



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:25 AM EDT

PDB ID : 6Y5W
Title : Crystal structure of the envelope glycoprotein complex of Andes virus in a near postfusion conformation
Authors : Serris, A.; Rey, F.A.; Guardado-Calvo, P.
Deposited on : 2020-02-26
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

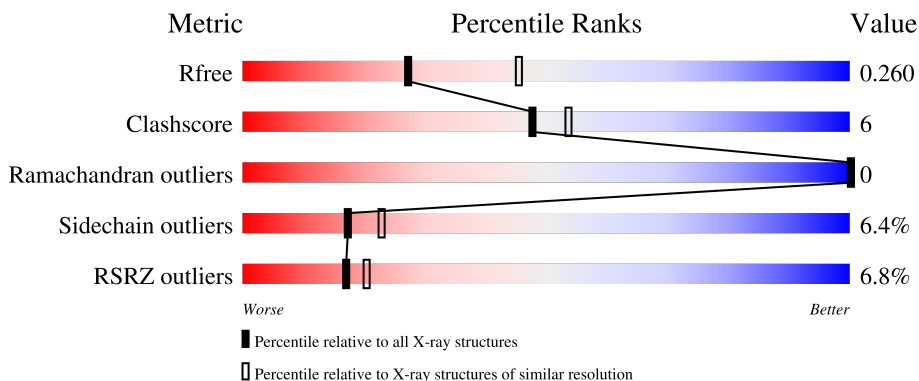
1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	892	<div> <div>5%</div> <div>30%</div> <div>9%</div> <div>61%</div> </div>
1	B	892	<div> <div>%</div> <div>37%</div> <div>8%</div> <div>55%</div> </div>
2	C	4	<div> <div>75%</div> <div>25%</div> </div>
3	D	4	<div> <div>25%</div> <div>75%</div> </div>
3	E	4	<div> <div>75%</div> <div>25%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5984 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 polypeptide, Envelope polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2676	1687	441	527	21			
1	B	405	Total	C	N	O	S	0	0	0
			3094	1942	522	597	33			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	GLY	-	linker	UNP A0A3Q8TA45
A	376	GLY	-	linker	UNP A0A3Q8TA45
A	377	SER	-	linker	UNP A0A3Q8TA45
A	378	GLY	-	linker	UNP A0A3Q8TA45
A	379	LEU	-	linker	UNP A0A3Q8TA45
A	380	VAL	-	linker	UNP A0A3Q8TA45
A	381	PRO	-	linker	UNP A0A3Q8TA45
A	382	ARG	-	linker	UNP A0A3Q8TA45
A	383	GLY	-	linker	UNP A0A3Q8TA45
A	384	SER	-	linker	UNP A0A3Q8TA45
A	385	GLY	-	linker	UNP A0A3Q8TA45
A	386	GLY	-	linker	UNP A0A3Q8TA45
A	387	GLY	-	linker	UNP A0A3Q8TA45
A	388	SER	-	linker	UNP A0A3Q8TA45
A	389	GLY	-	linker	UNP A0A3Q8TA45
A	390	GLY	-	linker	UNP A0A3Q8TA45
A	391	GLY	-	linker	UNP A0A3Q8TA45
A	392	SER	-	linker	UNP A0A3Q8TA45
A	393	TRP	-	linker	UNP A0A3Q8TA45
A	394	SER	-	linker	UNP A0A3Q8TA45
A	395	HIS	-	linker	UNP A0A3Q8TA45
A	396	PRO	-	linker	UNP A0A3Q8TA45
A	397	GLN	-	linker	UNP A0A3Q8TA45
A	398	PHE	-	linker	UNP A0A3Q8TA45
A	399	GLU	-	linker	UNP A0A3Q8TA45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LYS	-	linker	UNP A0A3Q8TA45
A	401	GLY	-	linker	UNP A0A3Q8TA45
A	402	GLY	-	linker	UNP A0A3Q8TA45
A	403	GLY	-	linker	UNP A0A3Q8TA45
A	404	THR	-	linker	UNP A0A3Q8TA45
A	405	GLY	-	linker	UNP A0A3Q8TA45
A	406	GLY	-	linker	UNP A0A3Q8TA45
A	407	GLY	-	linker	UNP A0A3Q8TA45
A	408	THR	-	linker	UNP A0A3Q8TA45
A	409	LEU	-	linker	UNP A0A3Q8TA45
A	410	VAL	-	linker	UNP A0A3Q8TA45
A	411	PRO	-	linker	UNP A0A3Q8TA45
A	412	ARG	-	linker	UNP A0A3Q8TA45
A	413	GLY	-	linker	UNP A0A3Q8TA45
A	414	SER	-	linker	UNP A0A3Q8TA45
A	415	GLY	-	linker	UNP A0A3Q8TA45
A	416	THR	-	linker	UNP A0A3Q8TA45
A	417	GLY	-	linker	UNP A0A3Q8TA45
A	418	GLY	-	linker	UNP A0A3Q8TA45
A	875	PRO	-	expression tag	UNP A0A3Q8TA45
A	876	PHE	-	expression tag	UNP A0A3Q8TA45
A	877	GLU	-	expression tag	UNP A0A3Q8TA45
A	878	ASP	-	expression tag	UNP A0A3Q8TA45
A	879	ASP	-	expression tag	UNP A0A3Q8TA45
A	880	ASP	-	expression tag	UNP A0A3Q8TA45
A	881	ASP	-	expression tag	UNP A0A3Q8TA45
A	882	LYS	-	expression tag	UNP A0A3Q8TA45
A	883	ALA	-	expression tag	UNP A0A3Q8TA45
A	884	GLY	-	expression tag	UNP A0A3Q8TA45
A	885	TRP	-	expression tag	UNP A0A3Q8TA45
A	886	SER	-	expression tag	UNP A0A3Q8TA45
A	887	HIS	-	expression tag	UNP A0A3Q8TA45
A	888	PRO	-	expression tag	UNP A0A3Q8TA45
A	889	GLN	-	expression tag	UNP A0A3Q8TA45
A	890	PHE	-	expression tag	UNP A0A3Q8TA45
A	891	GLU	-	expression tag	UNP A0A3Q8TA45
A	892	LYS	-	expression tag	UNP A0A3Q8TA45
A	893	GLY	-	expression tag	UNP A0A3Q8TA45
A	894	GLY	-	expression tag	UNP A0A3Q8TA45
A	895	GLY	-	expression tag	UNP A0A3Q8TA45
A	896	SER	-	expression tag	UNP A0A3Q8TA45
A	897	GLY	-	expression tag	UNP A0A3Q8TA45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	898	GLY	-	expression tag	UNP A0A3Q8TA45
A	899	GLY	-	expression tag	UNP A0A3Q8TA45
A	900	SER	-	expression tag	UNP A0A3Q8TA45
