



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:05 PM UTC

PDB ID : 7Q0I / pdb_00007q0i
Title : Crystal structure of the N-terminal domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-43
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-10-14
Resolution : 2.39 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

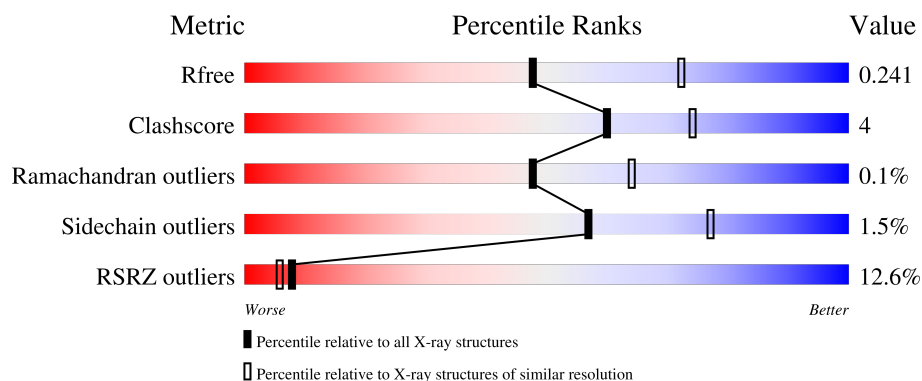
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	231	8% 92% 7%
1	H	231	6% 89% 10%
2	B	214	11% 93% 6%
2	L	214	9% 85% 14%
3	C	311	19% 78% 11% 10%

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Mol	Chain	Length	Quality of chain
3	D	311	15% 76% 13% 10%
4	E	2	100%
4	G	2	50% 50%
5	F	3	100%
6	I	2	100%
7	J	2	100%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 11604 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 Beta-43 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1721	1091	287	334	9			
1	A	229	Total	C	N	O	S	0	0	0
			1725	1094	288	334	9			

- Molecule 2 is a protein called Beta-43 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1600	1002	267	327	4			
2	B	212	Total	C	N	O	S	0	0	0
			1600	1002	267	327	4			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	280	Total	C	N	O	S	0	0	0
			2256	1468	369	411	8			
3	C	279	Total	C	N	O	S	0	0	0
			2256	1468	369	411	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	18	PHE	LEU	variant	UNP P0DTC2
D	80	ALA	ASP	variant	UNP P0DTC2
D	215	GLY	ASP	variant	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	ALA	deletion	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	243	ILE	ARG	variant	UNP P0DTC2
D	303	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	304	ASN	-	expression tag	UNP P0DTC2
D	305	ASP	-	expression tag	UNP P0DTC2
D	306	ILE	-	expression tag	UNP P0DTC2
D	307	PHE	-	expression tag	UNP P0DTC2
D	308	GLU	-	expression tag	UNP P0DTC2
D	309	ALA	-	expression tag	UNP P0DTC2
D	310	GLN	-	expression tag	UNP P0DTC2
D	311	LYS	-	expression tag	UNP P0DTC2
D	312	ILE	-	expression tag	UNP P0DTC2
D	313	GLU	-	expression tag	UNP P0DTC2
D	314	TRP	-	expression tag	UNP P0DTC2
D	315	HIS	-	expression tag	UNP P0DTC2
D	316	GLU	-	expression tag	UNP P0DTC2
D	317	LYS	-	expression tag	UNP P0DTC2
D	318	HIS	-	expression tag	UNP P0DTC2
D	319	HIS	-	expression tag	UNP P0DTC2
D	320	HIS	-	expression tag	UNP P0DTC2
D	321	HIS	-	expression tag	UNP P0DTC2
D	322	HIS	-	expression tag	UNP P0DTC2
D	323	HIS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	243	ILE	ARG	variant	UNP P0DTC2
C	303	LEU	-	expression tag	UNP P0DTC2
C	304	ASN	-	expression tag	UNP P0DTC2
C	305	ASP	-	expression tag	UNP P0DTC2
C	306	ILE	-	expression tag	UNP P0DTC2
C	307	PHE	-	expression tag	UNP P0DTC2
C	308	GLU	-	expression tag	UNP P0DTC2
C	309	ALA	-	expression tag	UNP P0DTC2
C	310	GLN	-	expression tag	UNP P0DTC2
C	311	LYS	-	expression tag	UNP P0DTC2
C	312	ILE	-	expression tag	UNP P0DTC2
C	313	GLU	-	expression tag	UNP P0DTC2
C	314	TRP	-	expression tag	UNP P0DTC2
C	315	HIS	-	expression tag	UNP P0DTC2
C	316	GLU	-	expression tag	UNP P0DTC2
C	317	LYS	-	expression tag	UNP P0DTC2

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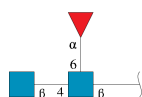
Chain	Residue	Modelled	Actual	Comment	Reference
C	318	HIS	-	expression tag	UNP P0DTC2
C	319	HIS	-	expression tag	UNP P0DTC2
C	320	HIS	-	expression tag	UNP P0DTC2
C	321	HIS	-	expression tag	UNP P0DTC2
C	322	HIS	-	expression tag	UNP P0DTC2
C	323	HIS	-	expression tag	UNP P0DTC2

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



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

- Molecule 5 is an oligosaccharide called 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
5	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

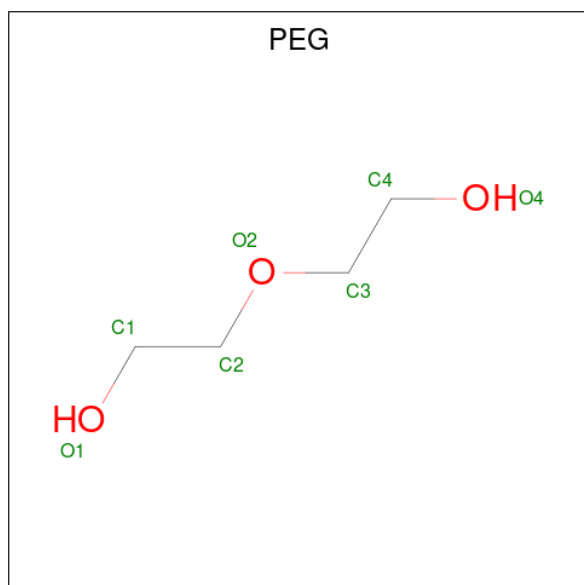
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

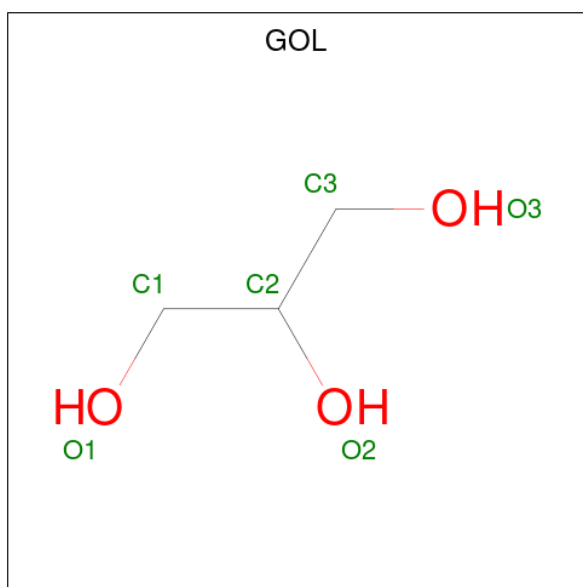
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	3	Total	Cl	0	0
			3	3		
8	L	1	Total	Cl	0	0
			1	1		
8	A	2	Total	Cl	0	0
			2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



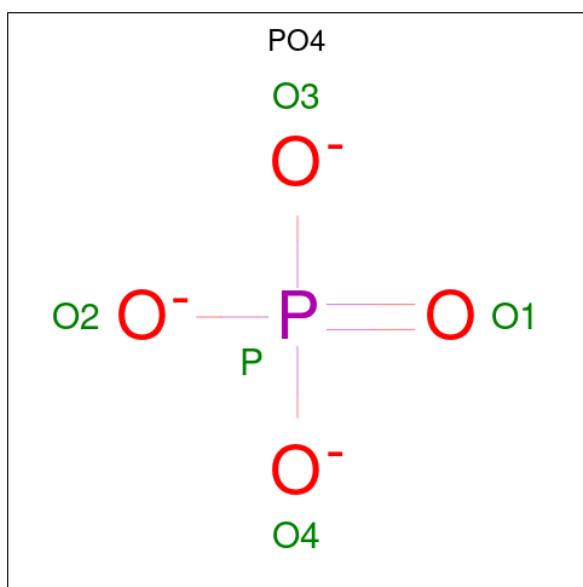
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



