



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 21, 2024 – 01:23 am GMT

PDB ID : 7BEP
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glycoprotein in a ternary complex with COVOX-384 and S309 Fabs
Authors : Zhou, D.; Zhao, Y.; Ren, J.; Stuart, D.
Deposited on : 2020-12-24
Resolution : 2.61 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 ⓘ 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

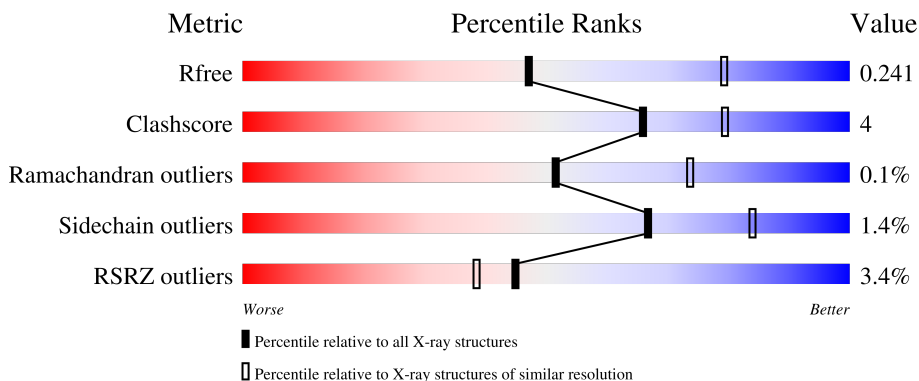
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	C	205	2% 85% 10% . .
1	E	205	2% 88% 7% .
2	A	243	2% 85% 9% 6%
2	D	243	% 84% 9% 7%
3	B	227	12% 84% 12% .

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Mol	Chain	Length	Quality of chain
3	F	227	
4	G	232	
4	H	232	
5	I	214	
5	L	214	
6	J	6	
6	K	6	

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
10	GLY	G	305	-	X	-	-
10	GLY	H	703	-	X	-	X
10	GLY	L	302	-	X	-	-
6	BMA	J	3	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 16957 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	197	1556	996	261	291	8	0	0	0
1	C	197	1556	996	261	291	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	527	LYS	PRO	engineered mutation	UNP P0DTC2
C	324	GLU	-	expression tag	UNP P0DTC2
C	325	THR	-	expression tag	UNP P0DTC2
C	326	GLY	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	527	LYS	PRO	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called COVOX-384 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	228	Total 1731	C 1099	N 289	O 335	S 8	0	2	0
2	D	227	Total 1725	C 1096	N 288	O 334	S 7	0	2	0

- Molecule 3 is a protein called COVOX-384 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	218	Total 1664	C 1044	N 279	O 336	S 5	0	1	0
3	F	218	Total 1671	C 1051	N 279	O 336	S 5	0	2	0

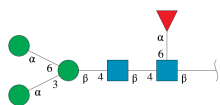
- Molecule 4 is a protein called S309 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	230	Total 1730	C 1089	N 292	O 341	S 8	0	1	0
4	G	232	Total 1745	C 1097	N 295	O 345	S 8	0	0	0

- Molecule 5 is a protein called S309 light chain.

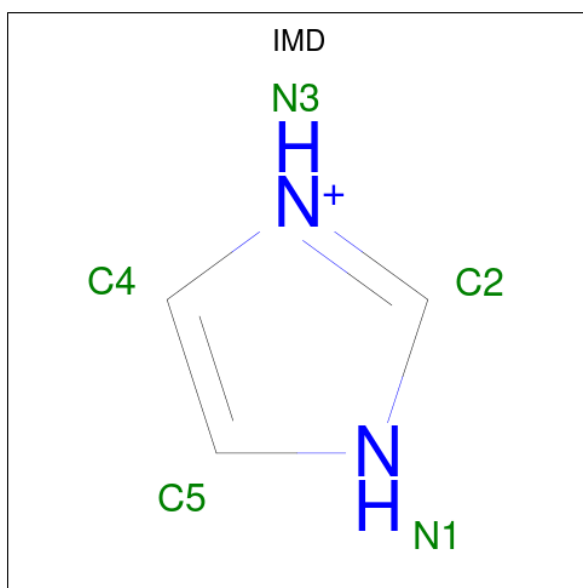
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	214	Total 1633	C 1016	N 278	O 333	S 6	0	1	0
5	I	214	Total 1634	C 1016	N 278	O 334	S 6	0	1	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
			Total	C	N	O			
6	J	6	Total 71	C 40	N 2	O 29	0	0	0
6	K	6	Total 71	C 40	N 2	O 29	0	0	0

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C N 5 3 2	0	0
7	H	1	Total C N 5 3 2	0	0
7	H	1	Total C N 5 3 2	0	0
7	C	1	Total C N 5 3 2	0	0
7	G	1	Total C N 5 3 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

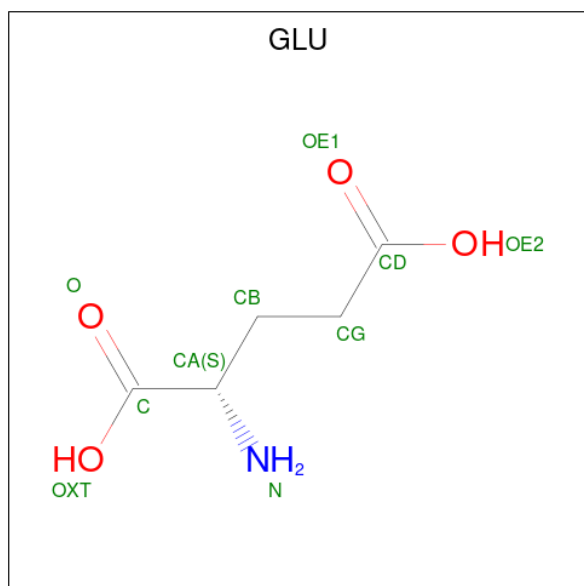
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	0
8	B	2	Total Cl 2 2	0	0
8	H	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0
8	D	2	Total Cl 2 2	0	0
8	F	1	Total Cl 1 1	0	0