A	901	GLY	-	expression tag	UNP A0A3Q8TA45
A	902	GLY	-	expression tag	UNP A0A3Q8TA45
A	903	GLY	-	expression tag	UNP A0A3Q8TA45
A	904	SER	-	expression tag	UNP A0A3Q8TA45
A	905	TRP	-	expression tag	UNP A0A3Q8TA45
A	906	SER	-	expression tag	UNP A0A3Q8TA45
A	907	HIS	-	expression tag	UNP A0A3Q8TA45
A	908	PRO	-	expression tag	UNP A0A3Q8TA45
A	909	GLN	-	expression tag	UNP A0A3Q8TA45
A	910	PHE	-	expression tag	UNP A0A3Q8TA45
A	911	GLU	-	expression tag	UNP A0A3Q8TA45
A	912	LYS	-	expression tag	UNP A0A3Q8TA45
B	608	GLY	-	linker	UNP A0A3Q8TA45
B	609	GLY	-	linker	UNP A0A3Q8TA45
B	610	SER	-	linker	UNP A0A3Q8TA45
B	611	GLY	-	linker	UNP A0A3Q8TA45
B	612	LEU	-	linker	UNP A0A3Q8TA45
B	613	VAL	-	linker	UNP A0A3Q8TA45
B	614	PRO	-	linker	UNP A0A3Q8TA45
B	615	ARG	-	linker	UNP A0A3Q8TA45
B	616	GLY	-	linker	UNP A0A3Q8TA45
B	617	SER	-	linker	UNP A0A3Q8TA45
B	618	GLY	-	linker	UNP A0A3Q8TA45
B	619	GLY	-	linker	UNP A0A3Q8TA45
B	620	GLY	-	linker	UNP A0A3Q8TA45
B	621	SER	-	linker	UNP A0A3Q8TA45
B	622	GLY	-	linker	UNP A0A3Q8TA45
B	623	GLY	-	linker	UNP A0A3Q8TA45
B	624	GLY	-	linker	UNP A0A3Q8TA45
B	625	SER	-	linker	UNP A0A3Q8TA45
B	626	TRP	-	linker	UNP A0A3Q8TA45
B	627	SER	-	linker	UNP A0A3Q8TA45
B	628	HIS	-	linker	UNP A0A3Q8TA45
B	629	PRO	-	linker	UNP A0A3Q8TA45
B	630	GLN	-	linker	UNP A0A3Q8TA45
B	631	PHE	-	linker	UNP A0A3Q8TA45
B	632	GLU	-	linker	UNP A0A3Q8TA45
B	633	LYS	-	linker	UNP A0A3Q8TA45
B	634	GLY	-	linker	UNP A0A3Q8TA45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	635	GLY	-	linker	UNP A0A3Q8TA45
B	636	GLY	-	linker	UNP A0A3Q8TA45
B	637	THR	-	linker	UNP A0A3Q8TA45
B	638	GLY	-	linker	UNP A0A3Q8TA45
B	639	GLY	-	linker	UNP A0A3Q8TA45
B	640	GLY	-	linker	UNP A0A3Q8TA45
B	641	THR	-	linker	UNP A0A3Q8TA45
B	642	LEU	-	linker	UNP A0A3Q8TA45
B	643	VAL	-	linker	UNP A0A3Q8TA45
B	644	PRO	-	linker	UNP A0A3Q8TA45
B	645	ARG	-	linker	UNP A0A3Q8TA45
B	646	GLY	-	linker	UNP A0A3Q8TA45
B	647	SER	-	linker	UNP A0A3Q8TA45
B	648	GLY	-	linker	UNP A0A3Q8TA45
B	649	THR	-	linker	UNP A0A3Q8TA45
B	650	GLY	-	linker	UNP A0A3Q8TA45
B	651	GLY	-	linker	UNP A0A3Q8TA45
B	1108	PRO	-	expression tag	UNP A0A3Q8TA45
B	1109	PHE	-	expression tag	UNP A0A3Q8TA45
B	1110	GLU	-	expression tag	UNP A0A3Q8TA45
B	1111	ASP	-	expression tag	UNP A0A3Q8TA45
B	1112	ASP	-	expression tag	UNP A0A3Q8TA45
B	1113	ASP	-	expression tag	UNP A0A3Q8TA45
B	1114	ASP	-	expression tag	UNP A0A3Q8TA45
B	1115	LYS	-	expression tag	UNP A0A3Q8TA45
B	1116	ALA	-	expression tag	UNP A0A3Q8TA45
B	1117	GLY	-	expression tag	UNP A0A3Q8TA45
B	1118	TRP	-	expression tag	UNP A0A3Q8TA45
B	1119	SER	-	expression tag	UNP A0A3Q8TA45
B	1120	HIS	-	expression tag	UNP A0A3Q8TA45
B	1121	PRO	-	expression tag	UNP A0A3Q8TA45
B	1122	GLN	-	expression tag	UNP A0A3Q8TA45
B	1123	PHE	-	expression tag	UNP A0A3Q8TA45
B	1124	GLU	-	expression tag	UNP A0A3Q8TA45
B	1125	LYS	-	expression tag	UNP A0A3Q8TA45
B	1126	GLY	-	expression tag	UNP A0A3Q8TA45
B	1127	GLY	-	expression tag	UNP A0A3Q8TA45
B	1128	GLY	-	expression tag	UNP A0A3Q8TA45
B	1129	SER	-	expression tag	UNP A0A3Q8TA45
B	1130	GLY	-	expression tag	UNP A0A3Q8TA45
B	1131	GLY	-	expression tag	UNP A0A3Q8TA45
B	1132	GLY	-	expression tag	UNP A0A3Q8TA45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1133	SER	-	expression tag	UNP A0A3Q8TA45
B	1134	GLY	-	expression tag	UNP A0A3Q8TA45
B	1135	GLY	-	expression tag	UNP A0A3Q8TA45
B	1136	GLY	-	expression tag	UNP A0A3Q8TA45
B	1137	SER	-	expression tag	UNP A0A3Q8TA45
B	1138	TRP	-	expression tag	UNP A0A3Q8TA45
B	1139	SER	-	expression tag	UNP A0A3Q8TA45
B	1140	HIS	-	expression tag	UNP A0A3Q8TA45
B	1141	PRO	-	expression tag	UNP A0A3Q8TA45
B	1142	GLN	-	expression tag	UNP A0A3Q8TA45
B	1143	PHE	-	expression tag	UNP A0A3Q8TA45
B	1144	GLU	-	expression tag	UNP A0A3Q8TA45
B	1145	LYS	-	expression tag	UNP A0A3Q8TA45

