	UNP A2T087
B	1189	SER	-	expression tag	UNP A2T087
B	1190	GLY	-	expression tag	UNP A2T087
B	1191	GLY	-	expression tag	UNP A2T087
B	1192	GLY	-	expression tag	UNP A2T087
B	1193	SER	-	expression tag	UNP A2T087
B	1194	TRP	-	expression tag	UNP A2T087
B	1195	SER	-	expression tag	UNP A2T087
B	1196	HIS	-	expression tag	UNP A2T087
B	1197	PRO	-	expression tag	UNP A2T087
B	1198	GLN	-	expression tag	UNP A2T087
B	1199	PHE	-	expression tag	UNP A2T087
B	1200	GLU	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	LYS	-	expression tag	UNP A2T087
B	1202	GLY	-	expression tag	UNP A2T087
B	1203	GLY	-	expression tag	UNP A2T087
B	1204	GLY	-	expression tag	UNP A2T087
B	1205	SER	-	expression tag	UNP A2T087
B	1206	GLY	-	expression tag	UNP A2T087
B	1207	GLY	-	expression tag	UNP A2T087
B	1208	GLY	-	expression tag	UNP A2T087
B	1209	SER	-	expression tag	UNP A2T087
B	1210	GLY	-	expression tag	UNP A2T087
B	1211	GLY	-	expression tag	UNP A2T087
B	1212	GLY	-	expression tag	UNP A2T087
B	1213	SER	-	expression tag	UNP A2T087
B	1214	TRP	-	expression tag	UNP A2T087
B	1215	SER	-	expression tag	UNP A2T087
B	1216	HIS	-	expression tag	UNP A2T087
B	1217	PRO	-	expression tag	UNP A2T087
B	1218	GLN	-	expression tag	UNP A2T087
B	1219	PHE	-	expression tag	UNP A2T087
B	1220	GLU	-	expression tag	UNP A2T087
B	1221	LYS	-	expression tag	UNP A2T087
C	821	HIS	TRP	engineered mutation	UNP A2T087
C	1159	ASP	-	expression tag	UNP A2T087
C	1160	PRO	-	expression tag	UNP A2T087
C	1161	THR	-	expression tag	UNP A2T087
C	1162	GLY	-	expression tag	UNP A2T087
C	1163	ASP	-	expression tag	UNP A2T087
C	1164	TYR	-	expression tag	UNP A2T087
C	1165	LYS	-	expression tag	UNP A2T087
C	1166	ASP	-	expression tag	UNP A2T087
C	1167	ASP	-	expression tag	UNP A2T087
C	1168	ASP	-	expression tag	UNP A2T087
C	1169	ASP	-	expression tag	UNP A2T087
C	1170	ALA	-	expression tag	UNP A2T087
C	1171	GLY	-	expression tag	UNP A2T087
C	1172	PRO	-	expression tag	UNP A2T087
C	1173	GLY	-	expression tag	UNP A2T087
C	1174	TRP	-	expression tag	UNP A2T087
C	1175	SER	-	expression tag	UNP A2T087
C	1176	HIS	-	expression tag	UNP A2T087
C	1177	PRO	-	expression tag	UNP A2T087
C	1178	GLN	-	expression tag	UNP A2T087

