wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2021 – 03:08 pm BST

PDB ID	:	7A59
Title	:	Crimean-Congo Hemorrhagic Fever Virus Envelope Glycoprotein Gc W1191H/W1197A/W1199A Mutant in Postfusion Conformation (Orthorhombic Crystal Form)
Authors	:	Hellert, J.; Guardado-Calvo, P.; Rey, F.A.
Deposited on	:	2020-08-20
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 (1)) were used in the production of this report:

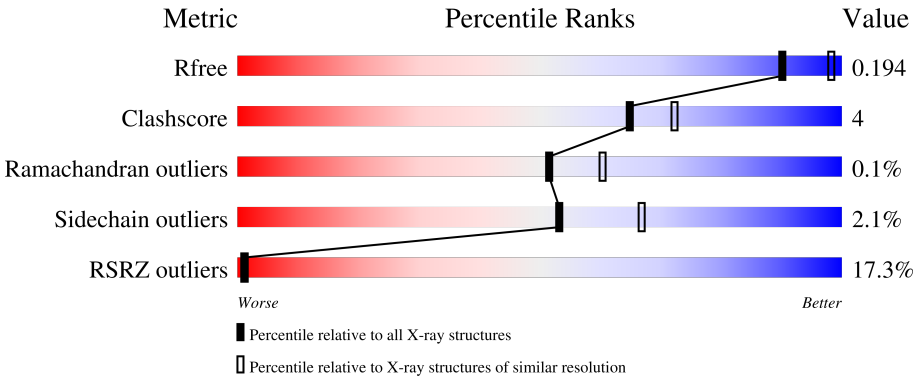
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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	538	19% 83% 10% 7%
1	B	538	16% 81% 14% 5%
1	C	538	14% 82% 11% 7%
2	D	5	40% 20% 40%

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	BMA	D	3	-	-	-	X
2	MAN	D	4	-	-	-	X
2	FUC	D	5	-	-	-	X
3	NAG	A	1601	-	-	-	X
3	NAG	B	1601	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12589 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3874	2430	659	750	35			
1	B	513	Total	C	N	O	S	0	0	0
			3998	2511	680	772	35			
1	C	501	Total	C	N	O	S	0	0	0
			3889	2439	662	753	35			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
A	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1562	GLU	-	expression tag	UNP Q8JSZ3
A	1563	ASN	-	expression tag	UNP Q8JSZ3
A	1564	LEU	-	expression tag	UNP Q8JSZ3
A	1565	TYR	-	expression tag	UNP Q8JSZ3
A	1566	PHE	-	expression tag	UNP Q8JSZ3
A	1567	GLN	-	expression tag	UNP Q8JSZ3
A	1568	SER	-	expression tag	UNP Q8JSZ3
A	1569	ALA	-	expression tag	UNP Q8JSZ3
A	1570	GLY	-	expression tag	UNP Q8JSZ3
A	1571	TRP	-	expression tag	UNP Q8JSZ3
A	1572	SER	-	expression tag	UNP Q8JSZ3
A	1573	HIS	-	expression tag	UNP Q8JSZ3
A	1574	PRO	-	expression tag	UNP Q8JSZ3
A	1575	GLN	-	expression tag	UNP Q8JSZ3
A	1576	PHE	-	expression tag	UNP Q8JSZ3
A	1577	GLU	-	expression tag	UNP Q8JSZ3
A	1578	LYS	-	expression tag	UNP Q8JSZ3
B	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
B	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3