- 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			

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



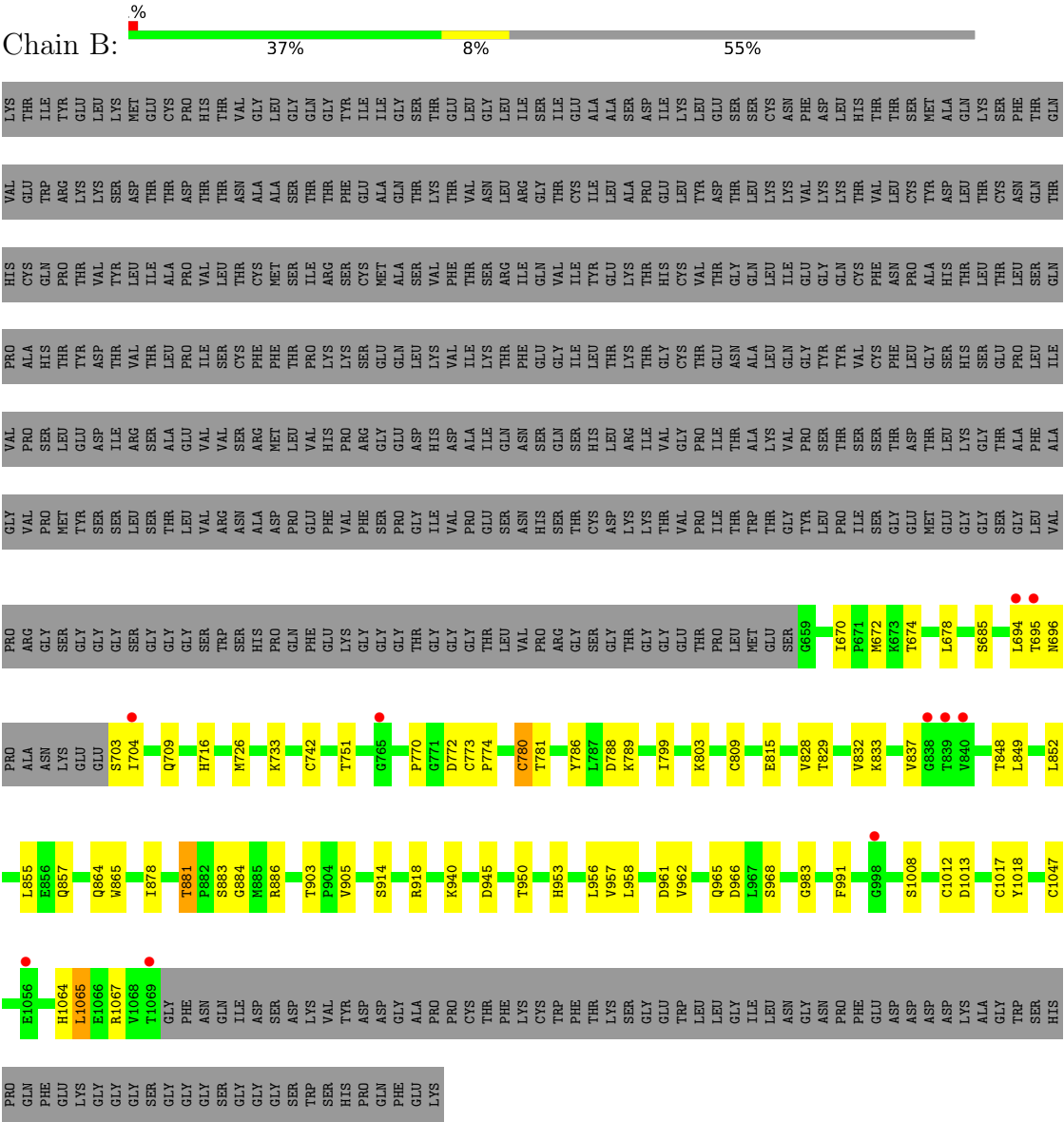
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is water.