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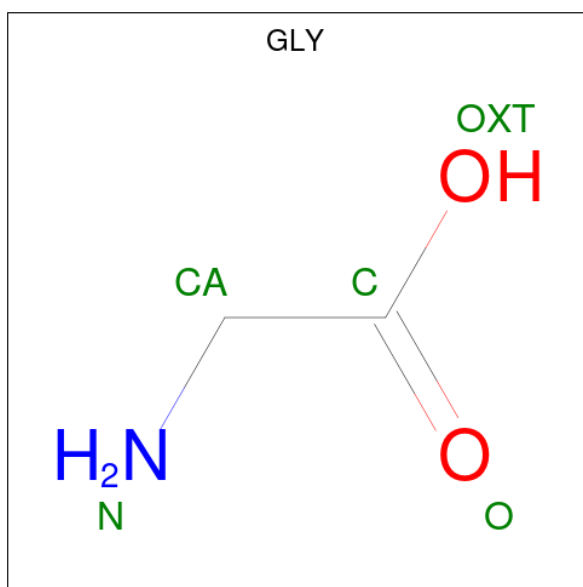
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	1	Total Cl 1 1	0	0

- Molecule 9 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



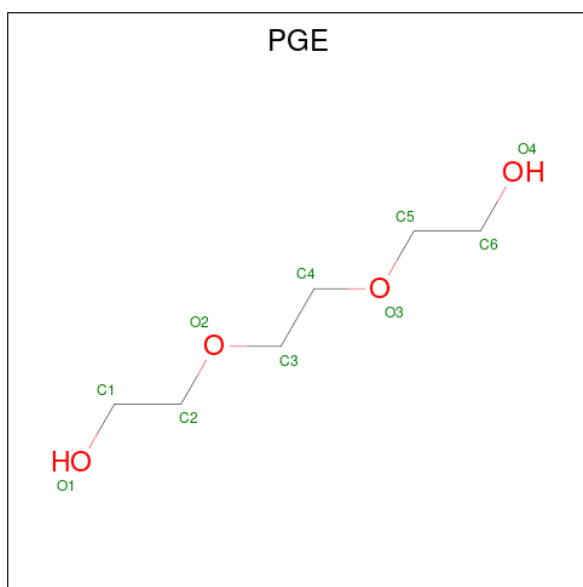
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 10 5 1 4	0	0
9	D	1	Total C N O 10 5 1 4	0	0

- Molecule 10 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



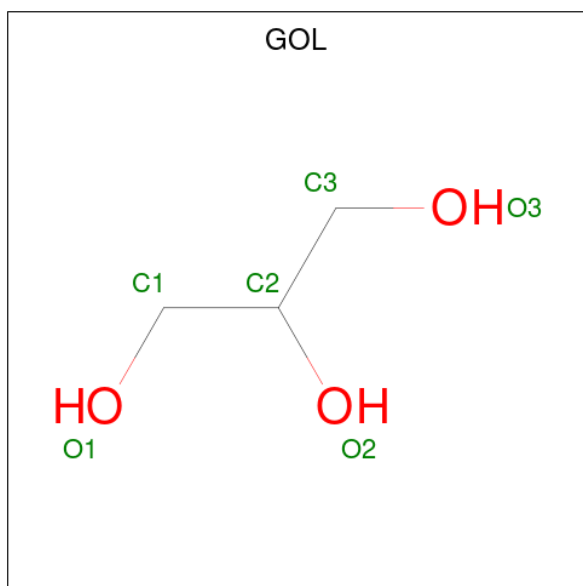
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			5	2	1	2		
10	H	1	Total	C	N	O	0	0
			5	2	1	2		
10	L	1	Total	C	N	O	0	0
			5	2	1	2		
10	F	1	Total	C	N	O	0	0
			5	2	1	2		
10	G	1	Total	C	N	O	0	0
			5	2	1	2		
10	G	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



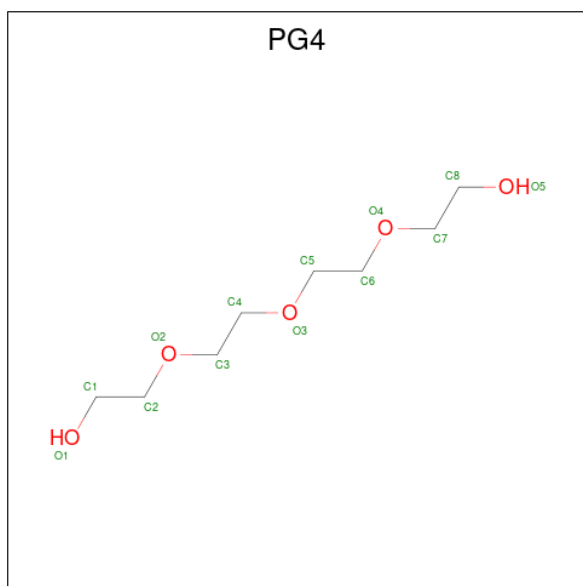
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	H	1	Total	C	O	0	0
			6	3	3		
12	F	1	Total	C	O	0	0
			6	3	3		
12	G	1	Total	C	O	0	0
			6	3	3		

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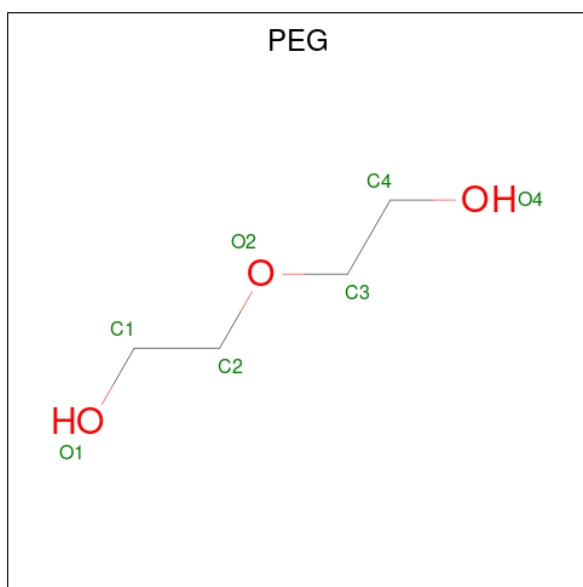
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 14 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			7	4	3		