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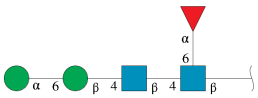
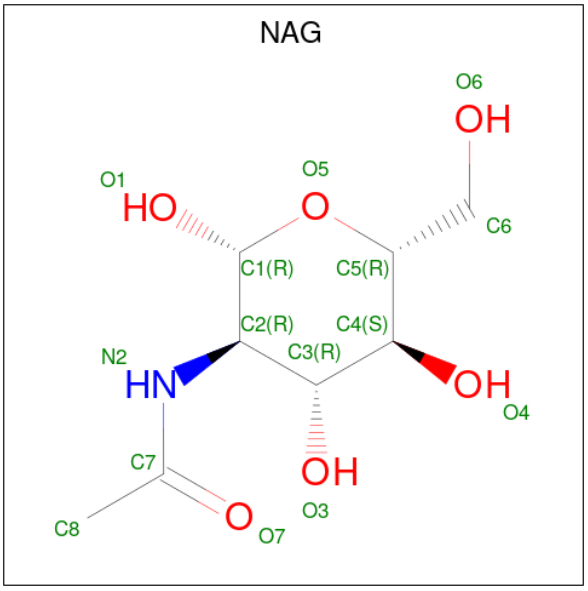
Chain	Residue	Modelled	Actual	Comment	Reference
B	1562	GLU	-	expression tag	UNP Q8JSZ3
B	1563	ASN	-	expression tag	UNP Q8JSZ3
B	1564	LEU	-	expression tag	UNP Q8JSZ3
B	1565	TYR	-	expression tag	UNP Q8JSZ3
B	1566	PHE	-	expression tag	UNP Q8JSZ3
B	1567	GLN	-	expression tag	UNP Q8JSZ3
B	1568	SER	-	expression tag	UNP Q8JSZ3
B	1569	ALA	-	expression tag	UNP Q8JSZ3
B	1570	GLY	-	expression tag	UNP Q8JSZ3
B	1571	TRP	-	expression tag	UNP Q8JSZ3
B	1572	SER	-	expression tag	UNP Q8JSZ3
B	1573	HIS	-	expression tag	UNP Q8JSZ3
B	1574	PRO	-	expression tag	UNP Q8JSZ3
B	1575	GLN	-	expression tag	UNP Q8JSZ3
B	1576	PHE	-	expression tag	UNP Q8JSZ3
B	1577	GLU	-	expression tag	UNP Q8JSZ3
B	1578	LYS	-	expression tag	UNP Q8JSZ3
C	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
C	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1562	GLU	-	expression tag	UNP Q8JSZ3
C	1563	ASN	-	expression tag	UNP Q8JSZ3
C	1564	LEU	-	expression tag	UNP Q8JSZ3
C	1565	TYR	-	expression tag	UNP Q8JSZ3
C	1566	PHE	-	expression tag	UNP Q8JSZ3
C	1567	GLN	-	expression tag	UNP Q8JSZ3
C	1568	SER	-	expression tag	UNP Q8JSZ3
C	1569	ALA	-	expression tag	UNP Q8JSZ3
C	1570	GLY	-	expression tag	UNP Q8JSZ3
C	1571	TRP	-	expression tag	UNP Q8JSZ3
C	1572	SER	-	expression tag	UNP Q8JSZ3
C	1573	HIS	-	expression tag	UNP Q8JSZ3
C	1574	PRO	-	expression tag	UNP Q8JSZ3
C	1575	GLN	-	expression tag	UNP Q8JSZ3
C	1576	PHE	-	expression tag	UNP Q8JSZ3
C	1577	GLU	-	expression tag	UNP Q8JSZ3
C	1578	LYS	-	expression tag	UNP Q8JSZ3

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	5	Total C N O 60 34 2 24	0	0	0

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

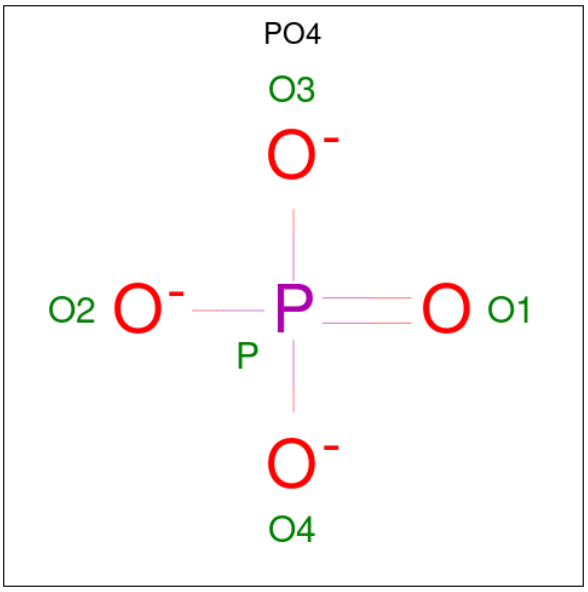


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

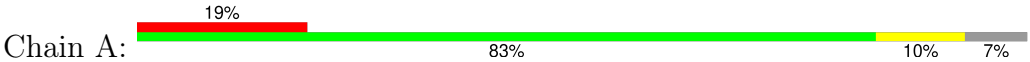
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	241	Total O 241 241	0	0
6	B	245	Total O 245 245	0	0
6	C	243	Total O 243 243	0	0