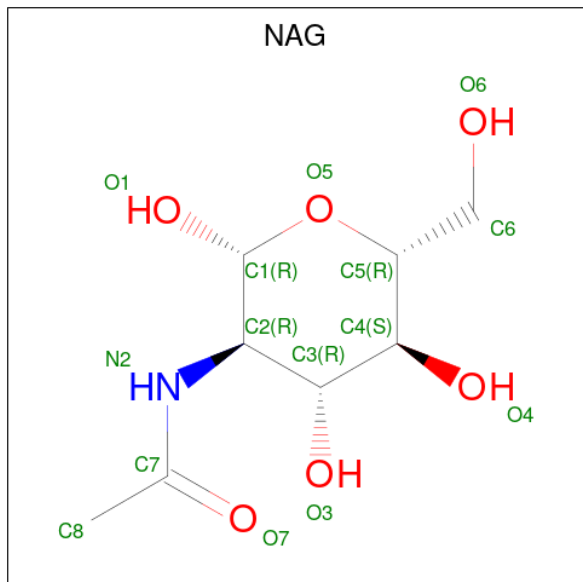
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



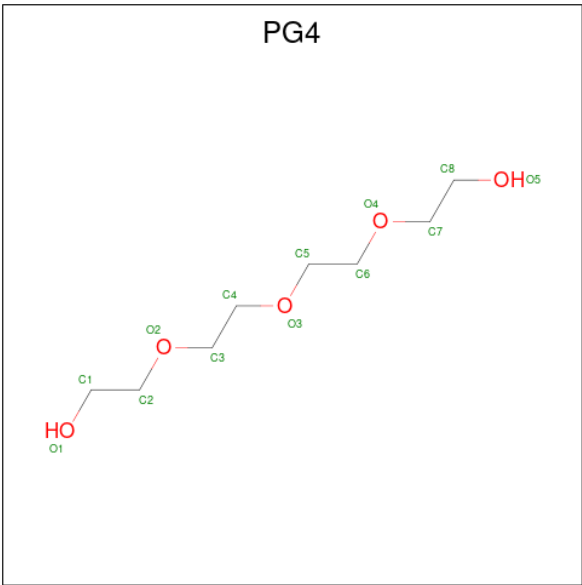
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	C	O	0	0
			13	8	5		

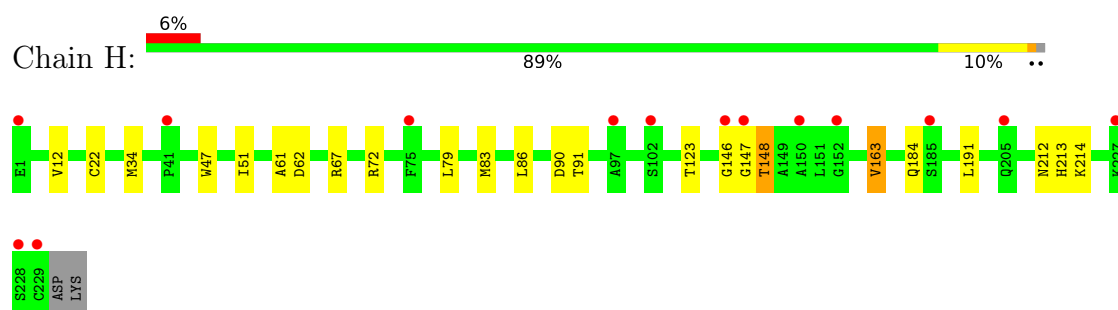
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	26	Total	O	0	0
			26	26		
14	L	27	Total	O	0	0
			27	27		
14	A	33	Total	O	0	0
			33	33		
14	B	19	Total	O	0	0
			19	19		
14	D	24	Total	O	0	0
			24	24		
14	C	28	Total	O	0	0
			28	28		

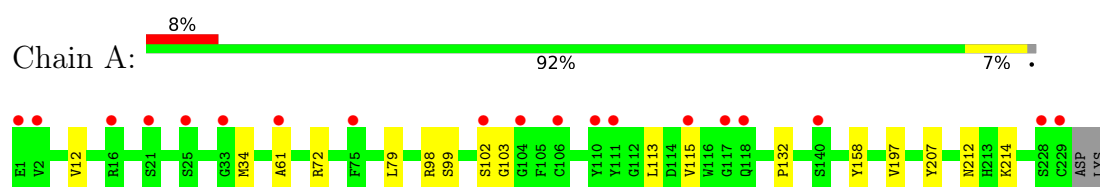
3 Residue-property plots [i](#)

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.

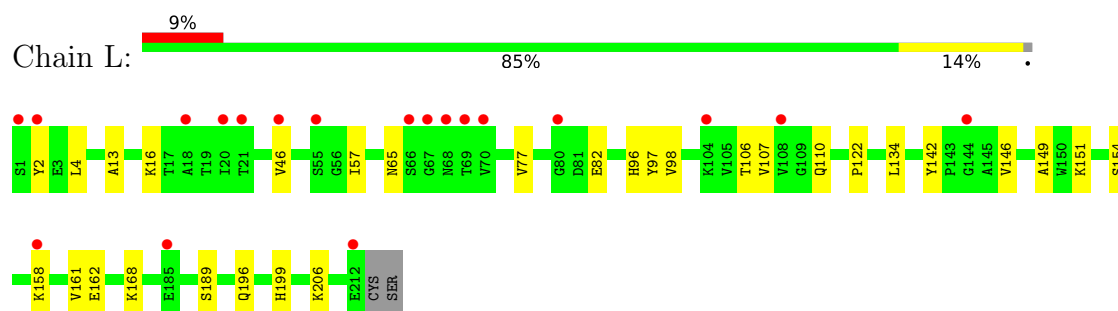
- Molecule 1: Beta-43 heavy chain



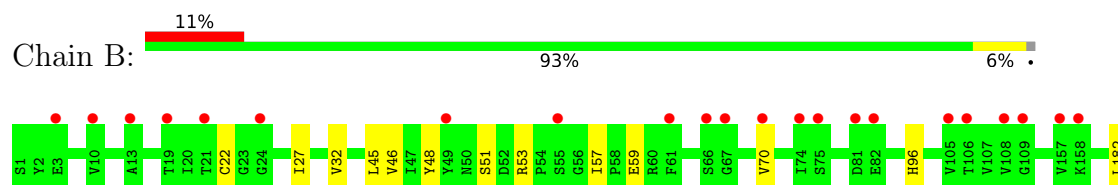
- Molecule 1: Beta-43 heavy chain

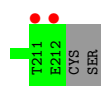


- Molecule 2: Beta-43 Fab light chain

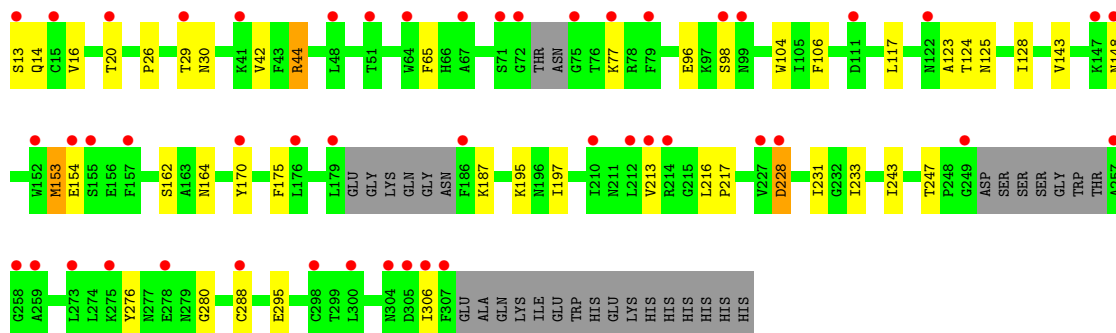
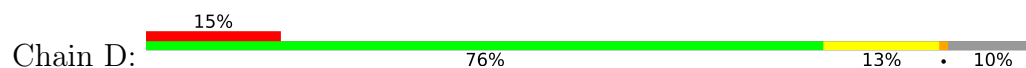


- Molecule 2: Beta-43 Fab light chain

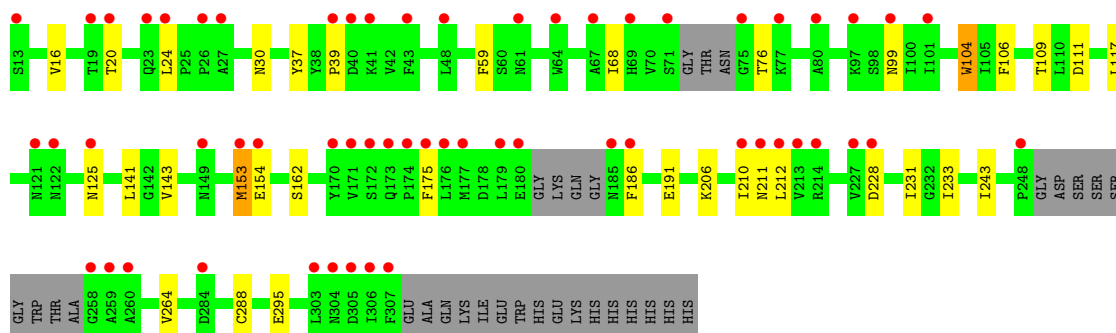
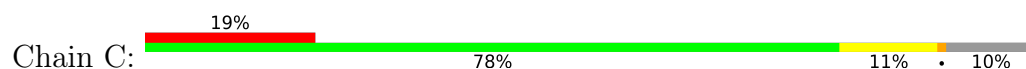




