wwPDB X-ray Structure Validation Summary Report (i)

Mar 15, 2023 – 06:26 pm GMT

PDB ID	:	8C3V
Title	:	SARS-CoV-2 Delta-RBD complexed with BA.2-13 Fab and C1 nanobody
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2022-12-28
Resolution	:	2.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

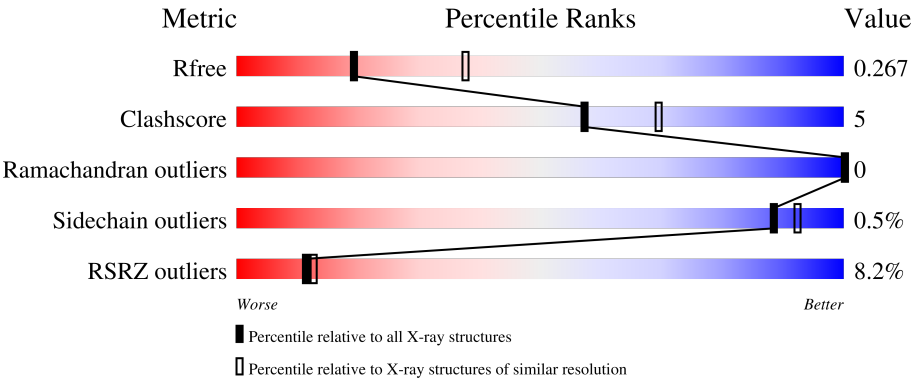
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	15% 79% 18% .
1	C	231	18% 78% 17% .
1	H	231	. 83% 14% .
2	B	213	8% 88% 12%
2	D	213	19% 93% 7%

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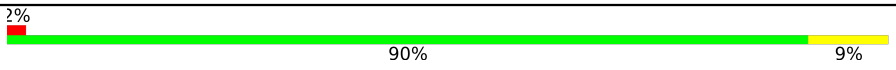
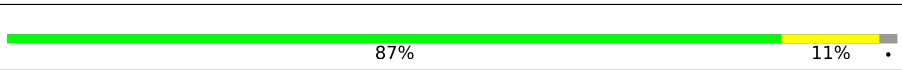
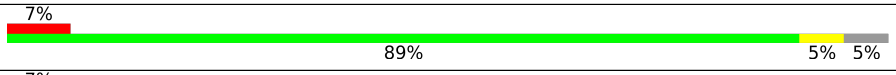
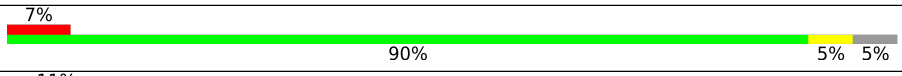
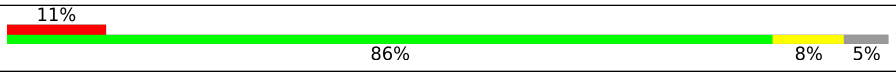
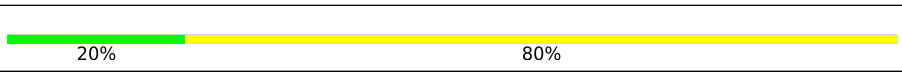
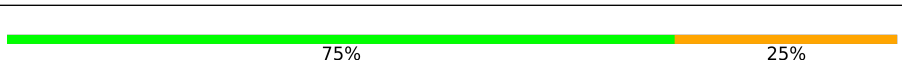
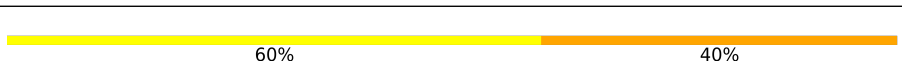
Mol	Chain	Length	Quality of chain
2	L	213	
3	R	202	
3	X	202	
3	Y	202	
4	I	131	
4	J	131	
4	K	131	
5	E	5	
6	F	4	
7	G	5	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17807 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 BA.2-13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	223	Total	C	N	O	S	0	0	0
			1679	1056	288	328	7			
1	A	224	Total	C	N	O	S	0	0	0
			1685	1059	289	330	7			
1	C	221	Total	C	N	O	S	0	0	0
			1668	1050	286	325	7			