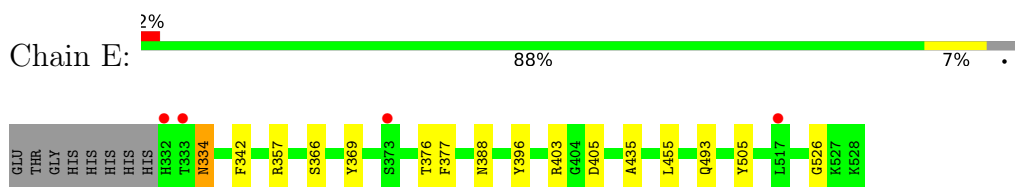
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	E	2	Total	O	0	0
			2	2		
15	A	2	Total	O	0	0
			2	2		
15	H	5	Total	O	0	0
			5	5		
15	L	1	Total	O	0	0
			1	1		
15	C	3	Total	O	0	0
			3	3		
15	D	1	Total	O	0	0
			1	1		
15	F	2	Total	O	0	0
			2	2		
15	G	2	Total	O	0	0
			2	2		

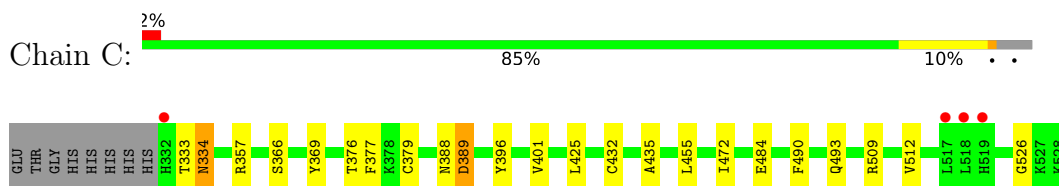
3 Residue-property plots [i](#)

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.

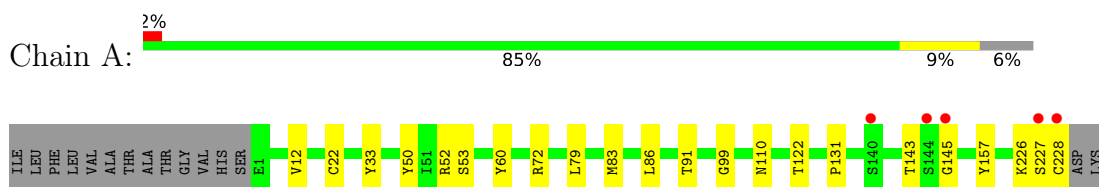
- Molecule 1: Spike glycoprotein



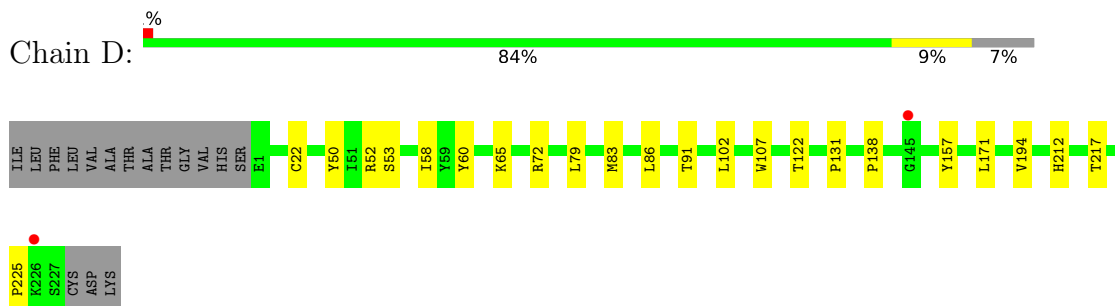
- Molecule 1: Spike glycoprotein



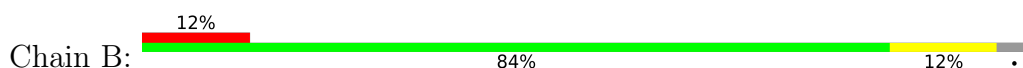
- Molecule 2: COVOX-384 heavy chain

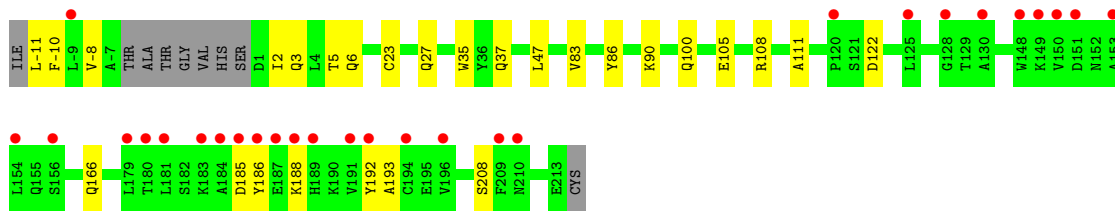


- Molecule 2: COVOX-384 heavy chain

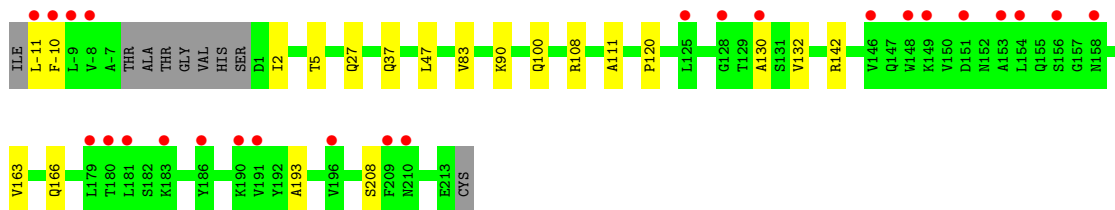
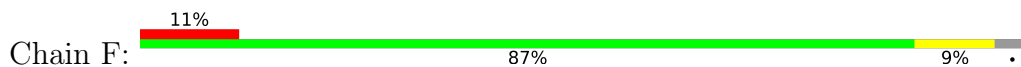