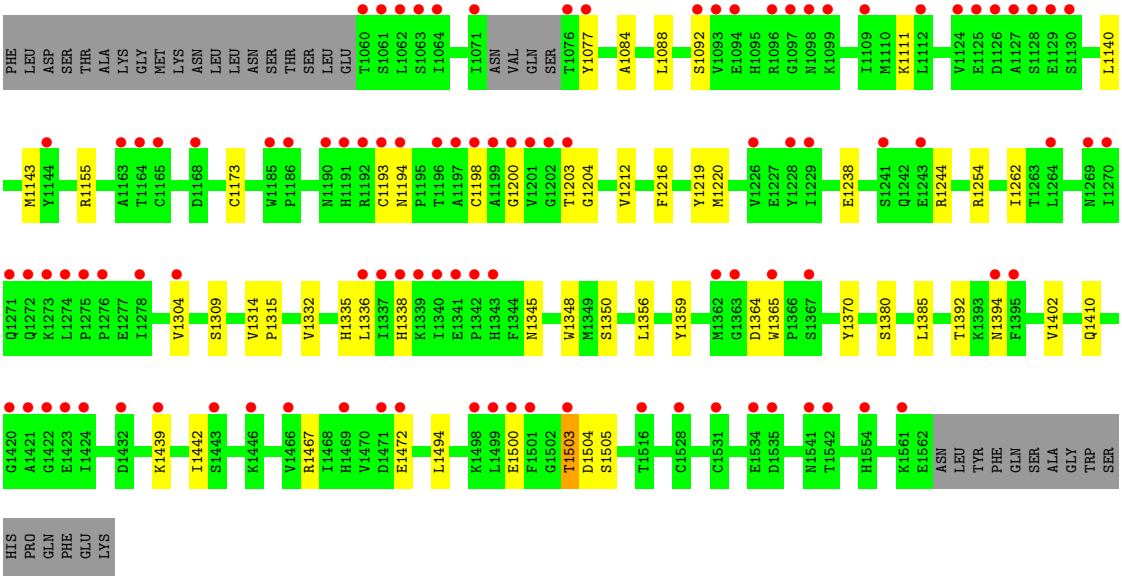
3 Residue-property plots (i)

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: Envelopment polyprotein

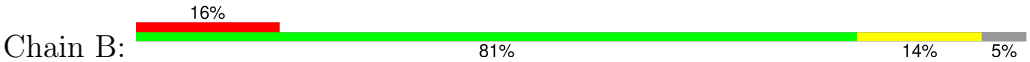
Chain A:

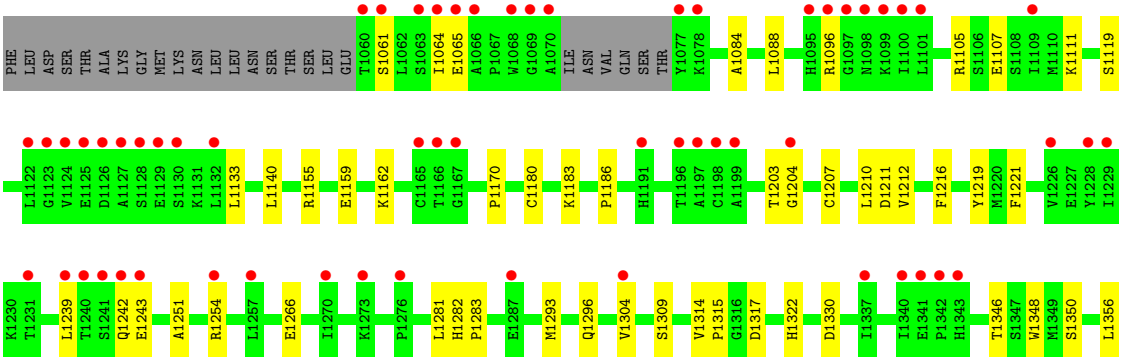


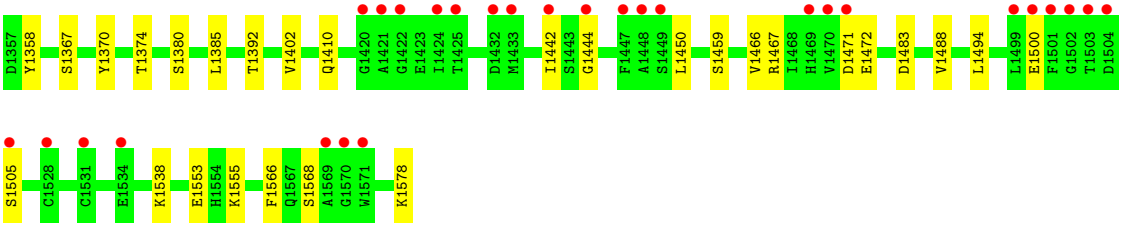


• Molecule 1: Envelopment polyprotein

Chain B:

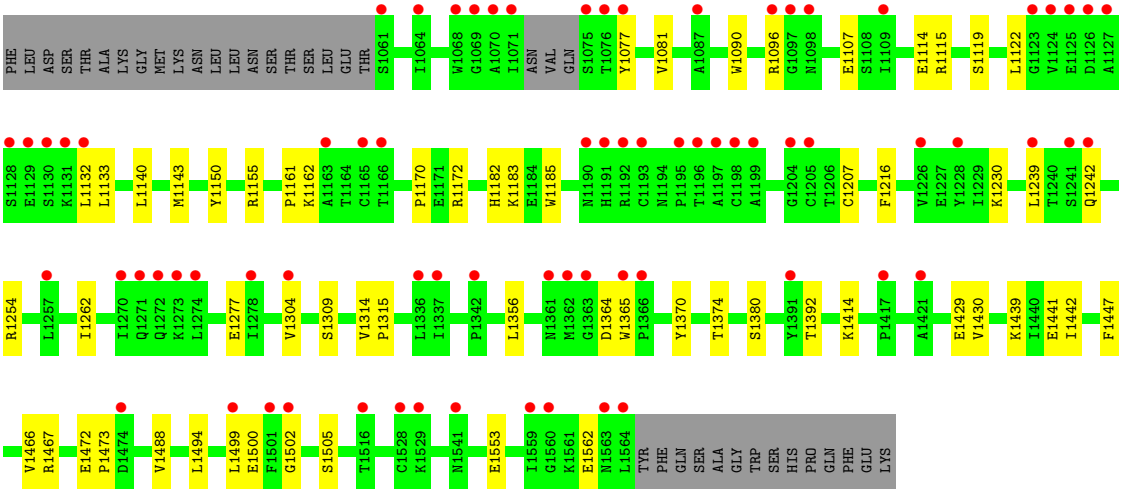






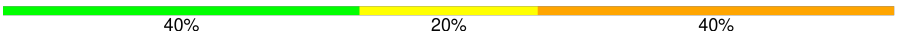
• Molecule 1: Envelopment polyprotein

Chain C:



• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.96Å 216.08Å 274.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.20 49.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-2.20) 92.1 (49.37-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.161 , 0.194 0.161 , 0.194	Depositor DCC
R_{free} test set	1997 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.97	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: CL, BMA, PO4, MAN, NAG, FUC

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	0.37	0/3960	0.54	0/5369
1	B	0.37	1/4091 (0.0%)	0.56	1/5545 (0.0%)
1	C	0.38	1/3975 (0.0%)	0.55	0/5389
All	All	0.37	2/12026 (0.0%)	0.55	1/16303 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1207	CYS	CB-SG	-5.44	1.73	1.81
1	C	1207	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1317	ASP	CB-CG-OD1	5.77	123.49	118.30

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	3874	0	3769	29	0
1	B	3998	0	3872	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3889	0	3784	35	0
2	D	60	0	52	1	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	0	0
6	A	241	0	0	1	0
6	B	245	0	0	4	0
6	C	243	0	0	2	0
All	All	12589	0	11503	96	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 96 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:1578:LYS:HG2	1:C:1172:ARG:HG2	1.62	0.79
1:A:1309:SER:HB2	1:C:1314:VAL:HG21	1.67	0.76
1:B:1254:ARG:NH1	6:B:1701:HOH:O	2.22	0.73
1:B:1315:PRO:HD3	1:B:1380:SER:HB3	1.72	0.70
1:A:1494:LEU:HD22	1:A:1505:SER:HB3	1.75	0.69

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	495/538 (92%)	485 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	509/538 (95%)	491 (96%)	18 (4%)	0	100 100
1	C	497/538 (92%)	483 (97%)	13 (3%)	1 (0%)	47 55
All	All	1501/1614 (93%)	1459 (97%)	41 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1161	PRO

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	442/477 (93%)	432 (98%)	10 (2%)	50 63
1	B	454/477 (95%)	444 (98%)	10 (2%)	52 65
1	C	444/477 (93%)	436 (98%)	8 (2%)	59 72
All	All	1340/1431 (94%)	1312 (98%)	28 (2%)	53 67