- Molecule 2 is a protein called BA.2-13 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1618	1008	273	331	6			
2	B	212	Total	C	N	O	S	0	0	0
			1618	1008	273	331	6			
2	D	212	Total	C	N	O	S	0	0	0
			1618	1008	273	331	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	197	Total	C	N	O	S	0	0	0
			1577	1008	271	290	8			
3	X	197	Total	C	N	O	S	0	0	0
			1577	1008	271	290	8			
3	Y	197	Total	C	N	O	S	0	0	0
			1577	1008	271	290	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	327	HIS	-	expression tag	UNP P0DTC2
R	328	HIS	-	expression tag	UNP P0DTC2

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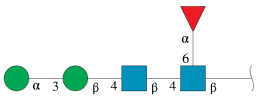
Chain	Residue	Modelled	Actual	Comment	Reference
R	329	HIS	-	expression tag	UNP P0DTC2
R	330	HIS	-	expression tag	UNP P0DTC2
R	331	HIS	-	expression tag	UNP P0DTC2
R	332	HIS	-	expression tag	UNP P0DTC2
R	452	ARG	LEU	conflict	UNP P0DTC2
R	478	LYS	THR	conflict	UNP P0DTC2
R	527	LYS	PRO	conflict	UNP P0DTC2
X	327	HIS	-	expression tag	UNP P0DTC2
X	328	HIS	-	expression tag	UNP P0DTC2
X	329	HIS	-	expression tag	UNP P0DTC2
X	330	HIS	-	expression tag	UNP P0DTC2
X	331	HIS	-	expression tag	UNP P0DTC2
X	332	HIS	-	expression tag	UNP P0DTC2
X	452	ARG	LEU	conflict	UNP P0DTC2
X	478	LYS	THR	conflict	UNP P0DTC2
X	527	LYS	PRO	conflict	UNP P0DTC2
Y	327	HIS	-	expression tag	UNP P0DTC2
Y	328	HIS	-	expression tag	UNP P0DTC2
Y	329	HIS	-	expression tag	UNP P0DTC2
Y	330	HIS	-	expression tag	UNP P0DTC2
Y	331	HIS	-	expression tag	UNP P0DTC2
Y	332	HIS	-	expression tag	UNP P0DTC2
Y	452	ARG	LEU	conflict	UNP P0DTC2
Y	478	LYS	THR	conflict	UNP P0DTC2
Y	527	LYS	PRO	conflict	UNP P0DTC2

- Molecule 4 is a protein called Nanobody C1.

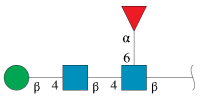
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	124	Total	C	N	O	S	0	0	0
			965	605	167	189	4			
4	J	124	Total	C	N	O	S	0	0	0
			965	605	167	189	4			
4	K	124	Total	C	N	O	S	0	0	0
			965	605	167	189	4			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



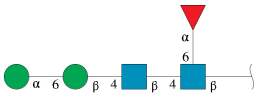
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	5	60	34	2	24	0	0	0

- Molecule 6 is an oligosaccharide called 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.



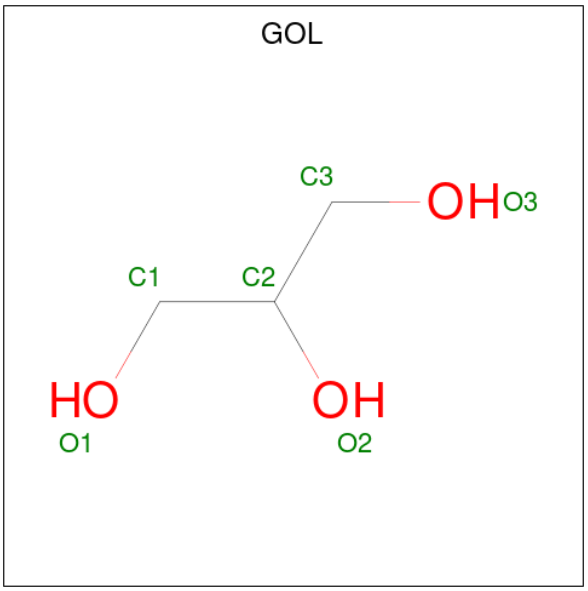
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	4	49	28	2	19	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