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



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



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



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain I:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.83Å 66.96Å 143.24Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	143.10 – 2.39 143.10 – 2.39	Depositor EDS
% Data completeness (in resolution range)	67.9 (143.10-2.39) 68.2 (143.10-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.202 , 0.242 0.203 , 0.241	Depositor DCC
R_{free} test set	2931 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11604	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: NAG, PG4, CL, FUC, PO4, PEG, GOL

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	0.14	0/1771	0.32	0/2411
1	H	0.13	0/1767	0.31	0/2407
2	B	0.15	0/1642	0.35	0/2249
2	L	0.13	0/1642	0.32	0/2249
3	C	0.17	0/2319	0.36	0/3154
3	D	0.18	0/2319	0.36	0/3153
All	All	0.15	0/11460	0.34	0/15623

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1663	11	0
1	H	1721	0	1652	19	0
2	B	1600	0	1537	9	0
2	L	1600	0	1537	23	0
3	C	2256	0	2186	17	0
3	D	2256	0	2187	28	0
4	E	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	24	0	22	1	0
5	F	38	0	34	0	0
6	I	28	0	25	0	0
7	J	28	0	25	0	0
8	A	2	0	0	0	0
8	H	3	0	0	0	0
8	L	1	0	0	0	0
9	L	7	0	10	0	0
10	A	6	0	8	0	0
10	B	6	0	8	0	0
10	L	6	0	8	0	0
11	B	5	0	0	0	0
12	C	42	0	39	0	0
12	D	56	0	52	1	0
13	D	13	0	18	0	0
14	A	33	0	0	0	0
14	B	19	0	0	0	0
14	C	28	0	0	0	0
14	D	24	0	0	0	0
14	H	26	0	0	0	0
14	L	27	0	0	1	0
All	All	11604	0	11033	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.

All (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:H:67:ARG:NH2	1:H:90:ASP:OD2	2.18	0.77
3:D:143:VAL:HG12	3:D:154:GLU:HB3	1.69	0.72
3:D:123:ALA:N	3:D:154:GLU:OE2	2.21	0.69
3:C:143:VAL:HG12	3:C:154:GLU:HB3	1.80	0.63
1:H:62:ASP:H	2:L:96:HIS:HE1	1.49	0.59
3:C:211:ASN:OD1	3:C:212:LEU:N	2.35	0.59
1:A:61:ALA:HA	2:B:96:HIS:CE1	2.38	0.58
3:D:187:LYS:NZ	3:D:213:VAL:O	2.37	0.57
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.86	0.57
1:A:132:PRO:HB3	1:A:158:TYR:HB3	1.88	0.55
3:C:141:LEU:HB3	3:C:243:ILE:HD12	1.87	0.55
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:228:ASP:N	3:D:228:ASP:OD1	2.40	0.55
2:B:22:CYS:HB3	2:B:70:VAL:HG13	1.88	0.55
3:C:109:THR:OG1	3:C:111:ASP:OD1	2.24	0.54
3:D:104:TRP:HB2	3:D:106:PHE:CE1	2.43	0.53
3:D:216:LEU:HD12	3:D:217:PRO:HD2	1.90	0.53
2:B:27:ILE:HD13	2:B:70:VAL:HG11	1.90	0.52
1:H:163:VAL:HG12	1:H:213:HIS:CD2	2.45	0.52
1:A:61:ALA:HA	2:B:96:HIS:HE1	1.75	0.52
3:D:128:ILE:HB	3:D:170:TYR:HB3	1.92	0.51
2:L:2:TYR:HB3	2:L:98:VAL:HG21	1.93	0.51
2:L:146:VAL:HG12	2:L:199:HIS:HB2	1.94	0.50
2:L:206:LYS:NZ	14:L:505:HOH:O	2.43	0.50
3:D:106:PHE:HB2	3:D:117:LEU:HB3	1.92	0.50
3:D:124:THR:O	3:D:175:PHE:N	2.40	0.50
2:L:82:GLU:OE1	2:L:168:LYS:NZ	2.43	0.50
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.93	0.49
1:H:34:MET:HG2	1:H:72:ARG:NH2	2.28	0.49
2:L:82:GLU:HG3	2:L:107:VAL:HG23	1.94	0.49
3:D:143:VAL:HG13	3:D:243:ILE:HD11	1.95	0.49
3:D:231:ILE:HD12	3:D:233:ILE:HG12	1.94	0.49
1:A:102:SER:HB2	3:D:247:THR:O	2.13	0.49
3:C:231:ILE:HD12	3:C:233:ILE:HG12	1.94	0.49
3:C:24:LEU:HD21	3:C:68:ILE:HD11	1.94	0.48
3:C:228:ASP:OD1	3:C:228:ASP:N	2.45	0.48
2:L:82:GLU:HG2	2:L:106:THR:HA	1.95	0.48
2:B:46:VAL:HA	2:B:57:ILE:HG13	1.94	0.48
3:C:20:THR:OG1	3:C:76:THR:O	2.25	0.48
2:L:122:PRO:HD3	2:L:134:LEU:HD23	1.94	0.48
3:D:125:ASN:HA	3:D:175:PHE:CE2	2.48	0.48
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.96	0.48
1:A:99:SER:HB3	1:A:113:LEU:HD23	1.97	0.47
1:H:47:TRP:CG	2:L:97:TYR:HB2	2.50	0.47
3:C:191:GLU:HG3	3:C:206:LYS:HB3	1.96	0.46
1:H:62:ASP:N	2:L:96:HIS:HE1	2.10	0.46
1:H:163:VAL:HG22	1:H:191:LEU:HD21	1.98	0.46
2:L:110:GLN:HB2	2:L:142:TYR:CE1	2.49	0.46
3:D:143:VAL:HA	3:D:154:GLU:HA	1.97	0.46
3:C:104:TRP:HB2	3:C:106:PHE:CE1	2.51	0.46
1:H:12:VAL:HG21	1:H:86:LEU:HD12	1.98	0.45
2:L:46:VAL:HA	2:L:57:ILE:HG13	1.97	0.45
3:D:20:THR:OG1	3:D:77:LYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:CYS:O	3:C:295:GLU:HG3	2.17	0.45
2:L:189:SER:HB3	3:D:42:VAL:HG13	1.99	0.45
3:D:29:THR:HG22	3:D:30:ASN:H	1.83	0.44
1:H:146:GLY:O	1:H:148:THR:N	2.47	0.44
3:C:30:ASN:OD1	3:C:59:PHE:HA	2.17	0.44
3:C:37:TYR:O	3:C:39:PRO:HD3	2.18	0.44
3:D:153:MET:HE2	3:D:153:MET:HB3	1.79	0.44
1:H:184:GLN:HG2	2:L:162:GLU:HG3	2.00	0.44
1:H:212:ASN:HD21	1:H:214:LYS:HE3	1.83	0.43
1:A:212:ASN:HD21	1:A:214:LYS:HE2	1.83	0.43
3:D:44:ARG:O	3:D:280:GLY:HA2	2.18	0.43
2:B:45:LEU:HD21	2:B:48:TYR:HB3	1.99	0.43
2:B:53:ARG:NH2	2:B:59:GLU:HG2	2.34	0.43
1:H:51:ILE:HD13	1:H:72:ARG:HG2	2.01	0.43
3:D:26:PRO:HB3	3:D:65:PHE:CE2	2.53	0.43
1:H:91:THR:HG23	1:H:123:THR:HA	2.01	0.42
2:L:16:LYS:O	2:L:77:VAL:HG23	2.19	0.42
1:A:34:MET:HG2	1:A:72:ARG:NH2	2.34	0.42
3:D:44:ARG:HB3	3:D:276:TYR:CG	2.55	0.42
3:D:164:ASN:CB	4:G:1:NAG:H82	2.50	0.42
1:H:61:ALA:HA	2:L:96:HIS:CE1	2.54	0.42
3:D:96:GLU:HG3	3:D:98:SER:O	2.19	0.42
3:C:153:MET:HE2	3:C:153:MET:HB3	1.73	0.42
1:H:62:ASP:H	2:L:96:HIS:CE1	2.33	0.42
3:D:288:CYS:O	3:D:295:GLU:HG3	2.19	0.42
12:D:404:NAG:O7	12:D:404:NAG:H3	2.20	0.42
3:D:195:LYS:HG2	3:D:197:ILE:HG12	2.02	0.42
2:B:32:VAL:HG21	2:B:70:VAL:HG21	2.03	0.41
1:A:197:VAL:HG11	1:A:207:TYR:CE1	2.55	0.41
2:B:51:SER:OG	3:D:148:ASN:ND2	2.47	0.41
2:L:107:VAL:O	2:L:142:TYR:OH	2.34	0.41
2:L:149:ALA:HB3	2:L:196:GLN:HB3	2.01	0.41
2:L:151:LYS:HE2	2:L:154:SER:HA	2.02	0.41
1:A:98:ARG:HG2	1:A:115:VAL:HB	2.03	0.41
1:H:47:TRP:CE2	2:L:97:TYR:HD2	2.38	0.41
3:C:210:ILE:HD12	3:C:210:ILE:HA	1.77	0.41
1:A:102:SER:OG	1:A:103:GLY:N	2.53	0.40
3:D:13:SER:OG	3:D:14:GLN:N	2.55	0.40
2:L:13:ALA:HB3	2:L:16:LYS:HD2	2.03	0.40
3:C:106:PHE:HB2	3:C:117:LEU:HB3	2.02	0.40
2:L:4:LEU:HD23	2:L:4:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:PRO:HB3	3:D:65:PHE:HE2	1.86	0.40
3:C:125:ASN:HA	3:C:175:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/231 (98%)	221 (97%)	6 (3%)	0	100	100
1	H	227/231 (98%)	217 (96%)	9 (4%)	1 (0%)	30	43
2	B	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
2	L	210/214 (98%)	200 (95%)	9 (4%)	1 (0%)	24	37
3	C	271/311 (87%)	258 (95%)	13 (5%)	0	100	100
3	D	272/311 (88%)	259 (95%)	13 (5%)	0	100	100
All	All	1417/1512 (94%)	1357 (96%)	58 (4%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	158	LYS
1	H	147	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	191/193 (99%)	190 (100%)	1 (0%)	81	91
1	H	190/193 (98%)	188 (99%)	2 (1%)	65	82
2	B	181/183 (99%)	180 (99%)	1 (1%)	78	89
2	L	181/183 (99%)	179 (99%)	2 (1%)	65	82
3	C	253/279 (91%)	246 (97%)	7 (3%)	38	60
3	D	252/279 (90%)	246 (98%)	6 (2%)	43	65
All	All	1248/1310 (95%)	1229 (98%)	19 (2%)	57	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	148	THR
1	H	163	VAL
2	L	65	ASN
2	L	161	VAL
1	A	12	VAL
2	B	182	LEU
3	D	16	VAL
3	D	44	ARG
3	D	153	MET
3	D	162	SER
3	D	228	ASP
3	D	306	ILE
3	C	16	VAL
3	C	99	ASN
3	C	104	TRP
3	C	153	MET
3	C	162	SER
3	C	186	PHE
3	C	264	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	96	HIS
2	L	110	GLN
2	L	186	GLN
2	B	96	HIS
3	D	121	ASN
3	C	49	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 ⓘ