- Molecule 3: COVOX-384 light chain

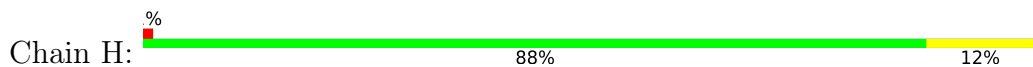




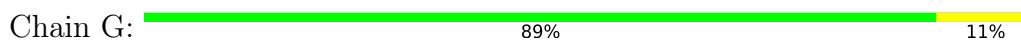
• Molecule 3: COVOX-384 light chain



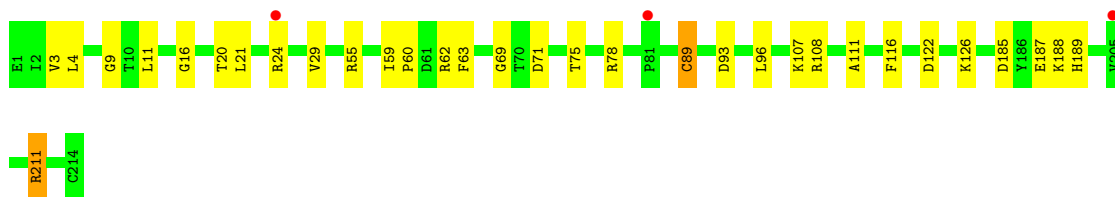
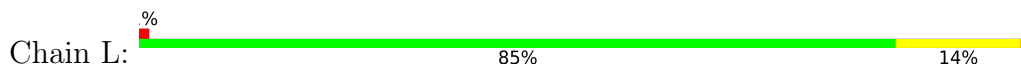
• Molecule 4: S309 heavy chain



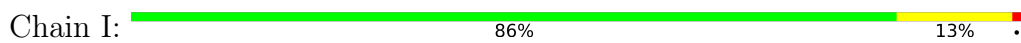
• Molecule 4: S309 heavy chain



• Molecule 5: S309 light chain



• Molecule 5: S309 light chain



- Molecule 6: alpha-D-mannopyranose-(1-3)-[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 J:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 6: alpha-D-mannopyranose-(1-3)-[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 K:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.76Å 113.22Å 302.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.93 – 2.61 62.93 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.93-2.61) 99.9 (62.93-2.61)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.203 , 0.241 0.203 , 0.241	Depositor DCC
R_{free} test set	5586 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.053 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16957	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: PEG, CL, GOL, FUC, PG4, PGE, BMA, NAG, MAN, IMD

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	C	0.27	0/1600	0.45	0/2178
1	E	0.27	0/1600	0.44	0/2178
2	A	0.27	0/1780	0.48	0/2422
2	D	0.27	0/1774	0.49	0/2414
3	B	0.27	0/1699	0.50	0/2306
3	F	0.27	0/1709	0.49	0/2320
4	G	0.28	0/1788	0.49	0/2433
4	H	0.27	0/1776	0.49	0/2419
5	I	0.28	0/1670	0.57	3/2266 (0.1%)
5	L	0.28	0/1669	0.50	0/2266
All	All	0.27	0/17065	0.49	3/23202 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	154	LEU	CB-CG-CD2	-7.78	97.78	111.00
5	I	13	LEU	CA-CB-CG	6.45	130.14	115.30
5	I	21	LEU	CA-CB-CG	5.54	128.04	115.30

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	C	1556	0	1463	12	0
1	E	1556	0	1463	9	1
2	A	1731	0	1708	12	0
2	D	1725	0	1703	14	0
3	B	1664	0	1636	15	0
3	F	1671	0	1654	13	0
4	G	1745	0	1699	17	1
4	H	1730	0	1687	17	0
5	I	1634	0	1590	19	0
5	L	1633	0	1590	23	0
6	J	71	0	61	1	0
6	K	71	0	61	0	0
7	C	5	0	5	0	0
7	E	5	0	5	0	0
7	G	5	0	5	0	0
7	H	10	0	10	0	0
8	A	2	0	0	1	0
8	B	2	0	0	2	0
8	C	1	0	0	0	0
8	D	2	0	0	0	0
8	F	1	0	0	1	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
9	A	10	0	5	1	0
9	D	10	0	5	2	0
10	A	5	0	2	0	0
10	F	5	0	2	0	0
10	G	10	0	4	1	0
10	H	5	0	2	1	0
10	L	5	0	2	0	0
11	B	10	0	14	0	0
12	F	6	0	8	0	0
12	G	12	0	16	1	0
12	H	6	0	8	0	0
13	I	13	0	18	0	0
13	L	13	0	18	0	0
14	D	7	0	10	1	0
15	A	2	0	0	0	0
15	C	3	0	0	0	0
15	D	1	0	0	0	0
15	E	2	0	0	0	0
15	F	2	0	0	0	0
15	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	5	0	0	0	0
15	L	1	0	0	0	0
All	All	16957	0	16454	134	1

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 134 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)
5:L:55:ARG:NH1	5:L:60:PRO:O	2.18	0.77
5:L:189:HIS:O	5:L:211:ARG:NH1	2.17	0.77
3:B:5:THR:HA	3:B:100:GLN:HE22	1.51	0.76
3:F:5:THR:HA	3:F:100:GLN:HE22	1.50	0.76
3:F:83:VAL:HG11	3:F:166:GLN:HB2	1.69	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:TYR:OH	4:G:205:THR:O[4_545]	2.13	0.07

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	C	195/205 (95%)	183 (94%)	12 (6%)	0	100	100
1	E	195/205 (95%)	182 (93%)	13 (7%)	0	100	100
2	A	228/243 (94%)	220 (96%)	7 (3%)	1 (0%)	34	55
2	D	227/243 (93%)	220 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	215/227 (95%)	203 (94%)	12 (6%)	0	100	100
3	F	216/227 (95%)	202 (94%)	14 (6%)	0	100	100
4	G	230/232 (99%)	227 (99%)	3 (1%)	0	100	100
4	H	229/232 (99%)	226 (99%)	3 (1%)	0	100	100
5	I	213/214 (100%)	206 (97%)	6 (3%)	1 (0%)	29	50
5	L	213/214 (100%)	205 (96%)	7 (3%)	1 (0%)	29	50
All	All	2161/2242 (96%)	2074 (96%)	84 (4%)	3 (0%)	51	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	69	GLY
2	A	227	SER
5	I	69	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	C	168/177 (95%)	164 (98%)	4 (2%)	49	72
1	E	168/177 (95%)	166 (99%)	2 (1%)	71	86
2	A	195/205 (95%)	192 (98%)	3 (2%)	65	82
2	D	194/205 (95%)	192 (99%)	2 (1%)	76	89
3	B	189/196 (96%)	187 (99%)	2 (1%)	73	88
3	F	191/196 (97%)	191 (100%)	0	100	100
4	G	194/194 (100%)	192 (99%)	2 (1%)	76	89
4	H	193/194 (100%)	191 (99%)	2 (1%)	76	89
5	I	186/185 (100%)	183 (98%)	3 (2%)	62	81
5	L	186/185 (100%)	181 (97%)	5 (3%)	44	69
All	All	1864/1914 (97%)	1839 (99%)	25 (1%)	67	85