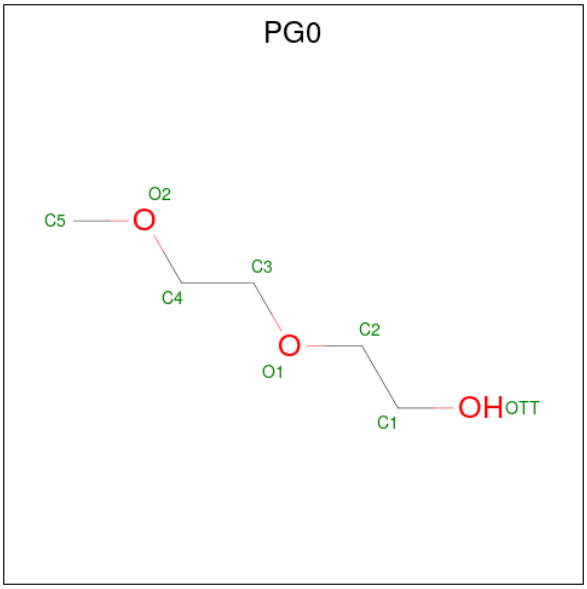
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	G	5	60	34	2	24	0	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



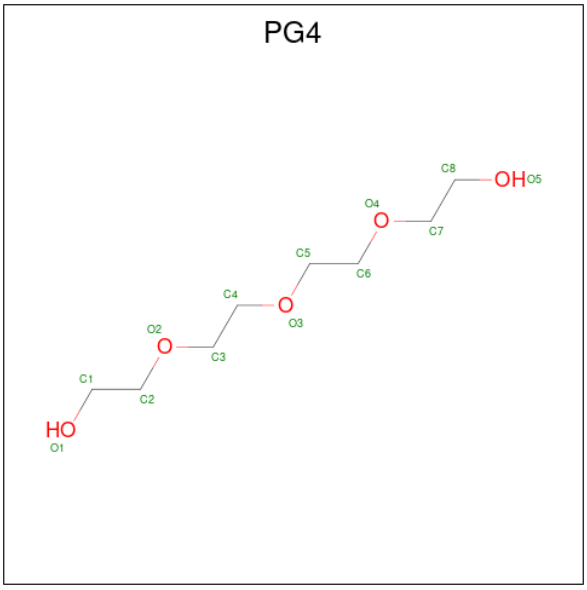
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	R	1	Total C O 6 3 3	0	0
8	R	1	Total C O 6 3 3	0	0
8	I	1	Total C O 6 3 3	0	0
8	I	1	Total C O 6 3 3	0	0
8	I	1	Total C O 6 3 3	0	0
8	X	1	Total C O 6 3 3	0	0
8	X	1	Total C O 6 3 3	0	0
8	J	1	Total C O 6 3 3	0	0
8	J	1	Total C O 6 3 3	0	0
8	Y	1	Total C O 6 3 3	0	0
8	Y	1	Total C O 6 3 3	0	0
8	K	1	Total C O 6 3 3	0	0
8	K	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

- Molecule 9 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	R	1	Total C O 8 5 3	0	0
9	J	1	Total C O 8 5 3	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

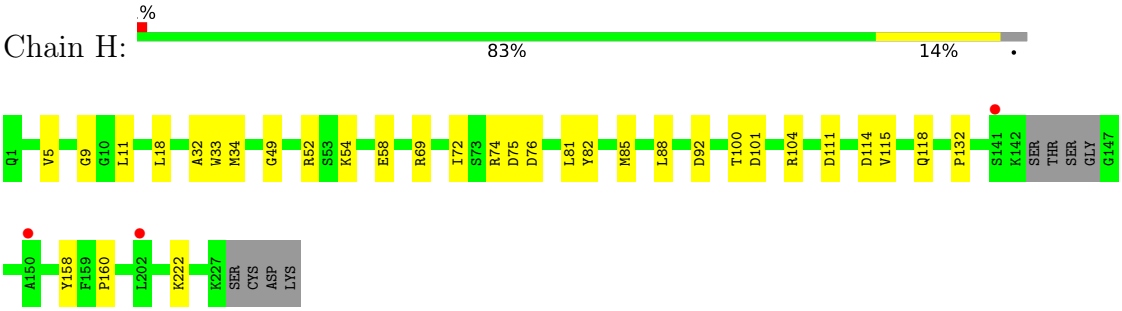


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	X	1	Total	C	O	0	0
			13	8	5		
10	Y	1	Total	C	O	0	0
			13	8	5		