11 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	$\# Z > 2$
4	NAG	E	1	3,4	14,14,15	0.28	0	17,19,21	0.51	0
4	FUC	E	2	4	10,10,11	0.74	0	14,14,16	0.78	0
5	NAG	F	1	3,5	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	F	2	5	14,14,15	0.36	0	17,19,21	0.51	0
5	FUC	F	3	5	10,10,11	0.92	0	14,14,16	0.70	0
4	NAG	G	1	3,4	14,14,15	0.40	0	17,19,21	0.50	0
4	FUC	G	2	4	10,10,11	0.80	0	14,14,16	0.80	0
6	NAG	I	1	3,6	14,14,15	0.15	0	17,19,21	0.56	0
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.44	0
7	NAG	J	1	3,7	14,14,15	0.22	0	17,19,21	0.56	0
7	NAG	J	2	7	14,14,15	0.21	0	19,19,21	0.30	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
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
5	NAG	F	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	F	3	5	-	-	0/1/1/1
4	NAG	G	1	3,4	-	0/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
6	NAG	I	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
7	NAG	J	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/22/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

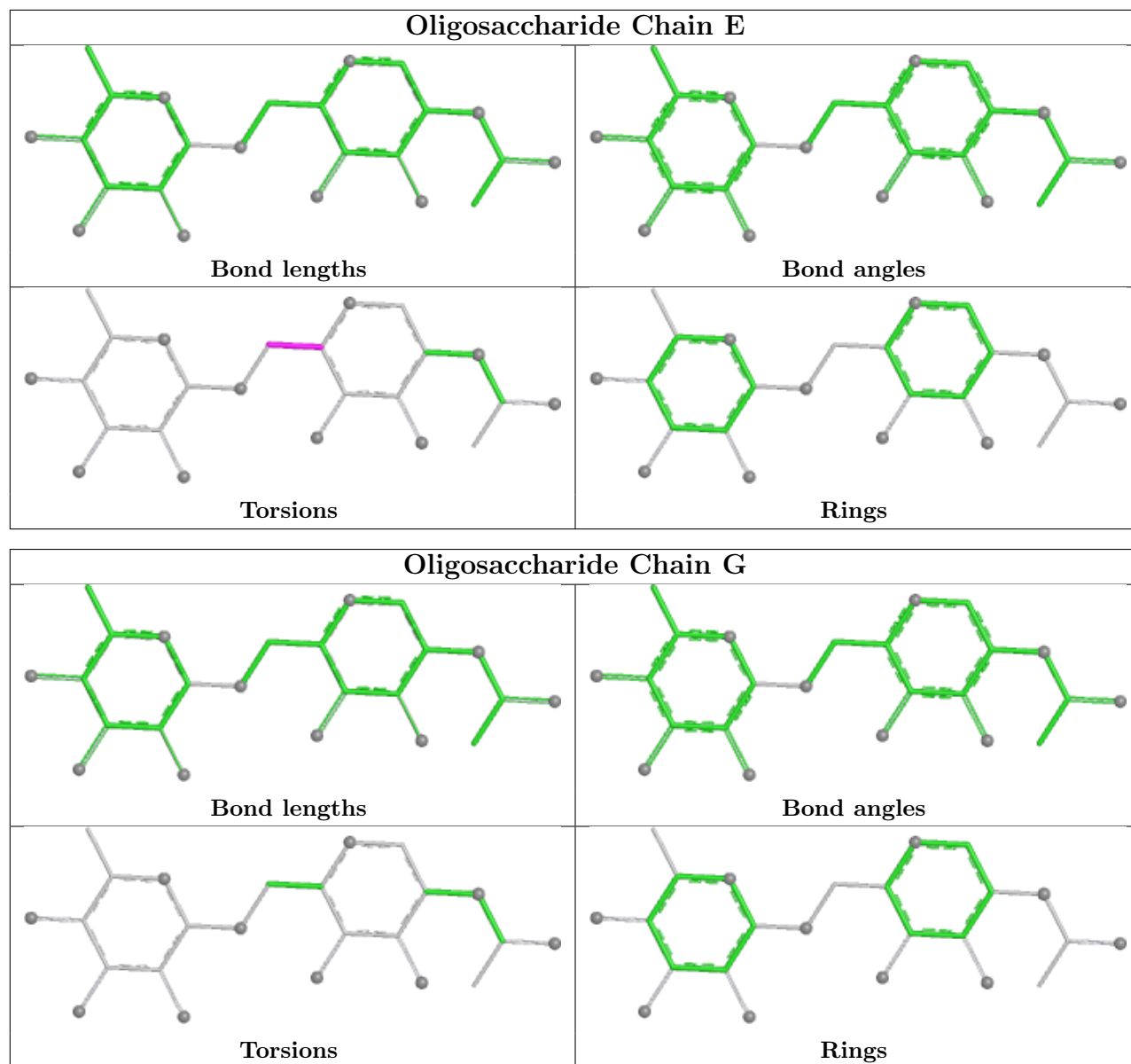
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6