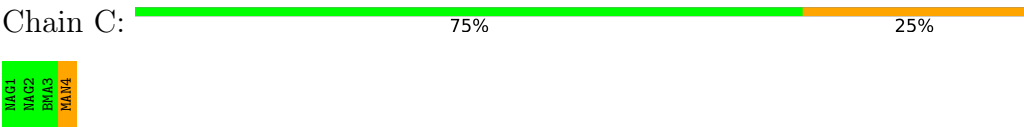
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	42	Total 42	O 42	0	0

TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 1: Envelope polyprotein,Envelope polyprotein



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



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





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

Chain E: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	130.33Å 130.33Å 129.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.62 – 2.55 37.62 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.3 (37.62-2.55) 97.3 (37.62-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.14rc3	Depositor
R, R_{free}	0.216 , 0.261 0.215 , 0.260	Depositor DCC
R_{free} test set	1360 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5984	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 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	0.25	0/2731	0.47	0/3718
1	B	0.24	0/3168	0.46	1/4294 (0.0%)
All	All	0.25	0/5899	0.46	1/8012 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	VAL	C-N-CA	5.75	136.07	121.70

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	2676	0	2648	42	0
1	B	3094	0	2972	37	0
2	C	50	0	43	1	0
3	D	50	0	43	0	0
3	E	50	0	43	0	0
4	A	22	0	0	0	0
4	B	42	0	0	0	0
All	All	5984	0	5749	71	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 6.

All (71) 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:A:334:ASN:ND2	1:A:338:GLU:OE2	2.16	0.78
1:B:881:THR:HG23	1:B:883:SER:H	1.51	0.75
1:B:966:ASP:OD1	1:B:968:SER:OG	2.05	0.74
1:A:75:GLN:HG3	1:A:110:ARG:HB2	1.70	0.71
1:A:221:SER:HB3	1:A:224:LEU:HB2	1.72	0.71
1:A:162:MET:HB3	1:A:169:ARG:HH12	1.57	0.70
1:B:716:HIS:HB2	1:B:803:LYS:HB2	1.74	0.68
1:B:833:LYS:HB3	1:B:957:VAL:HG22	1.83	0.60
1:B:1013:ASP:HB2	1:B:1018:TYR:HE2	1.69	0.58
1:A:266:ASP:HB3	1:A:269:SER:HB3	1.86	0.57
1:B:1012:CYS:HA	1:B:1017:CYS:HA	1.87	0.55
1:B:678:LEU:HB2	1:B:956:LEU:HB3	1.88	0.55
1:A:278:VAL:O	1:B:751:THR:OG1	2.26	0.54
1:A:259:LEU:HD13	1:A:268:ARG:HH12	1.73	0.54
1:A:328:LEU:HB3	1:A:361:ILE:HD12	1.90	0.54
1:A:194:HIS:CG	1:A:268:ARG:HE	2.26	0.53
1:A:306:PRO:O	1:A:308:THR:N	2.39	0.53
1:A:60:LEU:HD12	1:A:73:MET:HE1	1.91	0.53
1:A:267:ILE:H	1:A:267:ILE:HD13	1.74	0.53
1:A:178:HIS:O	1:A:178:HIS:ND1	2.43	0.52
1:B:961:ASP:OD1	1:B:962:VAL:N	2.43	0.52
1:B:832:VAL:HG22	1:B:958:LEU:HD13	1.92	0.52
1:A:242:ASN:HB3	1:A:332:VAL:HG12	1.92	0.51
1:A:85:LYS:HB3	1:B:774:PRO:HB3	1.91	0.51
1:A:292:GLN:OE1	2:C:4:MAN:O4	2.27	0.51
1:B:815:GLU:OE2	1:B:829:THR:HG23	2.10	0.51
1:B:886:ARG:HD3	1:B:1067:ARG:HD3	1.92	0.51
1:A:118:GLU:HA	1:A:121:ASP:HB2	1.93	0.50
1:B:829:THR:HG22	1:B:832:VAL:H	1.76	0.50
1:A:131:LEU:HD12	1:A:148:LEU:HD13	1.94	0.50
1:A:305:VAL:HG23	1:A:314:LEU:HB2	1.93	0.50
1:A:134:ASP:OD1	1:A:135:LEU:N	2.45	0.49
1:A:85:LYS:HA	1:A:100:PHE:HA	1.94	0.49
1:A:296:ARG:NH1	1:A:320:ALA:O	2.45	0.49
1:A:100:PHE:HB3	1:B:774:PRO:HG3	1.94	0.48
1:A:162:MET:HB3	1:A:169:ARG:NH1	2.26	0.48
1:A:84:ARG:O	1:A:101:GLU:N	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:O	1:A:170:ILE:N	2.41	0.48
1:B:780:CYS:SG	1:B:781:THR:N	2.87	0.48
1:A:284:ASP:HB3	1:B:789:LYS:HE3	1.94	0.47
1:A:202:ALA:HA	1:A:205:TYR:CZ	2.50	0.47
1:B:837:VAL:O	1:B:953:HIS:N	2.41	0.47
1:A:211:PRO:HB3	1:A:285:HIS:CD2	2.50	0.47
1:B:726:MET:HB2	1:B:878:ILE:HB	1.96	0.46
1:A:29:GLU:OE2	1:A:184:LEU:N	2.24	0.45
1:A:194:HIS:CD2	1:A:268:ARG:HE	2.34	0.45
1:A:59:LYS:HA	1:A:110:ARG:HH22	1.81	0.45
1:B:685:SER:HB3	1:B:945:ASP:O	2.17	0.45
1:B:983:GLY:HA3	1:B:991:PHE:HA	1.98	0.45
1:A:26:LEU:HD12	1:A:45:THR:HG22	1.99	0.44
1:A:132:CYS:SG	1:A:147:TYR:HB2	2.56	0.44
1:A:295:LEU:HD23	1:A:321:GLY:HA3	1.98	0.44
1:A:59:LYS:HG2	1:A:110:ARG:NH2	2.33	0.44
1:B:709:GLN:HB2	1:B:809:CYS:HB2	2.00	0.44
1:B:770:PRO:HB3	1:B:903:THR:HG22	1.98	0.44
1:B:881:THR:HG22	1:B:884:GLY:O	2.18	0.43
1:B:914:SER:O	1:B:918:ARG:HG3	2.19	0.43
1:A:78:PHE:CZ	1:A:114:ILE:HD11	2.54	0.43
1:A:203:HIS:HB2	1:B:855:LEU:HG	2.02	0.42
1:B:694:LEU:HD11	1:B:958:LEU:HD21	2.01	0.42
1:A:248:TYR:OH	1:A:360:PRO:O	2.28	0.42
1:B:848:THR:HG21	1:B:865:TRP:CD2	2.54	0.42
1:B:670:ILE:HG22	1:B:672:MET:HG2	2.02	0.42
1:A:294:HIS:CE1	1:B:905:VAL:HG13	2.55	0.41
1:A:320:ALA:HB1	1:B:772:ASP:HB3	2.02	0.41
1:B:966:ASP:C	1:B:968:SER:H	2.23	0.41
1:B:799:ILE:HD11	1:B:849:LEU:HD11	2.03	0.41
1:B:695:THR:HG22	1:B:703:SER:HB3	2.02	0.41
1:A:296:ARG:HD2	1:B:772:ASP:HB2	2.03	0.41
1:B:733:LYS:HB2	1:B:786:TYR:CE1	2.56	0.41
1:B:1064:HIS:O	1:B:1065:LEU:HD13	2.22	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	345/892 (39%)	319 (92%)	26 (8%)	0	100	100
1	B	401/892 (45%)	379 (94%)	22 (6%)	0	100	100
All	All	746/1784 (42%)	698 (94%)	48 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/761 (41%)	287 (92%)	25 (8%)	12	15
1	B	349/761 (46%)	332 (95%)	17 (5%)	25	34
All	All	661/1522 (43%)	619 (94%)	42 (6%)	17	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	CYS
1	A	66	PHE
1	A	71	THR
1	A	76	LYS
1	A	98	THR
1	A	104	THR
1	A	120	TYR
1	A	127	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	153	LEU
1	A	154	THR
1	A	165	VAL
1	A	166	PHE
1	A	167	THR
1	A	176	LYS
1	A	189	CYS
1	A	197	THR
1	A	200	GLN
1	A	223	GLN
1	A	236	LYS
1	A	240	THR
1	A	265	GLU
1	A	267	ILE
1	A	281	ARG
1	A	296	ARG
1	A	367	LEU
1	B	674	THR
1	B	696	ASN
1	B	704	ILE
1	B	742	CYS
1	B	773	CYS
1	B	780	CYS
1	B	788	ASP
1	B	852	LEU
1	B	857	GLN
1	B	864	GLN
1	B	881	THR
1	B	940	LYS
1	B	950	THR
1	B	965	GLN
1	B	1008	SER
1	B	1047	CYS
1	B	1065	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS

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 ⓘ

12 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	2,1	14,14,15	0.45	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	BMA	C	3	2	11,11,12	0.63	0	15,15,17	0.84	0
2	MAN	C	4	2	11,11,12	0.69	0	15,15,17	1.20	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.20	0	17,19,21	1.15	2 (11%)
3	BMA	D	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.22	1 (6%)
3	MAN	D	4	3	11,11,12	0.86	1 (9%)	15,15,17	1.40	3 (20%)
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.45	0
3	BMA	E	3	3	11,11,12	0.64	0	15,15,17	0.69	0
3	MAN	E	4	3	11,11,12	0.67	0	15,15,17	0.96	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	C	1	2,1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	C1-C2	2.55	1.58	1.52
3	D	3	BMA	C1-C2	2.28	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	3.53	116.98	112.19
3	D	4	MAN	C1-O5-C5	3.53	116.98	112.19
3	D	2	NAG	C1-O5-C5	3.52	116.96	112.19
3	D	3	BMA	C1-O5-C5	3.21	116.54	112.19
3	E	4	MAN	C1-O5-C5	2.34	115.36	112.19
3	D	2	NAG	O4-C4-C5	2.30	115.01	109.30
2	C	4	MAN	O2-C2-C3	-2.30	105.54	110.14
3	E	4	MAN	O2-C2-C3	-2.19	105.75	110.14
3	D	4	MAN	O2-C2-C3	-2.10	105.93	110.14
3	D	4	MAN	C1-C2-C3	2.00	112.13	109.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

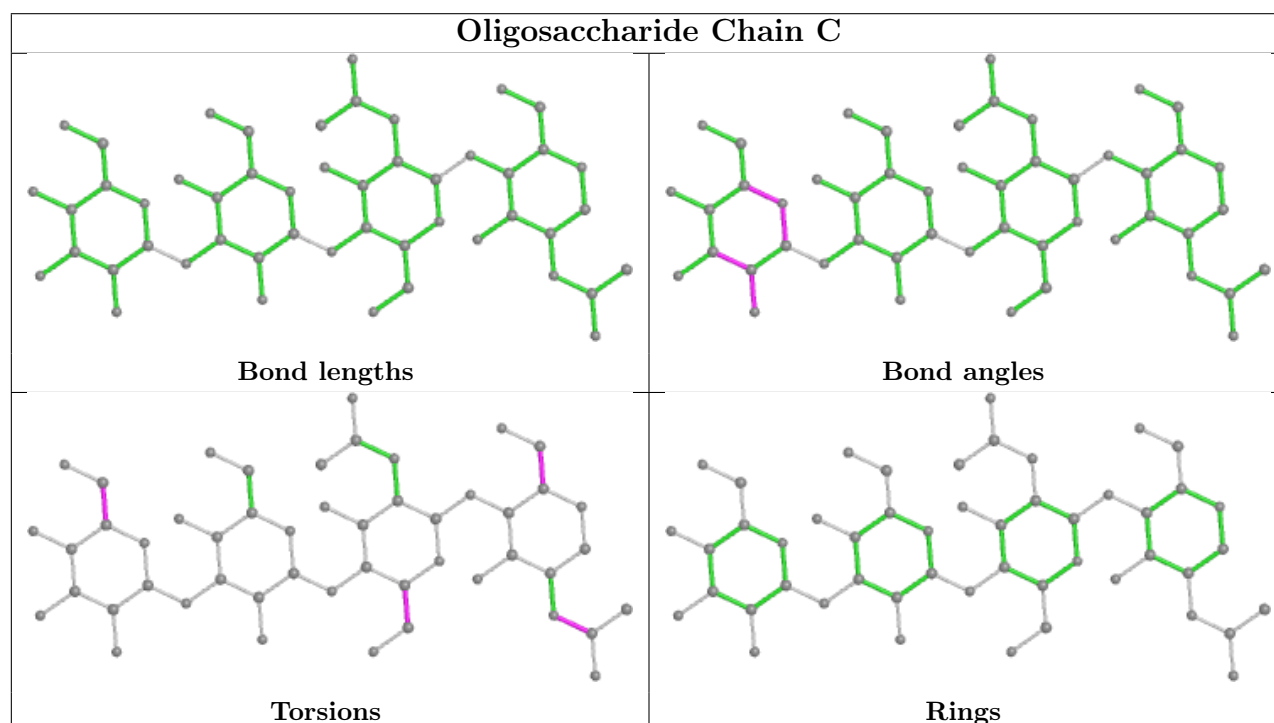
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