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	333	THR
1	C	389	ASP
5	I	89	CYS
1	C	377	PHE
2	D	50	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	$\# Z > 2$
6	NAG	J	1	6,1	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	J	2	6	14,14,15	0.41	0	17,19,21	0.58	0
6	BMA	J	3	6	11,11,12	0.60	0	15,15,17	1.62	3 (20%)
6	MAN	J	4	6	11,11,12	0.72	0	15,15,17	1.22	1 (6%)
6	MAN	J	5	6	11,11,12	0.74	0	15,15,17	1.29	2 (13%)
6	FUC	J	6	6	10,10,11	0.89	1 (10%)	14,14,16	0.73	0
6	NAG	K	1	6,1	14,14,15	0.28	0	17,19,21	0.52	0
6	NAG	K	2	6	14,14,15	0.35	0	17,19,21	0.55	0
6	BMA	K	3	6	11,11,12	0.49	0	15,15,17	1.49	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	K	4	6	11,11,12	0.83	0	15,15,17	1.27	1 (6%)
6	MAN	K	5	6	11,11,12	0.79	0	15,15,17	1.33	2 (13%)
6	FUC	K	6	6	10,10,11	0.89	0	14,14,16	0.83	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
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	1/2/19/22	0/1/1/1
6	FUC	J	6	6	-	-	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	1/2/19/22	0/1/1/1
6	FUC	K	6	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	6	FUC	O5-C1	-2.05	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	3	BMA	C1-C2-C3	4.41	115.08	109.67
6	K	5	MAN	C1-O5-C5	4.15	117.81	112.19
6	K	4	MAN	C1-O5-C5	3.88	117.45	112.19
6	J	5	MAN	C1-O5-C5	3.87	117.44	112.19
6	J	4	MAN	C1-O5-C5	3.67	117.17	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

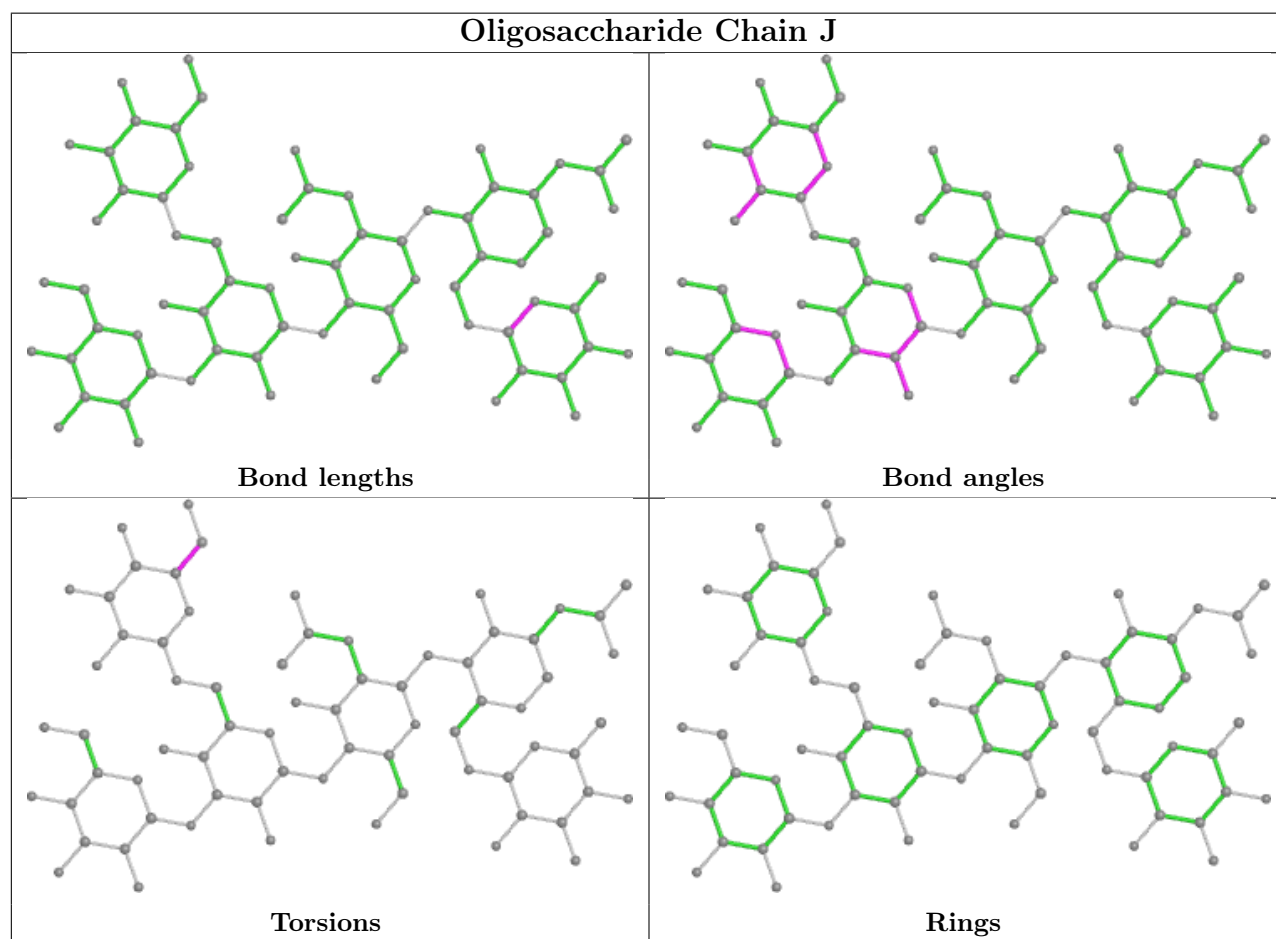
Mol	Chain	Res	Type	Atoms
6	J	5	MAN	O5-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6