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	PHE	-	expression tag	UNP A2T087
C	1180	GLU	-	expression tag	UNP A2T087
C	1181	LYS	-	expression tag	UNP A2T087
C	1182	GLY	-	expression tag	UNP A2T087
C	1183	GLY	-	expression tag	UNP A2T087
C	1184	GLY	-	expression tag	UNP A2T087
C	1185	SER	-	expression tag	UNP A2T087
C	1186	GLY	-	expression tag	UNP A2T087
C	1187	GLY	-	expression tag	UNP A2T087
C	1188	GLY	-	expression tag	UNP A2T087
C	1189	SER	-	expression tag	UNP A2T087
C	1190	GLY	-	expression tag	UNP A2T087
C	1191	GLY	-	expression tag	UNP A2T087
C	1192	GLY	-	expression tag	UNP A2T087
C	1193	SER	-	expression tag	UNP A2T087
C	1194	TRP	-	expression tag	UNP A2T087
C	1195	SER	-	expression tag	UNP A2T087
C	1196	HIS	-	expression tag	UNP A2T087
C	1197	PRO	-	expression tag	UNP A2T087
C	1198	GLN	-	expression tag	UNP A2T087
C	1199	PHE	-	expression tag	UNP A2T087
C	1200	GLU	-	expression tag	UNP A2T087
C	1201	LYS	-	expression tag	UNP A2T087
C	1202	GLY	-	expression tag	UNP A2T087
C	1203	GLY	-	expression tag	UNP A2T087
C	1204	GLY	-	expression tag	UNP A2T087
C	1205	SER	-	expression tag	UNP A2T087
C	1206	GLY	-	expression tag	UNP A2T087
C	1207	GLY	-	expression tag	UNP A2T087
C	1208	GLY	-	expression tag	UNP A2T087
C	1209	SER	-	expression tag	UNP A2T087
C	1210	GLY	-	expression tag	UNP A2T087
C	1211	GLY	-	expression tag	UNP A2T087
C	1212	GLY	-	expression tag	UNP A2T087
C	1213	SER	-	expression tag	UNP A2T087
C	1214	TRP	-	expression tag	UNP A2T087
C	1215	SER	-	expression tag	UNP A2T087
C	1216	HIS	-	expression tag	UNP A2T087
C	1217	PRO	-	expression tag	UNP A2T087
C	1218	GLN	-	expression tag	UNP A2T087
C	1219	PHE	-	expression tag	UNP A2T087
C	1220	GLU	-	expression tag	UNP A2T087

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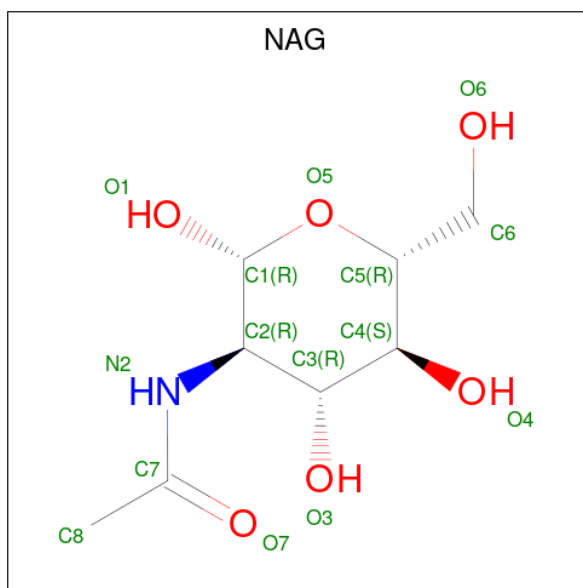| Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	LYS	-	expression tag	UNP A2T087

- Molecule 2 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

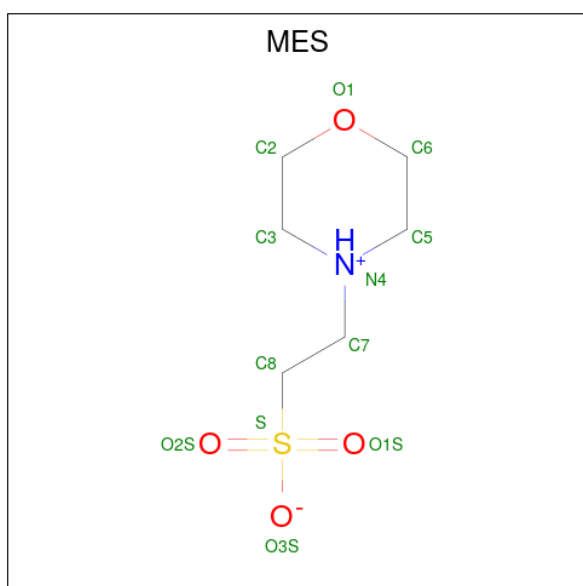- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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					