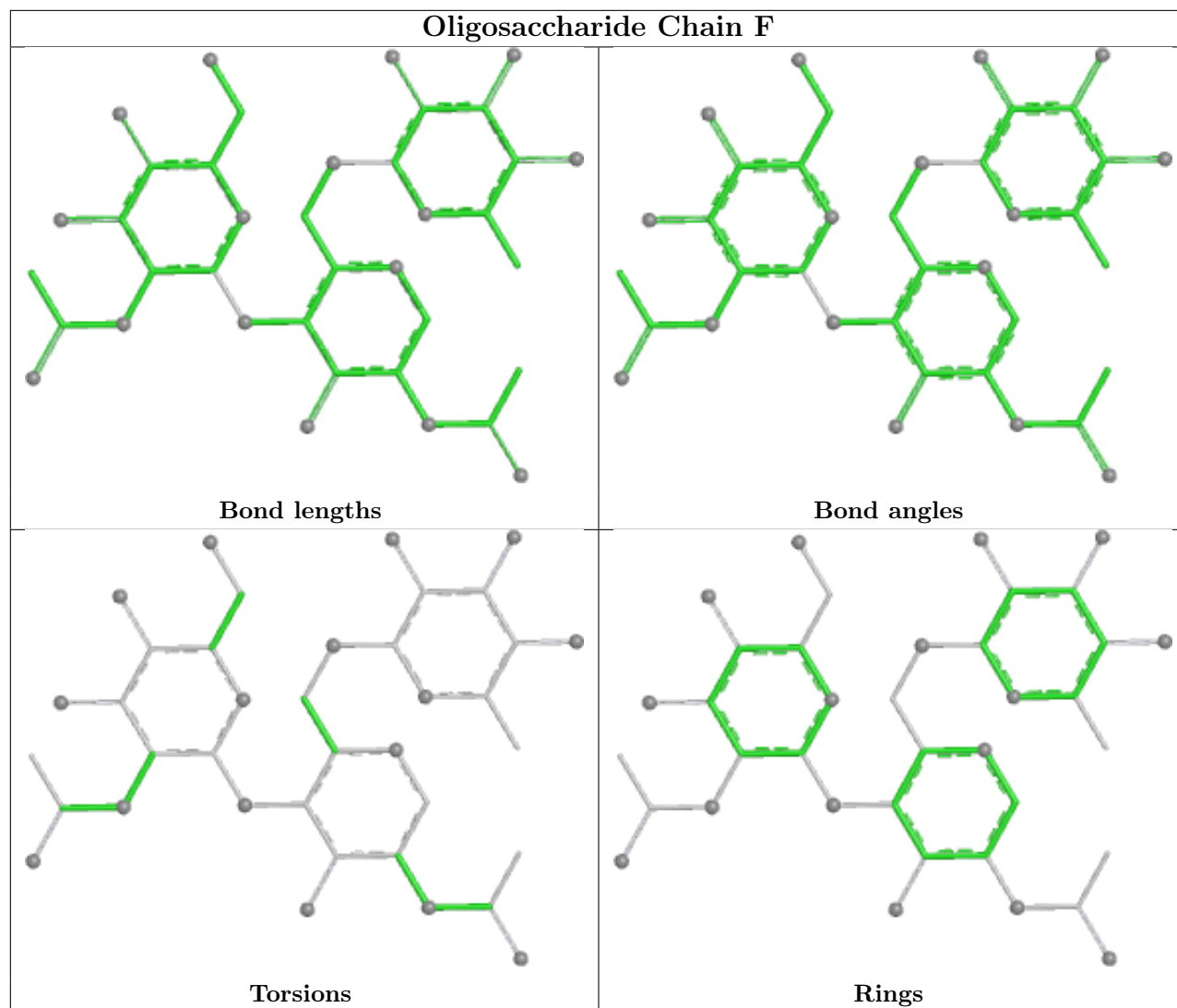
There are no ring outliers.

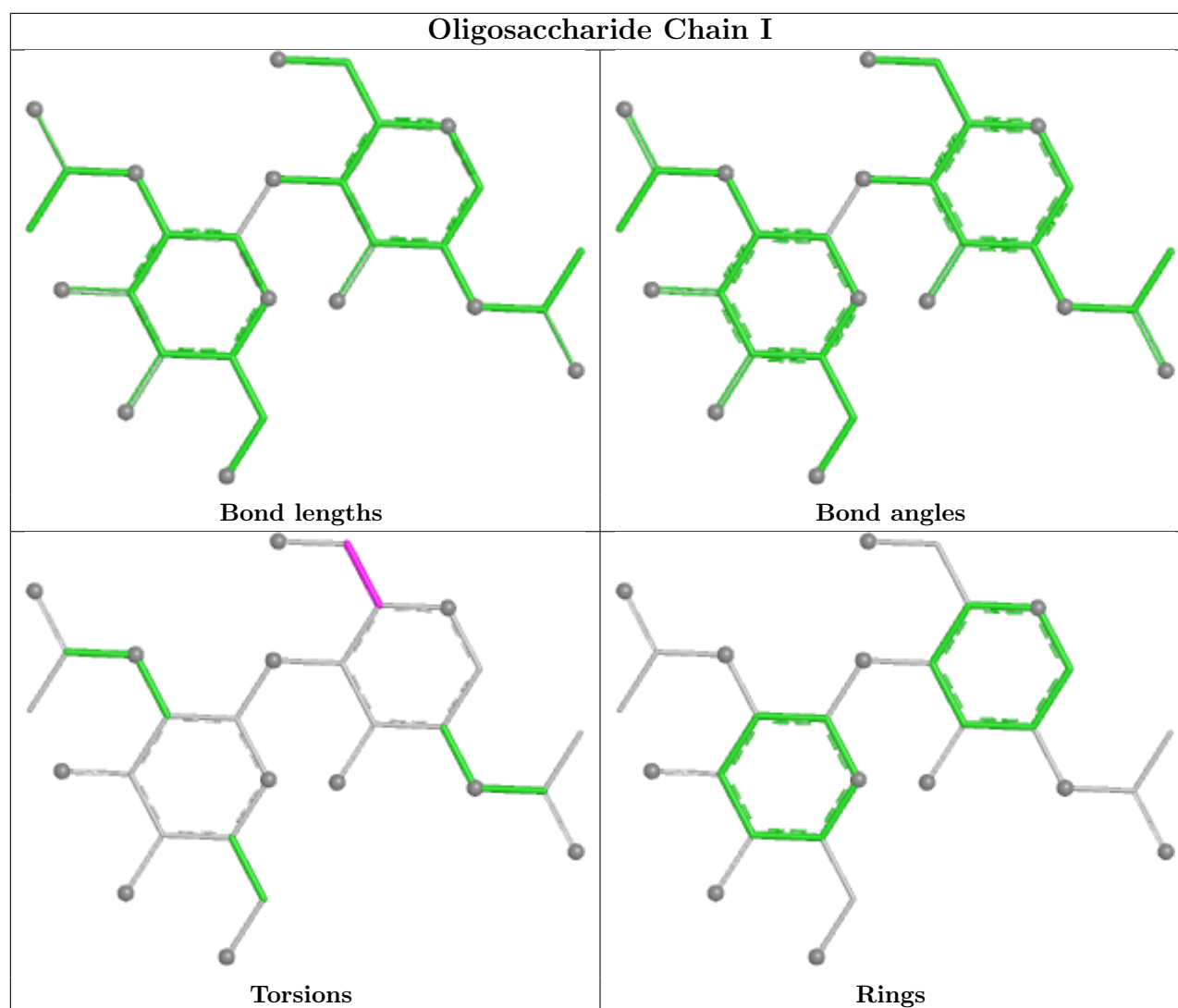
1 monomer is involved in 1 short contact:

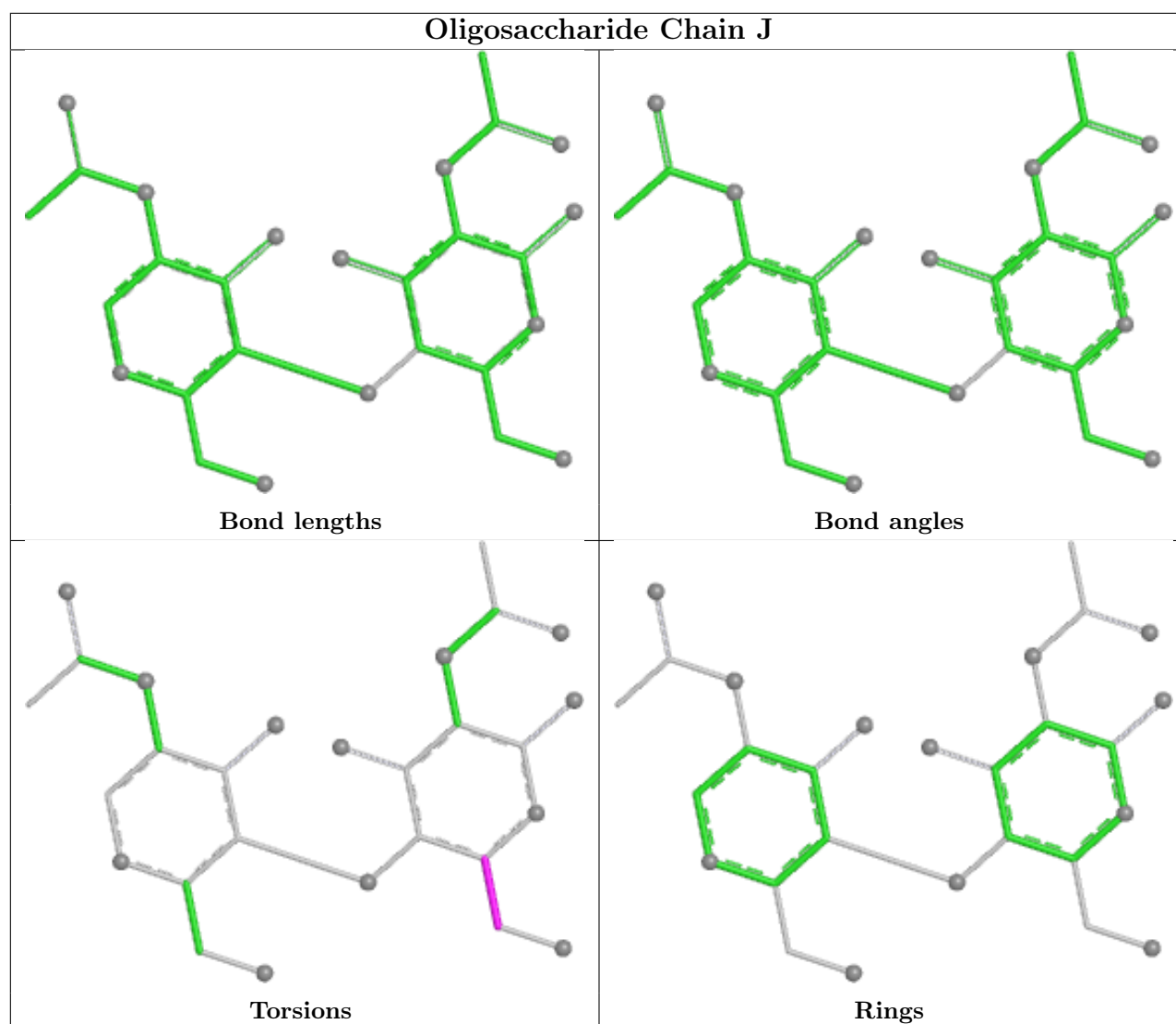
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

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](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\# Z > 2$
9	PEG	L	401	-	6,6,6	0.12	0	5,5,5	0.08	0
12	NAG	C	402	3	14,14,15	0.37	0	17,19,21	0.57	0
12	NAG	D	403	3	14,14,15	0.47	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	D	401	3	14,14,15	0.44	0	17,19,21	0.59	0
10	GOL	L	402	-	5,5,5	0.85	0	5,5,5	1.13	1 (20%)
10	GOL	B	301	-	5,5,5	0.90	0	5,5,5	1.12	1 (20%)
13	PG4	D	405	-	12,12,12	0.15	0	11,11,11	0.63	0
11	PO4	B	302	-	4,4,4	0.93	0	6,6,6	0.41	0
12	NAG	C	403	3	14,14,15	0.44	0	17,19,21	0.48	0
10	GOL	A	301	-	5,5,5	1.02	0	5,5,5	0.91	0
12	NAG	C	401	3	14,14,15	0.29	0	17,19,21	0.36	0
12	NAG	D	404	3	14,14,15	0.31	0	17,19,21	0.97	2 (11%)
12	NAG	D	402	3	14,14,15	0.36	0	17,19,21	0.52	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
9	PEG	L	401	-	-	3/4/4/4	-
12	NAG	C	402	3	-	0/6/23/26	0/1/1/1
12	NAG	D	403	3	-	0/6/23/26	0/1/1/1
12	NAG	D	401	3	-	1/6/23/26	0/1/1/1
10	GOL	L	402	-	-	4/4/4/4	-
10	GOL	B	301	-	-	2/4/4/4	-
13	PG4	D	405	-	-	6/10/10/10	-
12	NAG	C	403	3	-	0/6/23/26	0/1/1/1
10	GOL	A	301	-	-	3/4/4/4	-
12	NAG	C	401	3	-	1/6/23/26	0/1/1/1
12	NAG	D	404	3	-	1/6/23/26	0/1/1/1
12	NAG	D	402	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	404	NAG	C2-N2-C7	2.64	126.44	122.90
12	D	404	NAG	C1-O5-C5	2.31	115.28	112.19
10	B	301	GOL	C3-C2-C1	-2.02	104.37	111.80
10	L	402	GOL	C3-C2-C1	-2.01	104.44	111.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	402	GOL	O1-C1-C2-C3
10	L	402	GOL	C1-C2-C3-O3
12	D	404	NAG	C3-C2-N2-C7
13	D	405	PG4	O3-C5-C6-O4
13	D	405	PG4	O1-C1-C2-O2
12	D	402	NAG	O5-C5-C6-O6
9	L	401	PEG	C1-C2-O2-C3
10	A	301	GOL	C1-C2-C3-O3
10	B	301	GOL	C1-C2-C3-O3
10	L	402	GOL	O1-C1-C2-O2
10	L	402	GOL	O2-C2-C3-O3
13	D	405	PG4	O2-C3-C4-O3
9	L	401	PEG	O2-C3-C4-O4
10	B	301	GOL	O2-C2-C3-O3
13	D	405	PG4	C3-C4-O3-C5
12	D	402	NAG	C4-C5-C6-O6
13	D	405	PG4	C6-C5-O3-C4
10	A	301	GOL	O2-C2-C3-O3
9	L	401	PEG	O1-C1-C2-O2
12	D	401	NAG	C4-C5-C6-O6
12	C	401	NAG	C1-C2-N2-C7
10	A	301	GOL	O1-C1-C2-O2
13	D	405	PG4	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	404	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, 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	229/231 (99%)	0.70	19 (8%)	17 14	26, 46, 70, 119	0
1	H	229/231 (99%)	0.67	14 (6%)	27 23	30, 45, 67, 120	0
2	B	212/214 (99%)	0.83	24 (11%)	10 7	25, 49, 86, 103	0
2	L	212/214 (99%)	0.77	19 (8%)	15 12	34, 51, 80, 107	0
3	C	279/311 (89%)	1.30	58 (20%)	2 2	33, 51, 103, 129	0
3	D	280/311 (90%)	1.16	48 (17%)	4 3	27, 49, 85, 129	0
All	All	1441/1512 (95%)	0.93	182 (12%)	8 6	25, 48, 86, 129	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	257	ALA	8.3
3	C	307	PHE	7.4
3	C	67	ALA	7.4
3	D	72	GLY	7.3
3	D	306	ILE	6.5
3	C	180	GLU	6.3
3	C	306	ILE	6.2
3	C	212	LEU	6.0
1	A	75	PHE	5.8
3	D	307	PHE	5.7
3	C	71	SER	5.6
3	C	186	PHE	5.6
1	H	75	PHE	5.4
3	D	186	PHE	5.4
1	H	229	CYS	5.2
3	C	175	PHE	5.2
3	D	249	GLY	5.1
3	C	258	GLY	4.7
3	C	77	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	4.5
3	C	176	LEU	4.5
3	C	214	ARG	4.5
2	L	66	SER	4.2
3	C	177	MET	4.2
3	D	214	ARG	4.2
1	H	97	ALA	4.1
2	B	61	PHE	4.0
1	A	1	GLU	3.9
1	H	146	GLY	3.9
2	B	109	GLY	3.9
3	C	172	SER	3.8
3	D	213	VAL	3.8
3	D	305	ASP	3.8
2	B	70	VAL	3.8
3	C	303	LEU	3.7
3	C	170	TYR	3.7
1	A	33	GLY	3.7
3	D	170	TYR	3.7
3	C	260	ALA	3.6
2	L	158	LYS	3.6
2	L	20	ILE	3.6
3	C	75	GLY	3.6
1	A	111	TYR	3.5
2	L	212	GLU	3.5
1	H	102	SER	3.5
3	C	304	ASN	3.5
3	D	13	SER	3.4
2	B	81	ASP	3.4
3	D	77	LYS	3.4
2	L	68	ASN	3.4
3	C	149	ASN	3.4
3	D	228	ASP	3.4
3	C	121	ASN	3.4
3	C	305	ASP	3.4
3	C	101	ILE	3.3
3	C	210	ILE	3.3
3	D	67	ALA	3.3
3	C	211	ASN	3.3
3	C	13	SER	3.2
3	D	20	THR	3.2
3	C	173	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	210	ILE	3.1
2	L	1	SER	3.1
1	H	227	LYS	3.1
3	D	51	THR	3.1
3	C	20	THR	3.1
1	A	228	SER	3.1
2	B	105	VAL	3.1
2	B	108	VAL	3.1
3	D	176	LEU	3.1
3	C	41	LYS	3.0
3	C	259	ALA	3.0
3	D	273	LEU	3.0
2	B	49	TYR	3.0
3	D	71	SER	3.0
3	D	75	GLY	3.0
1	H	41	PRO	3.0
3	D	227	VAL	3.0
1	H	228	SER	3.0
2	L	55	SER	3.0
3	C	80	ALA	2.9
3	D	304	ASN	2.9
2	B	212	GLU	2.9
3	D	258	GLY	2.9
3	C	40	ASP	2.9
1	A	61	ALA	2.9
3	C	48	LEU	2.9
1	A	2	VAL	2.9
2	B	10	VAL	2.9
1	A	229	CYS	2.9
2	B	55	SER	2.8
1	A	110	TYR	2.8
3	C	39	PRO	2.8
1	A	118	GLN	2.8
2	B	106	THR	2.8
3	C	125	ASN	2.8
1	A	117	GLY	2.8
3	C	174	PRO	2.8
2	B	74	ILE	2.7
3	D	298	CYS	2.7
2	L	2	TYR	2.7
2	B	21	THR	2.7
3	D	98	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	26	PRO	2.7
2	L	70	VAL	2.7
3	C	171	VAL	2.7
3	D	300	LEU	2.6
2	B	13	ALA	2.6
3	D	259	ALA	2.6
1	A	16	ARG	2.6
2	B	75	SER	2.6
3	C	185	ASN	2.6
1	H	147	GLY	2.6
3	D	155	SER	2.6
1	H	150	ALA	2.5
3	C	153	MET	2.5
2	B	158	LYS	2.5
3	C	284	ASP	2.5
3	D	148	ASN	2.5
3	C	97	LYS	2.5
2	B	211	THR	2.5
1	A	115	VAL	2.5
3	C	213	VAL	2.5
3	D	179	LEU	2.5
3	D	122	ASN	2.5
2	L	21	THR	2.4
1	H	185	SER	2.4
2	B	66	SER	2.4
3	D	79	PHE	2.4
3	C	179	LEU	2.4
3	C	69	HIS	2.4
3	C	227	VAL	2.4
3	C	61	ASN	2.4
3	C	122	ASN	2.4
2	B	19	THR	2.4
2	B	157	VAL	2.4
3	D	64	TRP	2.4
2	B	3	GLU	2.4
3	C	248	PRO	2.4
3	D	99	ASN	2.3
2	L	108	VAL	2.3
3	D	157	PHE	2.3
3	D	48	LEU	2.3
1	A	102	SER	2.3
1	H	1	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	205	GLN	2.3
3	D	111	ASP	2.3
3	D	147	LYS	2.3
3	C	99	ASN	2.3
3	C	64	TRP	2.3
2	L	69	THR	2.3
3	D	278	GLU	2.3
3	D	41	LYS	2.3
3	C	24	LEU	2.3
3	C	228	ASP	2.3
2	L	80	GLY	2.2
3	C	23	GLN	2.2
3	C	19	THR	2.2
3	D	152	TRP	2.2
3	D	212	LEU	2.2
2	L	46	VAL	2.2
2	B	24	GLY	2.2
3	D	15	CYS	2.2
3	D	288	CYS	2.2
2	L	185	GLU	2.2
3	D	275	LYS	2.2
2	L	67	GLY	2.2
1	A	25	SER	2.2
1	A	140	SER	2.2
1	A	21	SER	2.1
2	B	82	GLU	2.1
3	C	43	PHE	2.1
2	B	67	GLY	2.1
3	D	29	THR	2.1
1	H	152	GLY	2.1
2	L	144	GLY	2.1
1	A	106	CYS	2.1
2	L	18	ALA	2.1
3	C	154	GLU	2.0
3	D	154	GLU	2.0
3	C	27	ALA	2.0
2	L	104	LYS	2.0