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1216	PHE
1	C	1562	GLU
1	B	1392	THR
1	C	1216	PHE
1	B	1304	VAL

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	1322	HIS
1	C	1546	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 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	2,1	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.77	0
2	BMA	D	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.04	1 (6%)
2	MAN	D	4	2	11,11,12	1.66	2 (18%)	15,15,17	1.63	3 (20%)
2	FUC	D	5	2	10,10,11	1.10	0	14,14,16	0.88	1 (7%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	FUC	D	5	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	C1-C2	4.65	1.62	1.52
2	D	3	BMA	C1-C2	2.61	1.58	1.52
2	D	4	MAN	C2-C3	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	MAN	C1-C2-C3	3.53	114.00	109.67
2	D	4	MAN	C1-O5-C5	3.51	116.95	112.19
2	D	4	MAN	O2-C2-C3	-2.24	105.65	110.14
2	D	5	FUC	O2-C2-C1	2.20	113.65	109.15
2	D	3	BMA	O5-C5-C6	2.19	110.64	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

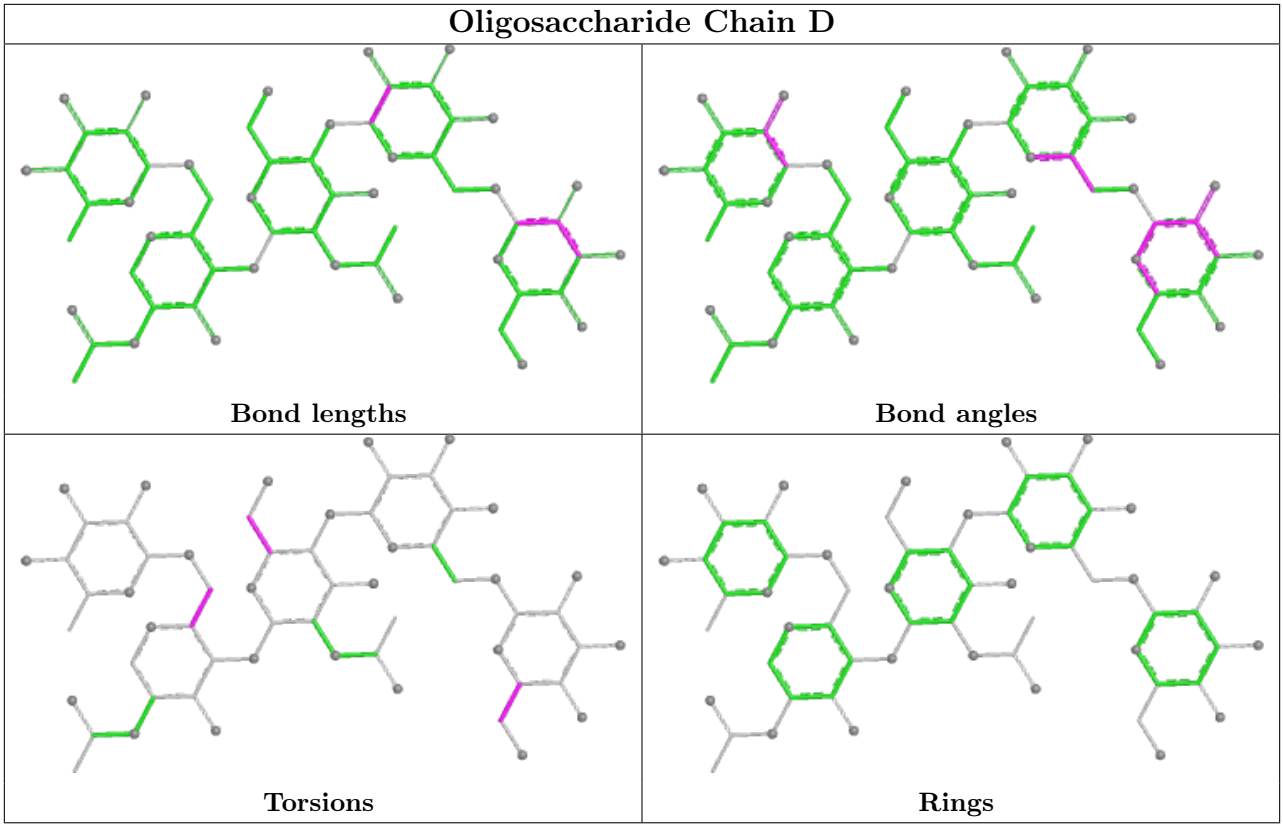
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