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

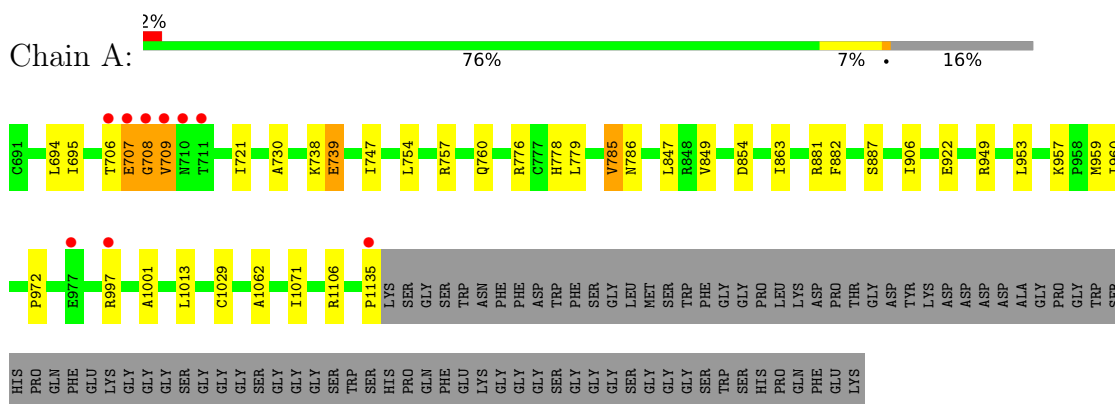| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total C N O S					0	0
			12 6 1 4 1						
4	C	1	Total C N O S					0	0
			12 6 1 4 1						

- Molecule 5 is water.

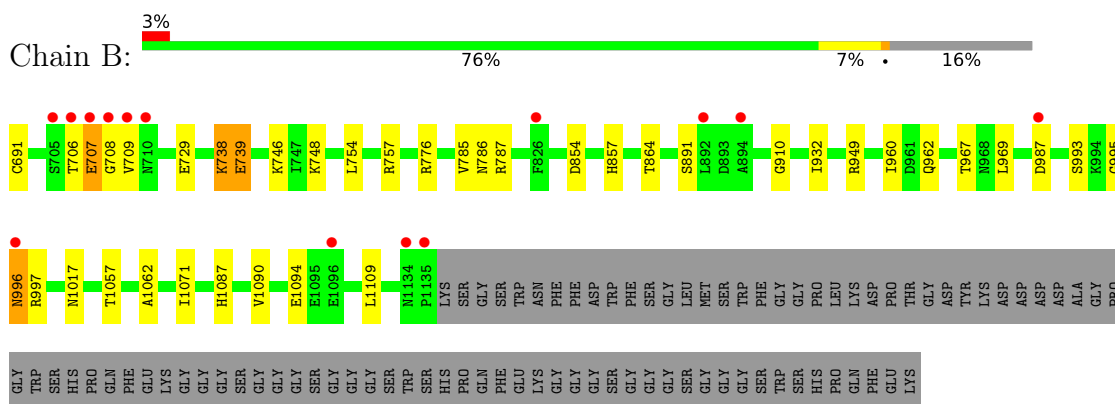| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total O		0	0
			105 105			
5	B	78	Total O		0	0
			78 78			
5	C	104	Total O		0	0
			104 104			

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.
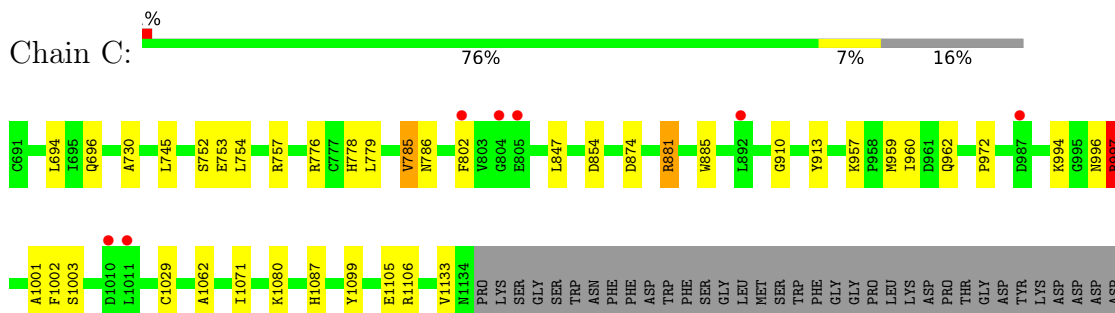
• Molecule 1: Glycoprotein