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

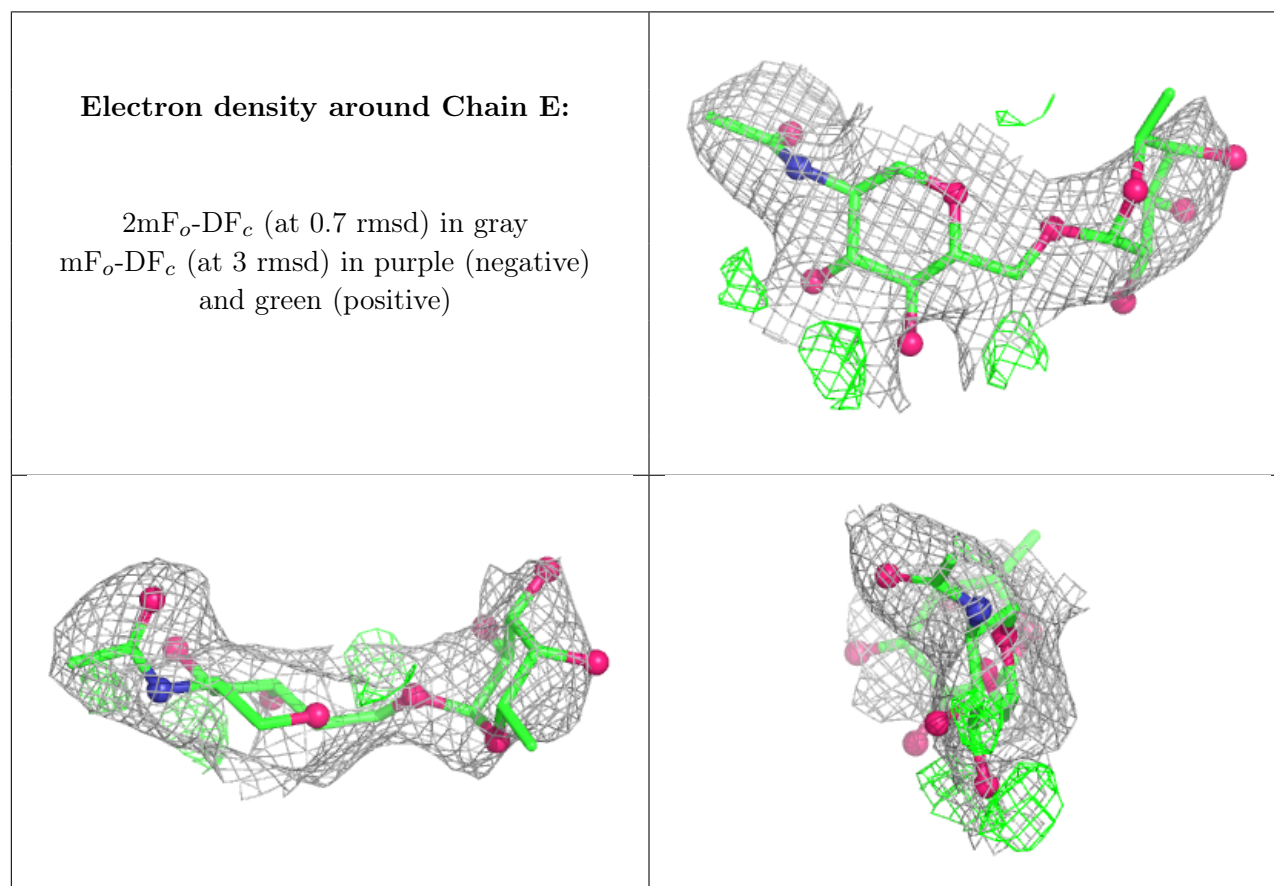
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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.

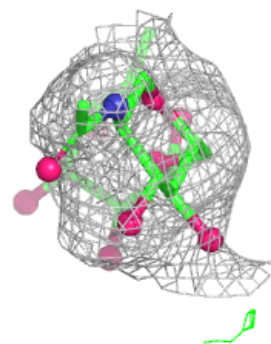
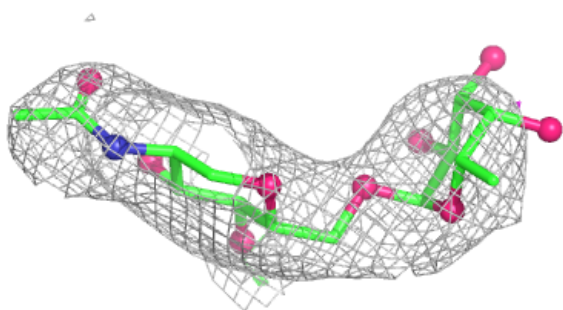
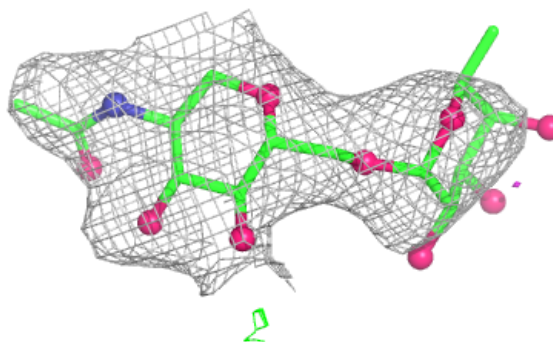
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	-	-	51,76,87,96	0
4	FUC	E	2	10/11	-	-	84,98,108,109	0
4	FUC	G	2	10/11	0.68	0.20	73,86,92,93	0
4	NAG	G	1	14/15	0.71	0.17	49,59,68,86	0
5	NAG	F	1	14/15	-	-	39,61,80,86	0
5	NAG	F	2	14/15	-	-	69,90,104,107	0
5	FUC	F	3	10/11	-	-	67,78,86,89	0
7	NAG	J	2	14/15	0.72	0.21	81,104,127,128	0
6	NAG	I	2	14/15	-	-	81,96,110,113	0
7	NAG	J	1	14/15	0.77	0.15	71,95,99,102	0
6	NAG	I	1	14/15	0.85	0.13	36,58,81,83	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.