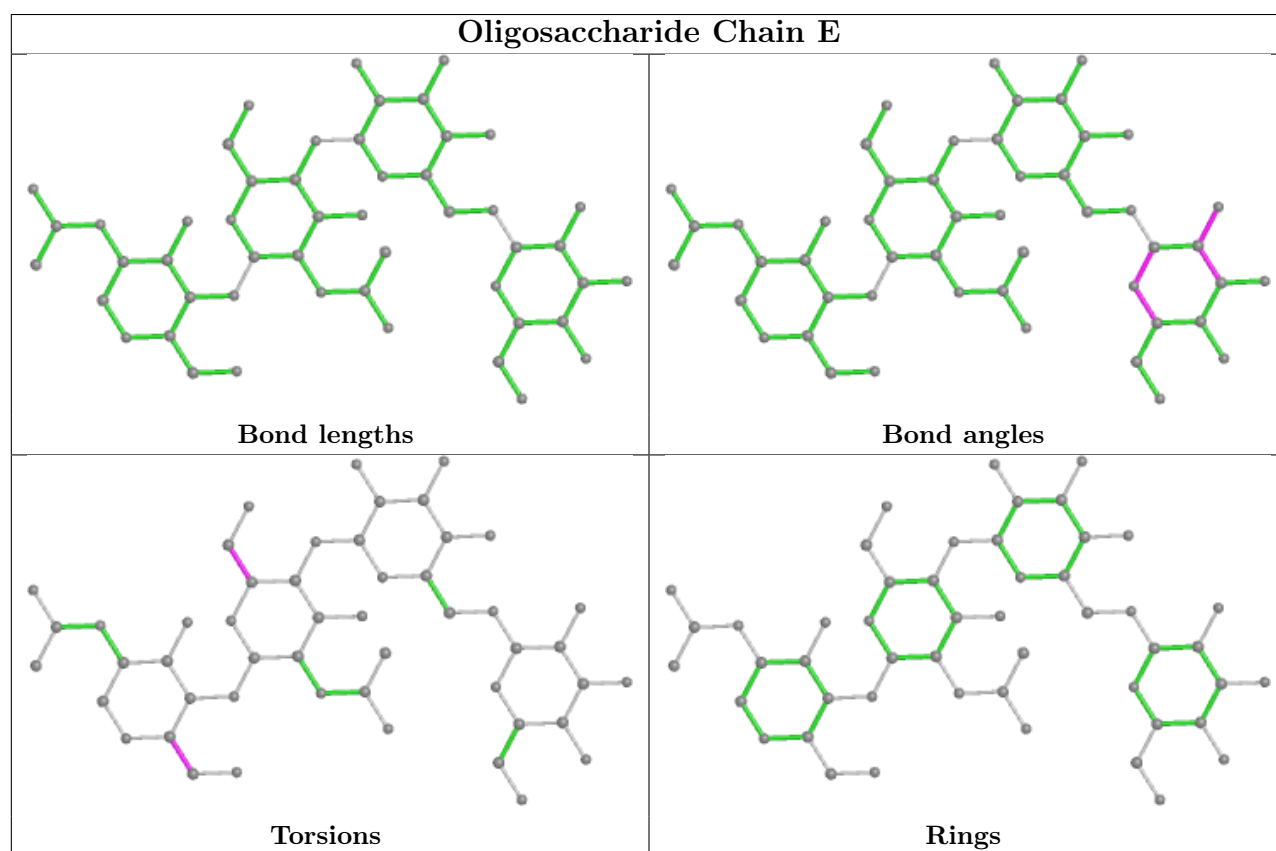
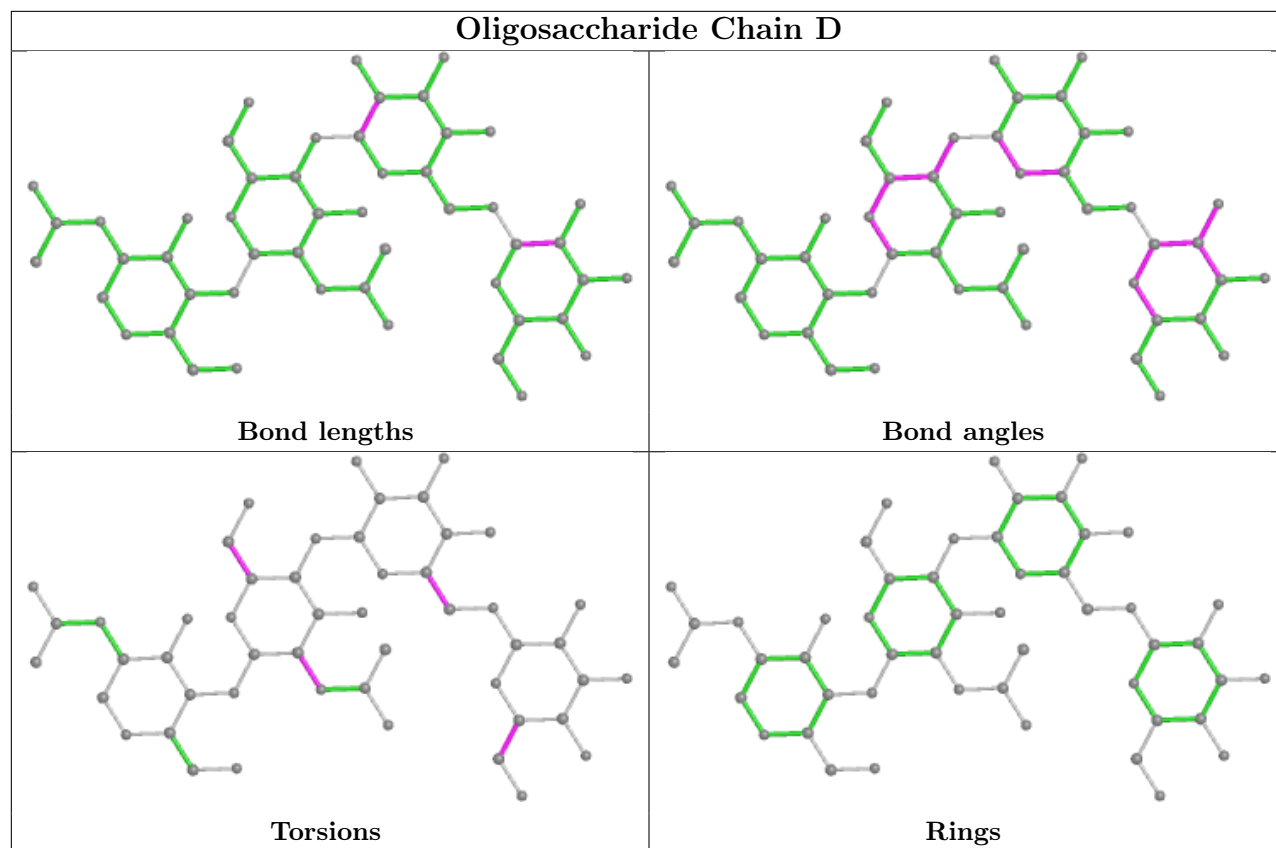
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	MAN	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