• Molecule 1: Glycoprotein

• Molecule 1: Glycoprotein

ALA GLY PRO GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 2: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

50%   50%

NAG1 FUL2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.31Å 102.03Å 198.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.50 38.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.50-2.50) 99.1 (38.44-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.3_1471	Depositor
R, R_{free}	0.196 , 0.235 0.201 , 0.239	Depositor DCC
R_{free} test set	2037 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.902	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10583	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MES, FUL, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.29	0/3448	0.50	1/4661 (0.0%)
1	B	0.28	0/3439	0.47	2/4649 (0.0%)
1	C	0.30	0/3431	0.49	1/4637 (0.0%)
All	All	0.29	0/10318	0.49	4/13947 (0.0%)

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
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	708	GLY	N-CA-C	-8.30	92.36	113.10
1	C	997	ARG	N-CA-C	5.36	125.46	111.00
1	B	708	GLY	N-CA-C	-5.24	100.01	113.10
1	B	739	GLU	OE1-CD-OE2	-5.16	117.11	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	707	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	709	VAL	Peptide
1	B	707	GLU	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	3387	0	3248	30	0
1	B	3378	0	3241	24	0
1	C	3371	0	3234	27	0
2	D	24	0	22	0	0
3	A	28	0	26	0	0
3	B	42	0	39	0	0
3	C	42	0	39	0	0
4	B	12	0	12	1	0
4	C	12	0	12	1	0
5	A	105	0	0	0	0
5	B	78	0	0	0	0
5	C	104	0	0	1	0
All	All	10583	0	9873	78	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 (78) 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:738:LYS:HE2	1:B:1017:ASN:HB3	1.37	1.05
1:A:707:GLU:HG2	1:A:708:GLY:H	1.42	0.84
1:C:913:TYR:OH	1:C:997:ARG:HG2	1.78	0.83
1:C:874:ASP:O	1:C:881:ARG:NH1	2.22	0.73
1:C:997:ARG:NH1	5:C:1401:HOH:O	2.21	0.73
1:B:739:GLU:OE1	1:B:739:GLU:N	2.21	0.72
1:A:786:ASN:ND2	1:B:962:GLN:OE1	2.23	0.70
1:A:1029:CYS:O	1:A:1106:ARG:NH2	2.28	0.66
1:A:747:ILE:HD13	1:A:863:ILE:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:VAL:HG13	1:C:786:ASN:H	1.60	0.65
1:B:706:THR:HG22	1:B:707:GLU:HG3	1.78	0.64
1:B:786:ASN:ND2	1:C:962:GLN:OE1	2.32	0.63
1:B:757:ARG:HB2	1:B:854:ASP:HB2	1.81	0.63
1:A:881:ARG:NH1	1:A:882:PHE:O	2.32	0.63
1:B:1094:GLU:HG2	1:B:1109:LEU:HD11	1.81	0.61
1:A:738:LYS:HG3	1:A:739:GLU:HG2	1.82	0.60
1:C:910:GLY:H	1:C:997:ARG:HH12	1.49	0.60
1:A:847:LEU:HD12	1:A:972:PRO:HB2	1.83	0.59
1:B:746:LYS:HB2	1:B:864:THR:HB	1.83	0.59
1:C:847:LEU:HD12	1:C:972:PRO:HB2	1.85	0.59
1:C:757:ARG:HB2	1:C:854:ASP:HB2	1.85	0.58
1:C:996:ASN:OD1	1:C:997:ARG:HB2	2.03	0.58
1:A:997:ARG:HH11	1:A:997:ARG:HG3	1.69	0.57