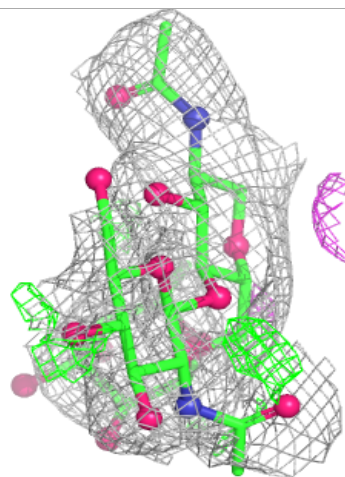
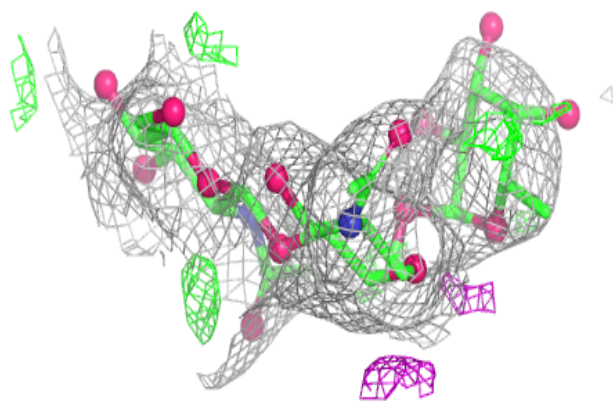
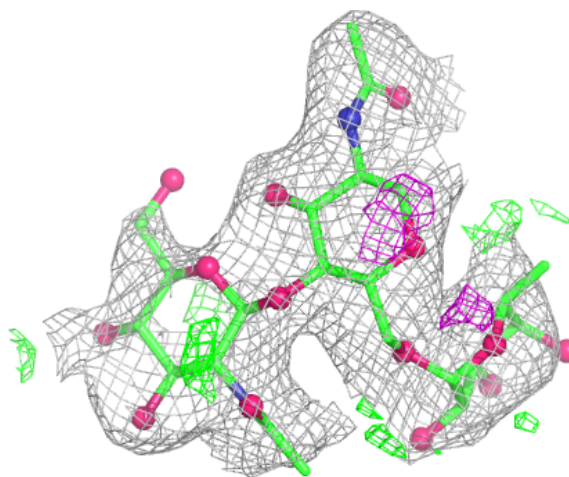
Electron density around Chain G:

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



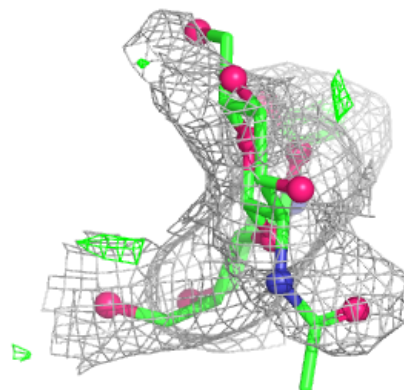
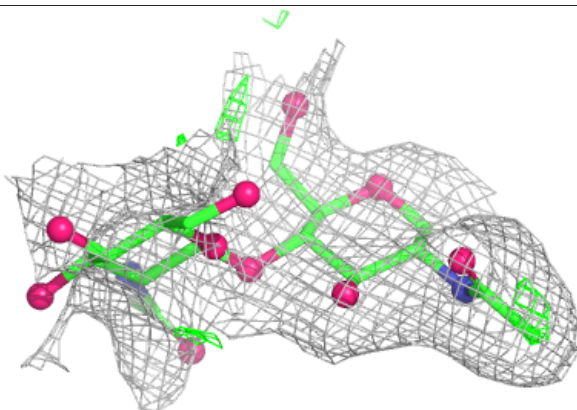
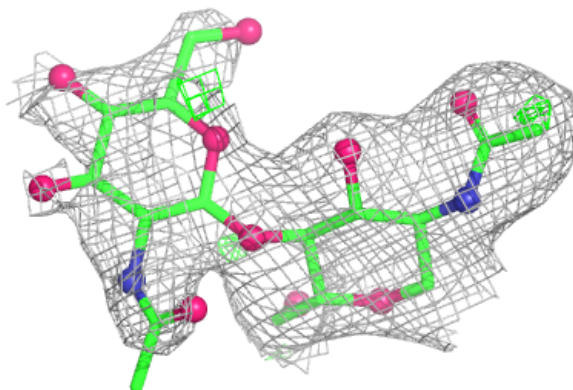
Electron density around Chain F:

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

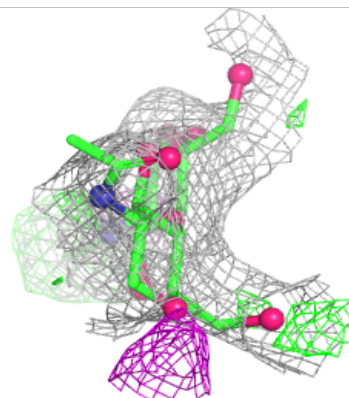
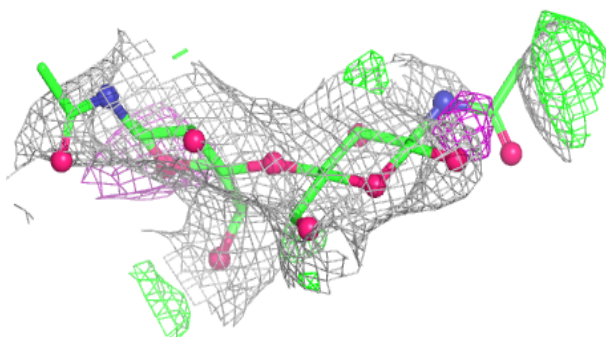
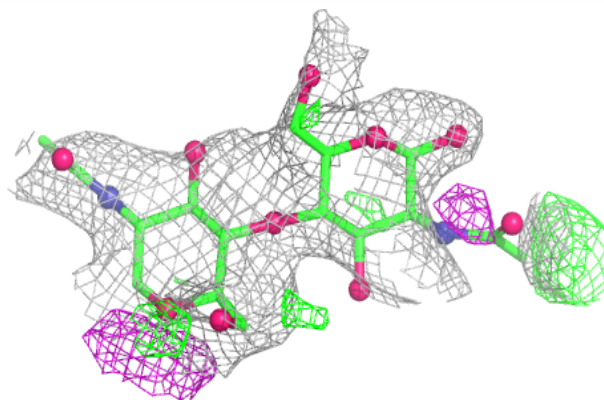


Electron density around Chain I:

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

**Electron density around Chain J:**

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



6.4 Ligands [i](#)

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
12	NAG	C	403	14/15	0.42	0.22	77,96,103,103	0
12	NAG	C	401	14/15	0.47	0.25	101,124,132,133	0
12	NAG	D	403	14/15	0.48	0.26	77,103,113,121	0
12	NAG	C	402	14/15	0.50	0.20	70,82,94,96	0
12	NAG	D	402	14/15	0.50	0.21	69,102,110,115	0
12	NAG	D	401	14/15	0.63	0.21	57,71,79,85	0
12	NAG	D	404	14/15	0.65	0.20	89,106,115,115	0
8	CL	H	303	1/1	0.82	0.22	83,83,83,83	0
10	GOL	L	402	6/6	0.84	0.19	62,70,73,73	0
9	PEG	L	401	7/7	0.84	0.19	59,61,68,71	0
11	PO4	B	302	5/5	0.85	0.24	48,54,59,108	0
13	PG4	D	405	13/13	0.87	0.17	46,53,65,74	0
10	GOL	B	301	6/6	0.88	0.14	43,51,52,69	0
10	GOL	A	301	6/6	0.88	0.17	38,50,57,66	0
8	CL	A	303	1/1	0.92	0.32	90,90,90,90	0
8	CL	L	403	1/1	0.95	0.09	68,68,68,68	0
8	CL	A	302	1/1	0.95	0.10	68,68,68,68	0
8	CL	H	302	1/1	0.95	0.16	61,61,61,61	0
8	CL	H	301	1/1	0.95	0.15	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.