There are no ligands in this entry.

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	349/892 (39%)	0.64	41 (11%) 4 6	45, 83, 133, 195	0
1	B	405/892 (45%)	0.02	10 (2%) 57 63	30, 53, 88, 124	0
All	All	754/1784 (42%)	0.31	51 (6%) 17 20	30, 67, 113, 195	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	THR	9.3
1	A	288	ILE	6.6
1	A	71	THR	5.8
1	A	198	LEU	4.6
1	A	23	ILE	4.6
1	B	839	THR	3.9
1	A	238	GLY	3.5
1	B	704	ILE	3.3
1	A	159	ARG	3.2
1	B	838	GLY	3.2
1	A	287	ALA	3.1
1	A	290	ASN	3.0
1	B	840	VAL	3.0
1	A	53	GLU	2.9
1	A	169	ARG	2.8
1	A	303	ALA	2.8
1	A	56	SER	2.8
1	B	694	LEU	2.8
1	B	765	GLY	2.8
1	A	239	CYS	2.7
1	A	265	GLU	2.7
1	A	90	THR	2.5
1	A	177	THR	2.5
1	A	64	CYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	167	THR	2.5
1	B	1069	THR	2.5
1	A	372	GLU	2.4
1	A	84	ARG	2.4
1	A	113	CYS	2.4
1	A	61	GLU	2.3
1	A	310	SER	2.3
1	B	695	THR	2.3
1	A	311	THR	2.3
1	A	179	CYS	2.3
1	A	36	LEU	2.3
1	A	34	VAL	2.3
1	A	28	MET	2.3
1	B	998	GLY	2.3
1	A	203	HIS	2.2
1	A	200	GLN	2.2
1	A	65	ASN	2.2
1	A	201	PRO	2.2
1	A	88	ASP	2.1
1	A	27	LYS	2.1
1	A	55	ALA	2.1
1	A	166	PHE	2.1
1	A	286	ASP	2.1
1	A	105	LYS	2.1
1	A	234	LEU	2.1
1	A	118	GLU	2.1
1	B	1056	GLU	2.1

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.