1:A:707:GLU:HG2	1:A:708:GLY:N	2.16	0.55
1:B:691:CYS:N	1:B:1057:THR:O	2.42	0.53
1:A:754:LEU:HB2	1:A:1001:ALA:HB3	1.91	0.52
1:A:949:ARG:HB2	1:A:953:LEU:HD12	1.93	0.51
1:C:957:LYS:HE3	1:C:959:MET:HE3	1.92	0.51
1:B:891:SER:HB2	1:C:696:GLN:HE21	1.76	0.51
1:A:957:LYS:HE3	1:A:959:MET:HE3	1.93	0.51
1:C:694:LEU:HD12	1:C:730:ALA:HB2	1.93	0.50
1:C:752:SER:HB3	1:C:1003:SER:HB2	1.94	0.50
1:A:882:PHE:CD1	1:A:887:SER:HB3	2.47	0.50
1:C:1062:ALA:HB3	1:C:1071:ILE:HB	1.93	0.49
1:B:993:SER:HB2	1:B:996:ASN:HB3	1.93	0.49
1:C:802:PHE:CE2	1:C:1133:VAL:HG11	2.48	0.49
1:B:1062:ALA:HB3	1:B:1071:ILE:HB	1.95	0.49
1:A:709:VAL:HG12	1:A:709:VAL:O	2.14	0.48
1:B:738:LYS:HE3	1:B:739:GLU:OE1	2.15	0.47
1:A:785:VAL:HG23	1:A:786:ASN:H	1.78	0.47
1:C:996:ASN:OD1	1:C:997:ARG:N	2.48	0.47
1:A:776:ARG:HH21	1:A:1135:PRO:HA	1.80	0.47
1:B:854:ASP:OD2	1:C:1087:HIS:ND1	2.44	0.46
1:C:745:LEU:HD21	1:C:885:TRP:CE2	2.50	0.46
1:B:738:LYS:CE	1:B:1017:ASN:HB3	2.27	0.45
1:B:776:ARG:HD3	1:B:776:ARG:HA	1.76	0.45
1:B:787:ARG:HA	1:B:787:ARG:HD2	1.84	0.45
1:C:754:LEU:HB2	1:C:1001:ALA:HB3	2.00	0.44
1:A:721:ILE:HD13	1:A:1013:LEU:HD11	1.99	0.44
1:A:738:LYS:HG3	1:A:739:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ARG:HB2	1:A:854:ASP:HB2	2.00	0.43
1:A:776:ARG:HD3	1:A:776:ARG:HA	1.64	0.43
1:B:932:ILE:HG12	1:B:949:ARG:HB3	2.00	0.43
1:A:760:GLN:OE1	1:A:922:GLU:HG3	2.19	0.43
1:C:778:HIS:O	1:C:779:LEU:HB2	2.19	0.43
4:C:1304:MES:H81	4:C:1304:MES:H31	1.85	0.43
1:B:754:LEU:HD23	1:B:857:HIS:HA	2.01	0.42
1:A:849:VAL:HG22	1:A:906:ILE:HG12	2.00	0.42
1:B:910:GLY:H	1:B:997:ARG:HH22	1.66	0.42
1:B:967:THR:HB	1:B:969:LEU:HG	2.01	0.42
1:B:738:LYS:H	1:B:738:LYS:HG3	1.45	0.42
1:C:913:TYR:CZ	1:C:997:ARG:HG2	2.52	0.42
1:C:1029:CYS:O	1:C:1106:ARG:NH2	2.53	0.42
1:A:997:ARG:HG3	1:A:997:ARG:NH1	2.33	0.42
1:A:1062:ALA:HB3	1:A:1071:ILE:HB	2.00	0.42
1:A:854:ASP:OD2	1:B:1087:HIS:ND1	2.52	0.42
4:B:1304:MES:H82	4:B:1304:MES:H31	1.63	0.42
1:A:695:ILE:HA	1:A:721:ILE:HG22	2.02	0.41
1:B:729:GLU:HG3	1:B:748:LYS:HB2	2.01	0.41
1:A:778:HIS:O	1:A:779:LEU:HB2	2.20	0.41
1:C:994:LYS:HE2	1:C:994:LYS:HB3	1.79	0.41
1:A:707:GLU:CG	1:A:708:GLY:N	2.84	0.41
1:C:753:GLU:HG2	1:C:1002:PHE:CD1	2.56	0.41
1:C:802:PHE:HE2	1:C:1133:VAL:HG11	1.85	0.41
1:A:738:LYS:HG3	1:A:739:GLU:N	2.36	0.40
1:A:694:LEU:HD12	1:A:730:ALA:HB2	2.03	0.40
1:C:1099:TYR:O	1:C:1105:GLU:HA	2.21	0.40
1:C:776:ARG:HA	1:C:776:ARG:HD3	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/531 (84%)	432 (97%)	10 (2%)	2 (0%)	29	48
1	B	443/531 (83%)	419 (95%)	19 (4%)	5 (1%)	14	26
1	C	442/531 (83%)	431 (98%)	9 (2%)	2 (0%)	29	48
All	All	1329/1593 (83%)	1282 (96%)	38 (3%)	9 (1%)	22	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	709	VAL
1	C	785	VAL
1	A	785	VAL
1	A	960	ILE
1	B	785	VAL
1	B	960	ILE
1	C	960	ILE
1	B	996	ASN
1	B	995	GLY