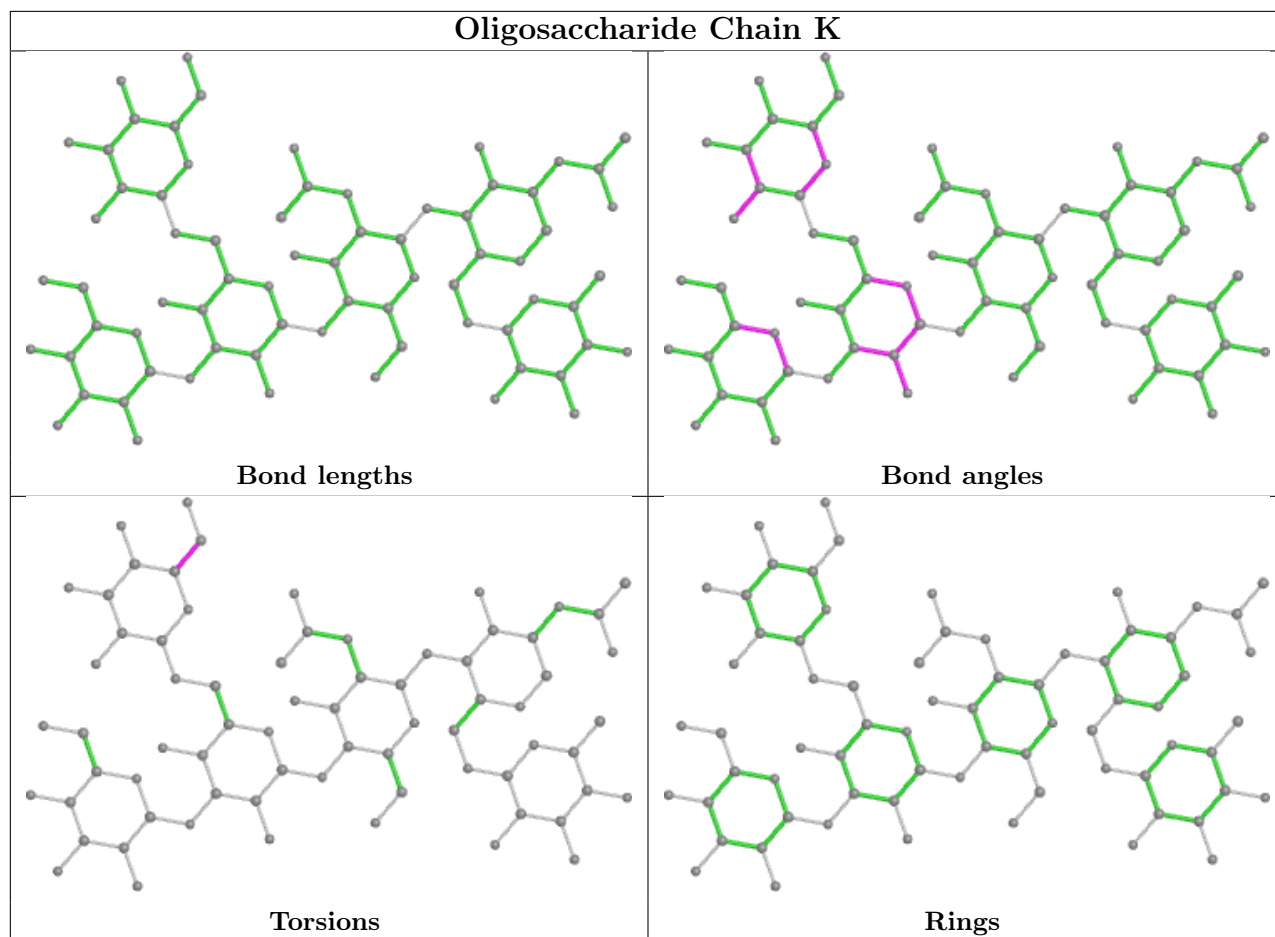
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	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 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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$
10	GLY	L	302	-	4,4,4	1.13	1 (25%)	3,4,4	1.66	1 (33%)
7	IMD	C	701	-	3,5,5	0.41	0	4,5,5	0.59	0
11	PGE	B	301	-	9,9,9	0.37	0	8,8,8	0.29	0
7	IMD	E	801	-	3,5,5	0.41	0	4,5,5	0.58	0
10	GLY	G	305	-	4,4,4	1.10	1 (25%)	3,4,4	1.72	1 (33%)
9	GLU	D	304	-	8,9,9	1.08	1 (12%)	10,11,11	1.44	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	IMD	G	304	-	3,5,5	0.41	0	4,5,5	0.58	0
10	GLY	G	303	-	4,4,4	1.14	1 (25%)	3,4,4	1.62	1 (33%)
9	GLU	A	303	-	8,9,9	1.13	1 (12%)	10,11,11	1.41	2 (20%)
13	PG4	L	301	-	12,12,12	0.53	0	11,11,11	0.48	0
12	GOL	F	302	-	5,5,5	0.97	0	5,5,5	0.92	0
14	PEG	D	303	-	6,6,6	0.49	0	5,5,5	0.26	0
10	GLY	F	303	-	4,4,4	1.12	1 (25%)	3,4,4	1.83	2 (66%)
7	IMD	H	702	-	3,5,5	0.40	0	4,5,5	0.59	0
12	GOL	H	701	-	5,5,5	0.94	0	5,5,5	0.91	0
12	GOL	G	301	-	5,5,5	0.94	0	5,5,5	0.99	0
10	GLY	H	703	-	4,4,4	1.07	1 (25%)	3,4,4	1.76	2 (66%)
7	IMD	H	704	-	3,5,5	0.41	0	4,5,5	0.60	0
10	GLY	A	304	-	4,4,4	1.12	1 (25%)	3,4,4	1.66	1 (33%)
13	PG4	I	301	-	12,12,12	0.53	0	11,11,11	0.28	0
12	GOL	G	302	-	5,5,5	0.90	0	5,5,5	0.99	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
10	GLY	L	302	-	-	2/2/2/2	-
11	PGE	B	301	-	-	4/7/7/7	-
7	IMD	C	701	-	-	-	0/1/1/1
10	GLY	G	305	-	-	2/2/2/2	-
7	IMD	E	801	-	-	-	0/1/1/1
9	GLU	D	304	-	-	3/9/9/9	-
7	IMD	G	304	-	-	-	0/1/1/1
10	GLY	G	303	-	-	0/2/2/2	-
9	GLU	A	303	-	-	4/9/9/9	-
13	PG4	L	301	-	-	5/10/10/10	-
12	GOL	F	302	-	-	2/4/4/4	-
14	PEG	D	303	-	-	1/4/4/4	-
10	GLY	F	303	-	-	0/2/2/2	-
7	IMD	H	702	-	-	-	0/1/1/1
12	GOL	H	701	-	-	2/4/4/4	-
12	GOL	G	301	-	-	0/4/4/4	-
10	GLY	H	703	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IMD	H	704	-	-	-	0/1/1/1
10	GLY	A	304	-	-	0/2/2/2	-
13	PG4	I	301	-	-	5/10/10/10	-
12	GOL	G	302	-	-	4/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	303	GLY	OXT-C	-2.15	1.23	1.30
10	F	303	GLY	OXT-C	-2.15	1.23	1.30
10	L	302	GLY	OXT-C	-2.12	1.23	1.30
10	A	304	GLY	OXT-C	-2.11	1.23	1.30
10	G	305	GLY	OXT-C	-2.10	1.23	1.30