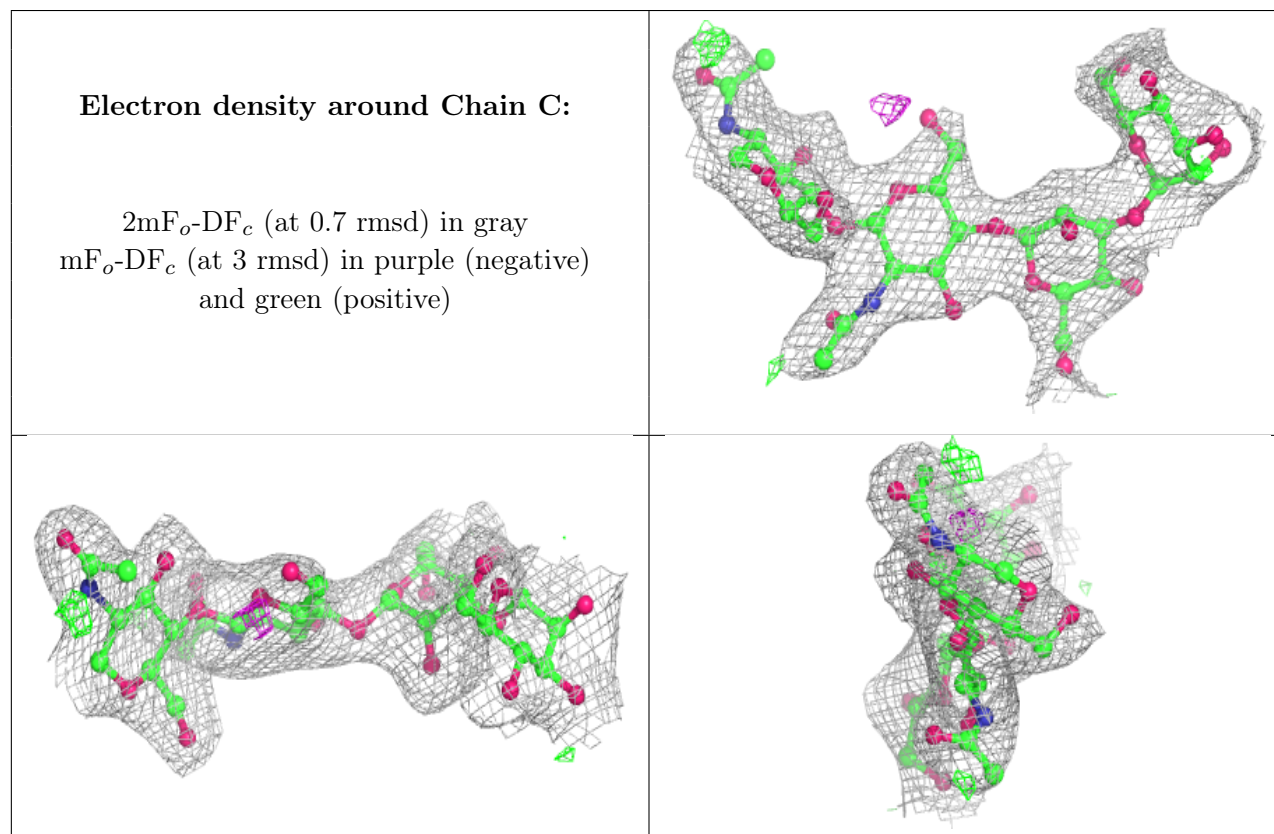
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	D	4	11/12	0.54	0.32	109,114,122,123	0

Continued on next page...

Continued from previous page...

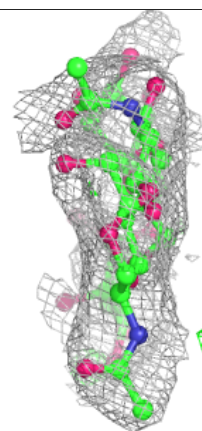
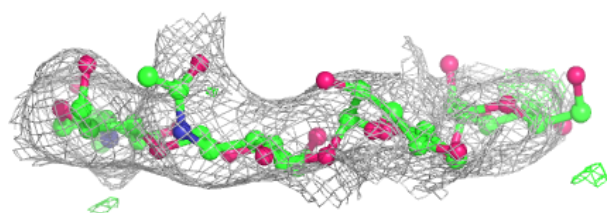
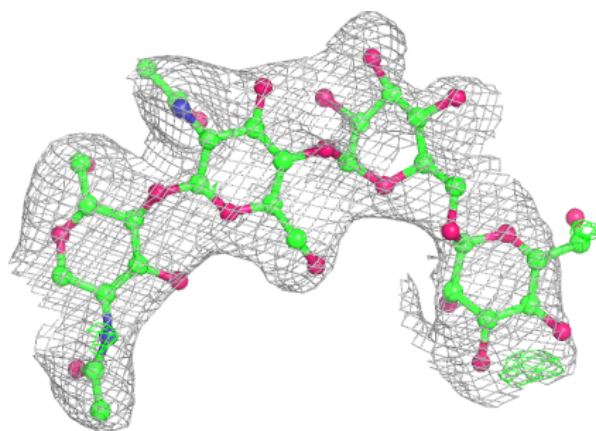
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.68	0.15	81,90,96,97	0
3	MAN	E	4	11/12	0.71	0.25	100,106,109,110	0
3	BMA	D	3	11/12	0.75	0.30	120,122,127,130	0
3	NAG	D	2	14/15	0.81	0.23	83,91,105,117	0
3	BMA	E	3	11/12	0.83	0.12	72,84,89,97	0
2	BMA	C	3	11/12	0.88	0.16	78,84,93,95	0
3	NAG	E	2	14/15	0.92	0.14	54,60,74,77	0
3	NAG	D	1	14/15	0.92	0.13	47,59,78,82	0
2	NAG	C	2	14/15	0.92	0.16	69,75,84,87	0
2	NAG	C	1	14/15	0.93	0.13	47,59,65,71	0
3	NAG	E	1	14/15	0.96	0.13	31,43,50,53	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.

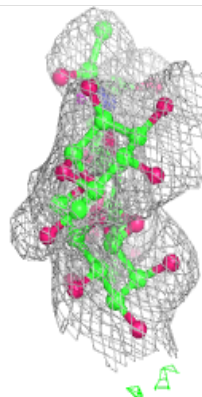
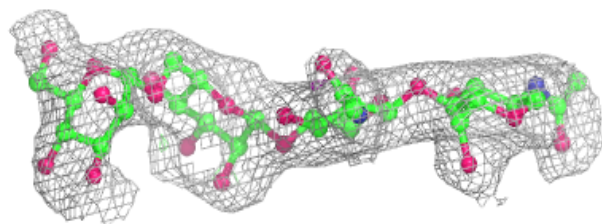
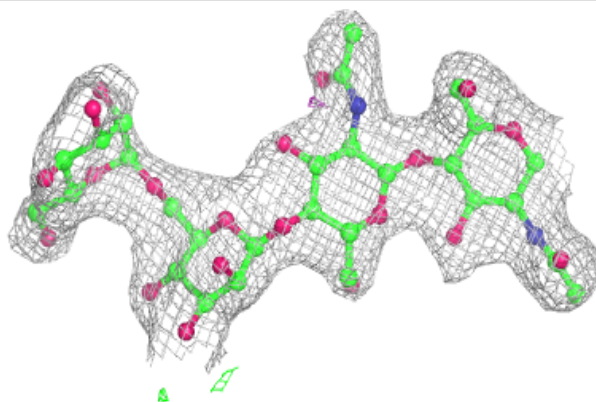


Electron density around Chain D:

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

**Electron density around Chain E:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.