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	384/443 (87%)	382 (100%)	2 (0%)	88	96
1	B	383/443 (86%)	380 (99%)	3 (1%)	81	93
1	C	382/443 (86%)	379 (99%)	3 (1%)	81	93
All	All	1149/1329 (86%)	1141 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	706	THR
1	A	739	GLU
1	B	738	LYS
1	B	987	ASP

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Mol	Chain	Res	Type
1	B	1090	VAL
1	C	881	ARG
1	C	997	ARG
1	C	1080	LYS

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

Mol	Chain	Res	Type
1	B	1134	ASN
1	C	696	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 ⓘ

2 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	D	1	1,2	14,14,15	0.26	0	17,19,21	0.45	0
2	FUL	D	2	2	10,10,11	0.81	0	14,14,16	1.13	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	FUL	D	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

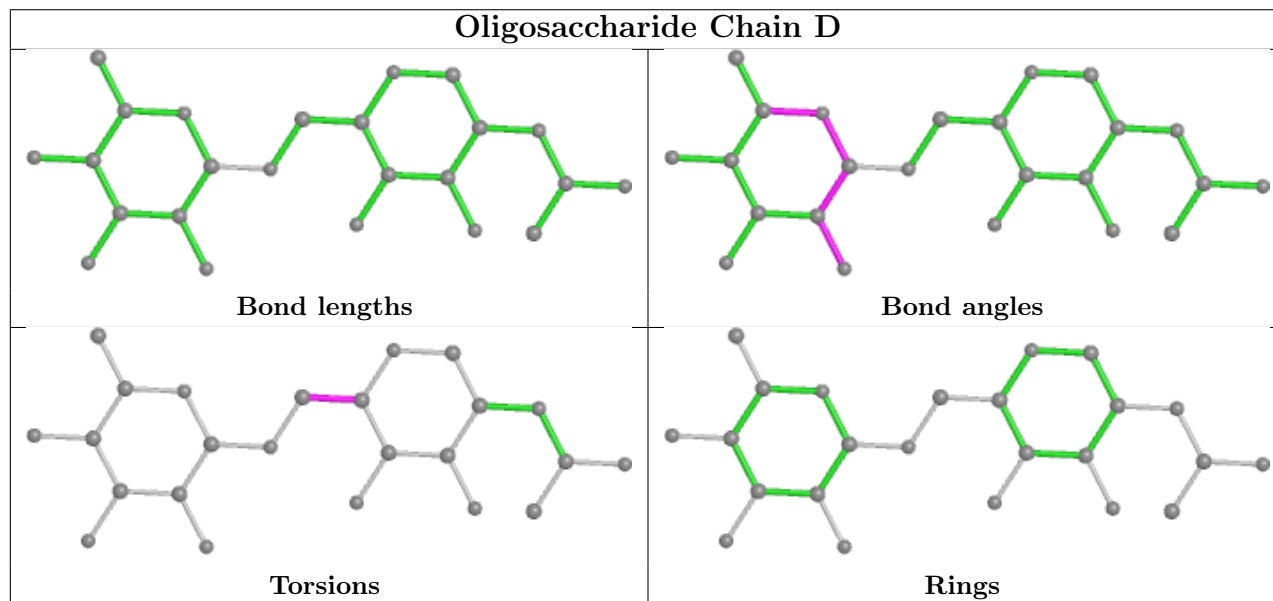| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	FUL	C1-O5-C5	2.16	117.66	112.78
2	D	2	FUL	O2-C2-C1	2.13	113.50	109.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.45	0
4	MES	B	1304	-	12,12,12	2.33	1 (8%)	14,16,16	2.37	7 (50%)
3	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	C	1303	1	14,14,15	0.36	0	17,19,21	0.42	0
3	NAG	B	1301	1	14,14,15	0.33	0	17,19,21	0.77	0
3	NAG	C	1302	1	14,14,15	0.51	0	17,19,21	0.48	0
4	MES	C	1304	-	12,12,12	2.28	1 (8%)	14,16,16	2.16	6 (42%)
3	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.59	0
3	NAG	A	1302	1	14,14,15	0.40	0	17,19,21	0.45	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	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	MES	B	1304	-	-	5/6/14/14	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	MES	C	1304	-	-	4/6/14/14	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1304	MES	C8-S	-7.77	1.66	1.77
4	C	1304	MES	C8-S	-7.64	1.66	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1304	MES	C5-N4-C3	5.08	120.27	108.83