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	304	GLU	OXT-C-O	-3.31	116.58	124.09
9	A	303	GLU	OXT-C-O	-3.25	116.72	124.09
9	D	304	GLU	OXT-C-CA	2.49	121.86	113.38
10	F	303	GLY	OXT-C-O	-2.43	117.25	123.30
9	A	303	GLU	OXT-C-CA	2.29	121.17	113.38

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	303	GLU	N-CA-CB-CG
9	A	303	GLU	C-CA-CB-CG
10	H	703	GLY	O-C-CA-N
10	H	703	GLY	OXT-C-CA-N
10	L	302	GLY	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	304	GLU	2	0
10	G	303	GLY	1	0
9	A	303	GLU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	303	PEG	1	0
10	H	703	GLY	1	0
12	G	302	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	197/205 (96%)	0.09	4 (2%) 65 60	69, 92, 136, 179	0
1	E	197/205 (96%)	0.13	4 (2%) 65 60	70, 93, 138, 174	0
2	A	228/243 (93%)	0.06	5 (2%) 62 57	64, 90, 141, 214	0
2	D	227/243 (93%)	0.04	2 (0%) 84 82	64, 90, 124, 193	0
3	B	218/227 (96%)	0.57	28 (12%) 3 2	64, 103, 167, 189	0
3	F	218/227 (96%)	0.51	25 (11%) 4 3	64, 102, 165, 187	0
4	G	232/232 (100%)	-0.07	1 (0%) 92 91	72, 87, 113, 188	0
4	H	230/232 (99%)	-0.01	2 (0%) 84 82	67, 89, 113, 163	0
5	I	214/214 (100%)	-0.00	0 100 100	73, 103, 129, 155	0
5	L	214/214 (100%)	0.00	3 (1%) 75 71	71, 97, 127, 168	0
All	All	2175/2242 (97%)	0.13	74 (3%) 45 38	64, 93, 151, 214	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	148	TRP	7.3
3	F	181	LEU	6.6
3	B	181	LEU	6.5
3	B	191	VAL	5.9
2	A	145	GLY	5.3

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

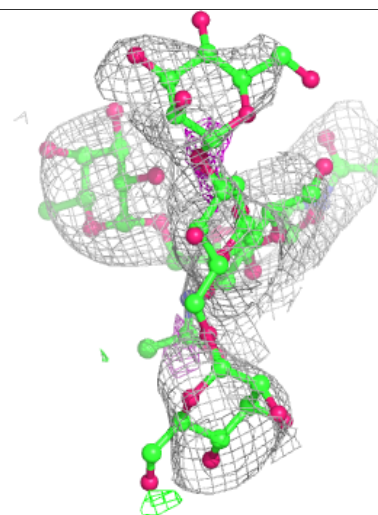
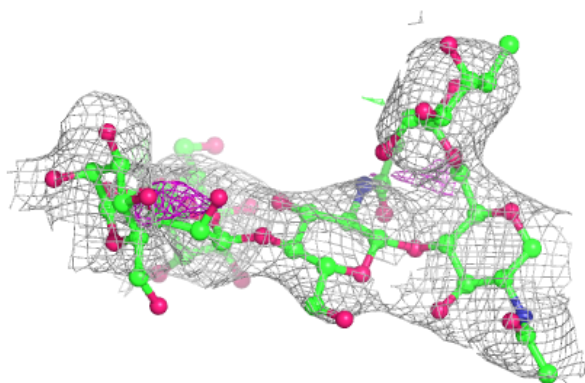
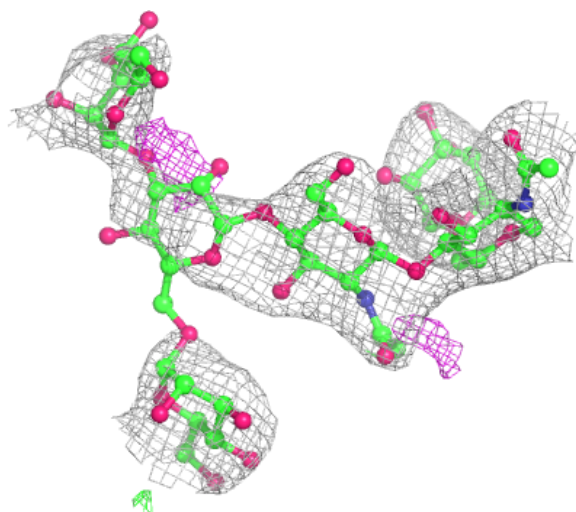
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