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

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



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	1601	1	14,14,15	0.47	0	17,19,21	0.37	0
5	PO4	A	1605	-	4,4,4	0.81	0	6,6,6	0.44	0
3	NAG	B	1601	1	14,14,15	0.87	1 (7%)	17,19,21	1.34	2 (11%)

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	1601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1601	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1601	NAG	C1-C2	2.40	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1601	NAG	C2-N2-C7	4.23	128.92	122.90
3	B	1601	NAG	C1-O5-C5	2.32	115.33	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1601	NAG	O5-C5-C6-O6
3	A	1601	NAG	C4-C5-C6-O6
3	B	1601	NAG	C8-C7-N2-C2
3	B	1601	NAG	O7-C7-N2-C2
3	B	1601	NAG	O5-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	1601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	499/538 (92%)	1.05	101 (20%)	1	1	37, 67, 131, 211	0
1	B	513/538 (95%)	0.95	87 (16%)	1	1	37, 66, 130, 184	0
1	C	501/538 (93%)	0.80	74 (14%)	2	2	36, 65, 124, 184	0
All	All	1513/1614 (93%)	0.93	262 (17%)	1	1	36, 66, 128, 211	0

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1127	ALA	14.6
1	B	1501	PHE	11.6
1	C	1128	SER	11.5
1	B	1064	ILE	10.1
1	A	1126	ASP	9.0

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, 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	MAN	D	4	11/12	0.46	0.57	131,148,154,154	0
2	FUC	D	5	10/11	0.52	0.44	136,139,142,144	0
2	NAG	D	2	14/15	0.65	0.36	111,125,136,144	0

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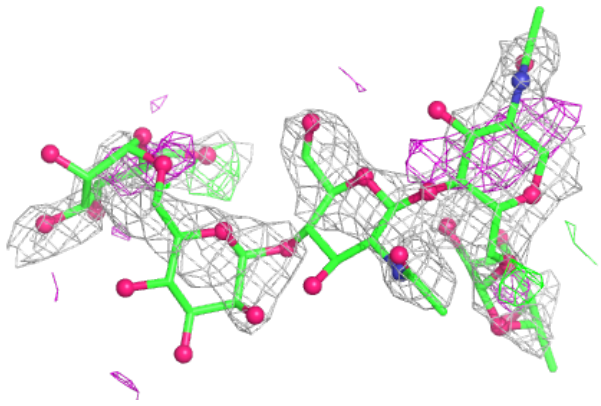
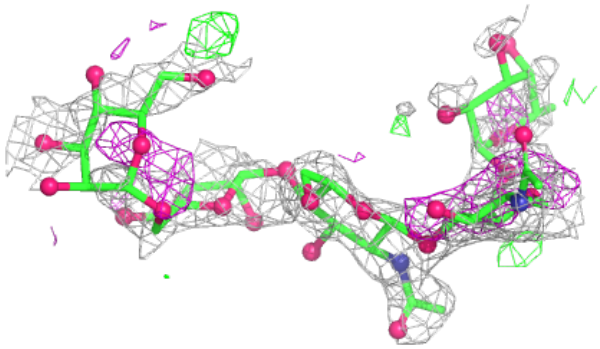
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.68	0.49	150,154,157,158	0
2	NAG	D	1	14/15	0.78	0.40	72,101,116,128	0

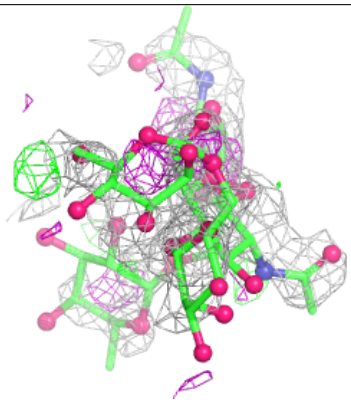
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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, 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	B	1601	14/15	0.15	0.58	106,120,124,125	0
3	NAG	A	1601	14/15	0.35	0.81	117,135,139,140	0
4	CL	C	1601	1/1	0.82	0.23	94,94,94,94	0
4	CL	C	1602	1/1	0.89	0.11	90,90,90,90	0
4	CL	A	1604	1/1	0.90	0.29	84,84,84,84	0
4	CL	B	1602	1/1	0.92	0.09	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	A	1605	5/5	0.93	0.12	111,112,116,116	0
4	CL	A	1603	1/1	0.97	0.16	49,49,49,49	0
4	CL	A	1602	1/1	0.99	0.26	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.