4	C	1304	MES	C5-N4-C3	4.40	118.74	108.83
4	C	1304	MES	C7-N4-C3	3.22	119.47	111.23
4	B	1304	MES	C7-N4-C5	3.13	119.23	111.23
4	B	1304	MES	C7-N4-C3	2.93	118.72	111.23
4	B	1304	MES	C2-C3-N4	-2.88	105.73	110.10
4	C	1304	MES	C6-C5-N4	-2.77	105.90	110.10
4	C	1304	MES	O3S-S-C8	2.67	110.08	105.77
4	B	1304	MES	C6-C5-N4	-2.63	106.12	110.10
4	B	1304	MES	O1S-S-C8	2.41	109.82	106.92
4	C	1304	MES	C7-N4-C5	2.34	117.23	111.23
4	C	1304	MES	O1S-S-C8	2.19	109.55	106.92
4	B	1304	MES	O3S-S-C8	2.10	109.16	105.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1304	MES	C8-C7-N4-C5
4	B	1304	MES	C7-C8-S-O1S
4	C	1304	MES	C8-C7-N4-C3
4	C	1304	MES	C7-C8-S-O2S
4	C	1304	MES	C7-C8-S-O3S
3	B	1301	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
4	B	1304	MES	C7-C8-S-O3S
3	B	1301	NAG	C1-C2-N2-C7
4	B	1304	MES	C8-C7-N4-C3
4	B	1304	MES	C7-C8-S-O2S
4	C	1304	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1304	MES	1	0
4	C	1304	MES	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	445/531 (83%)	-0.03	9 (2%)	65	68	18, 30, 57, 114	0
1	B	445/531 (83%)	0.07	14 (3%)	49	52	18, 33, 62, 111	0
1	C	444/531 (83%)	-0.00	7 (1%)	72	74	17, 31, 51, 106	0
All	All	1334/1593 (83%)	0.01	30 (2%)	62	65	17, 31, 56, 114	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	706	THR	6.5
1	B	709	VAL	5.9
1	C	804	GLY	5.0
1	B	710	ASN	4.8
1	C	802	PHE	4.8
1	A	707	GLU	4.5
1	A	709	VAL	4.3
1	A	708	GLY	4.1
1	A	997	ARG	3.8
1	A	1135	PRO	3.6
1	B	708	GLY	3.6
1	B	707	GLU	3.6
1	B	892	LEU	3.4
1	A	710	ASN	3.2
1	B	996	ASN	2.6
1	A	711	THR	2.5
1	C	892	LEU	2.5
1	B	826	PHE	2.5
1	B	1135	PRO	2.4
1	A	977	GLU	2.4
1	B	705	SER	2.4
1	B	1096	GLU	2.4
1	B	706	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1011	LEU	2.3
1	C	1010	ASP	2.3
1	B	894	ALA	2.2
1	C	987	ASP	2.2
1	C	805	GLU	2.1
1	B	1134	ASN	2.1
1	B	987	ASP	2.0