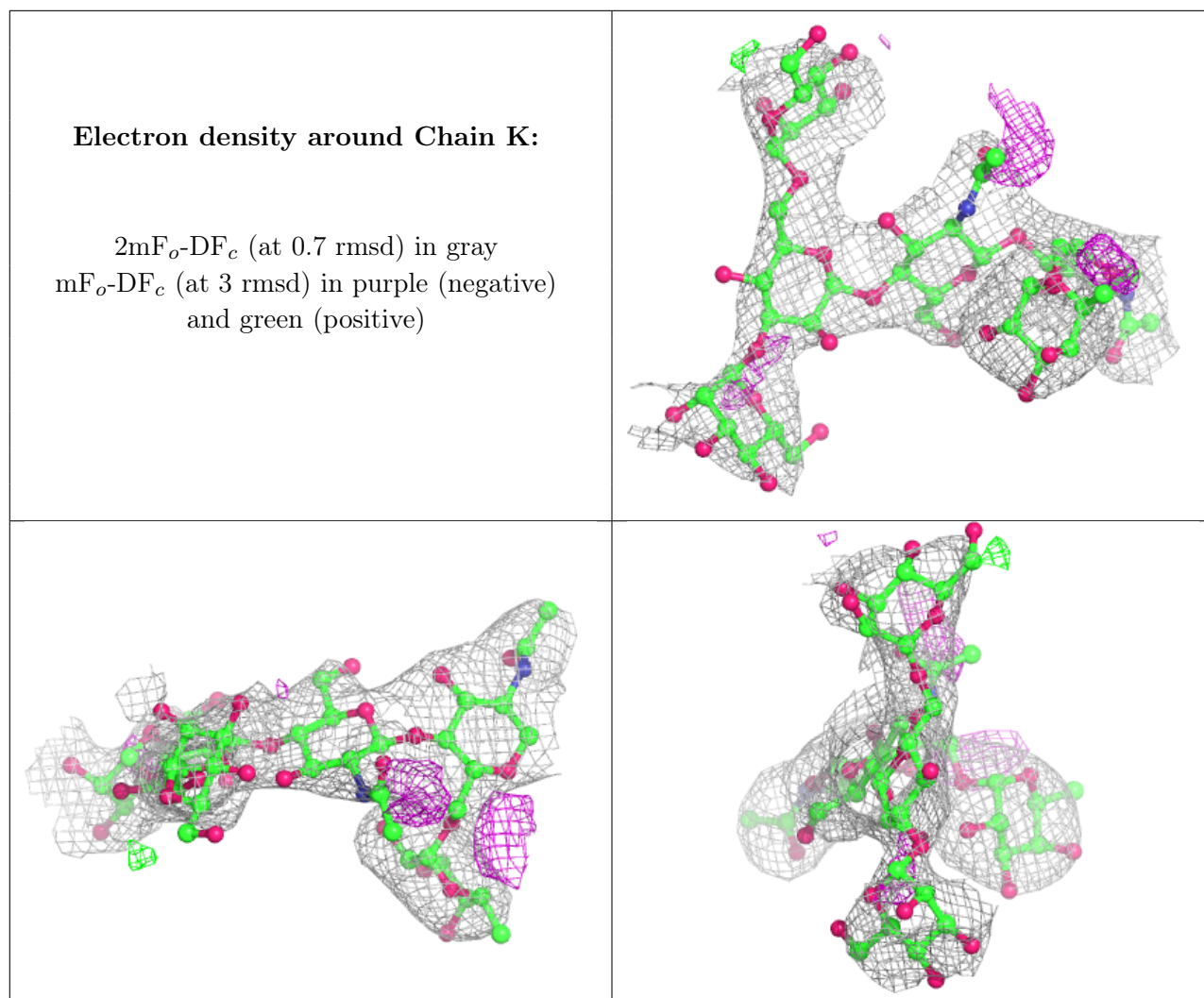
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	K	4	11/12	0.66	0.40	148,162,180,181	0
6	BMA	J	3	11/12	0.69	0.41	164,177,181,181	0
6	MAN	J	4	11/12	0.74	0.36	137,159,176,183	0
6	MAN	K	5	11/12	0.74	0.26	158,168,175,177	0
6	MAN	J	5	11/12	0.75	0.22	181,185,190,192	0
6	BMA	K	3	11/12	0.85	0.33	154,158,166,169	0
6	NAG	K	2	14/15	0.90	0.26	101,128,142,147	0
6	NAG	J	2	14/15	0.91	0.23	113,126,142,164	0
6	NAG	K	1	14/15	0.94	0.16	78,89,108,110	0
6	NAG	J	1	14/15	0.95	0.16	82,98,117,119	0
6	FUC	K	6	10/11	0.96	0.22	90,97,99,104	0
6	FUC	J	6	10/11	0.97	0.23	94,106,115,118	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 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
10	GLY	G	303	5/5	0.56	0.34	110,119,122,126	0
10	GLY	H	703	5/5	0.65	0.46	85,109,130,132	0
14	PEG	D	303	7/7	0.71	0.28	102,108,118,120	0
12	GOL	F	302	6/6	0.74	0.25	90,98,121,123	0
8	CL	I	302	1/1	0.76	0.22	97,97,97,97	0
8	CL	C	702	1/1	0.77	0.11	120,120,120,120	0
10	GLY	G	305	5/5	0.77	0.37	105,115,118,125	0
9	GLU	A	303	10/10	0.78	0.38	117,117,124,126	0
13	PG4	L	301	13/13	0.79	0.20	78,98,119,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PGE	B	301	10/10	0.80	0.26	88,106,117,119	0
8	CL	H	705	1/1	0.80	0.13	109,109,109,109	0
8	CL	B	303	1/1	0.81	0.09	116,116,116,116	0
9	GLU	D	304	10/10	0.83	0.42	130,130,131,142	0
7	IMD	H	702	5/5	0.83	0.37	104,107,114,123	0
8	CL	D	302	1/1	0.84	0.11	84,84,84,84	0
12	GOL	G	302	6/6	0.86	0.34	88,95,101,103	0
10	GLY	A	304	5/5	0.86	0.18	120,126,135,135	0
10	GLY	F	303	5/5	0.86	0.23	86,114,127,129	0
7	IMD	E	801	5/5	0.88	0.23	103,106,109,112	0
12	GOL	H	701	6/6	0.88	0.15	94,103,105,106	0
7	IMD	H	704	5/5	0.89	0.46	133,134,139,143	0
7	IMD	C	701	5/5	0.90	0.28	105,109,115,116	0
13	PG4	I	301	13/13	0.90	0.16	78,96,111,112	0
7	IMD	G	304	5/5	0.90	0.24	127,128,133,136	0
8	CL	A	301	1/1	0.91	0.10	86,86,86,86	0
12	GOL	G	301	6/6	0.91	0.17	97,98,101,103	0
8	CL	A	302	1/1	0.92	0.12	92,92,92,92	0
8	CL	D	301	1/1	0.93	0.07	83,83,83,83	0
10	GLY	L	302	5/5	0.96	0.26	90,92,96,99	0
8	CL	F	301	1/1	0.97	0.07	77,77,77,77	0
8	CL	B	302	1/1	0.98	0.10	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.