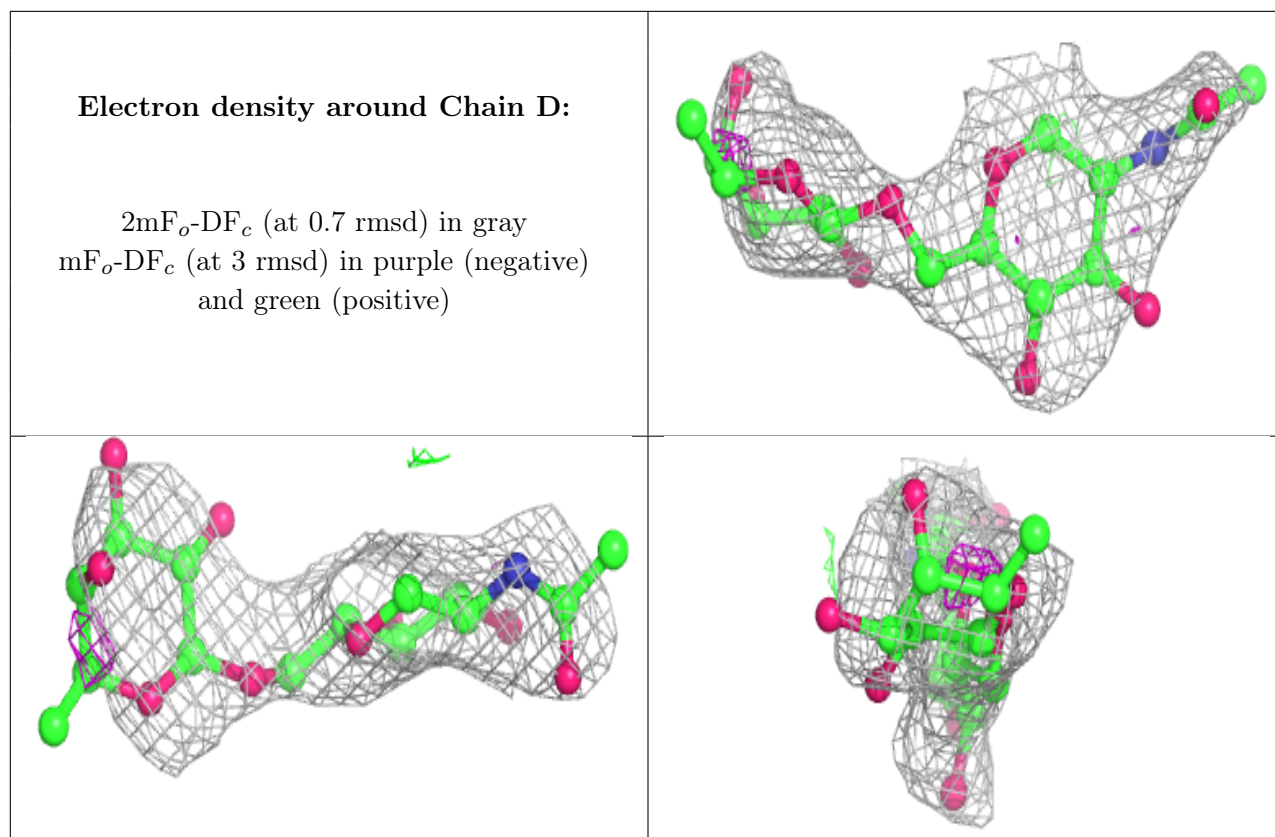## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	FUL	D	2	10/11	0.85	0.39	65,72,74,74	0
2	NAG	D	1	14/15	0.88	0.38	49,55,59,63	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 D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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, 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	C	1303	14/15	0.73	0.43	55,61,64,65	0
3	NAG	B	1301	14/15	0.74	0.26	52,58,61,62	0
3	NAG	C	1301	14/15	0.76	0.24	49,55,61,65	0
3	NAG	B	1303	14/15	0.78	0.40	59,66,68,69	0
4	MES	B	1304	12/12	0.80	0.40	80,81,90,91	12
3	NAG	A	1301	14/15	0.84	0.21	43,49,52,55	0
4	MES	C	1304	12/12	0.90	0.23	41,43,59,59	12
3	NAG	A	1302	14/15	0.92	0.21	33,37,40,40	0
3	NAG	B	1302	14/15	0.92	0.13	32,34,38,39	0
3	NAG	C	1302	14/15	0.92	0.17	34,36,42,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.