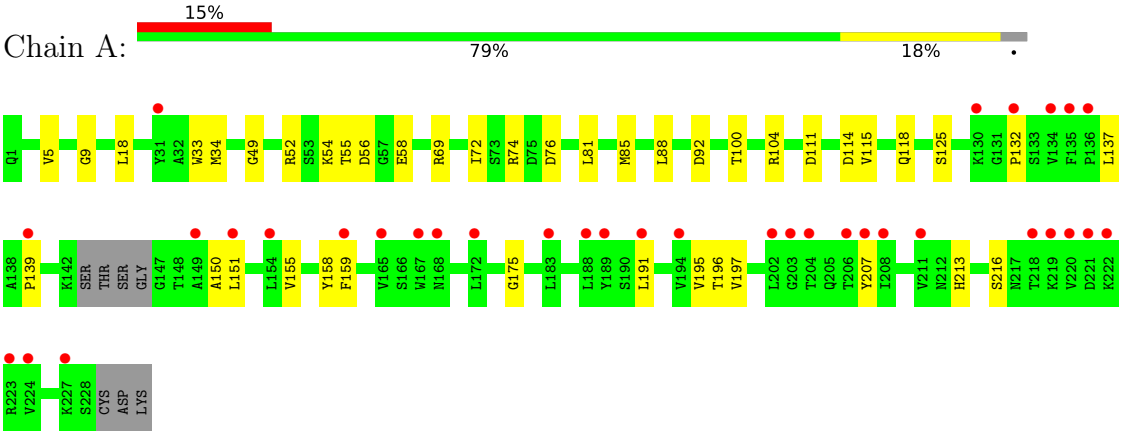
3 Residue-property plots (i)

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.

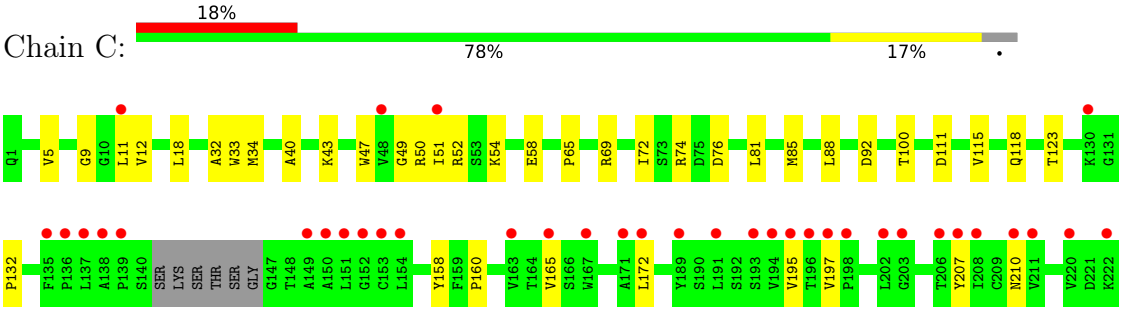
• Molecule 1: BA.2-13 heavy chain

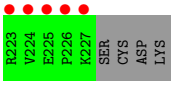


• Molecule 1: BA.2-13 heavy chain



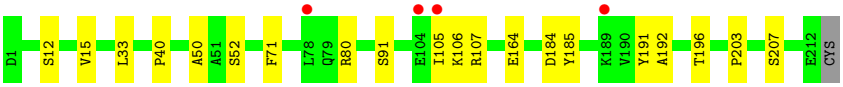
• Molecule 1: BA.2-13 heavy chain





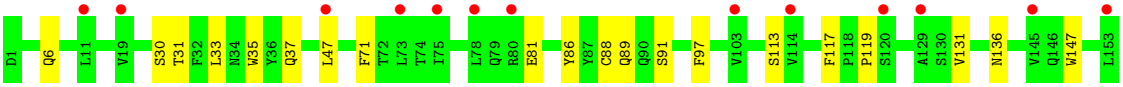
• Molecule 2: BA.2-13 light chain

Chain L:



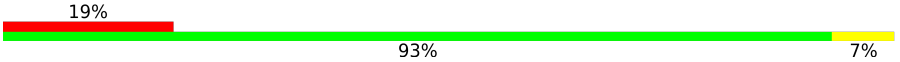
• Molecule 2: BA.2-13 light chain

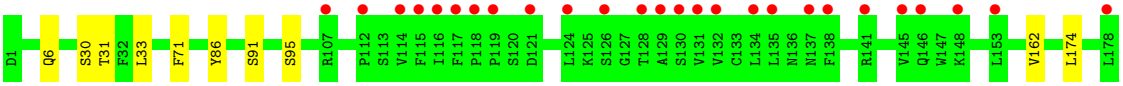
Chain B:

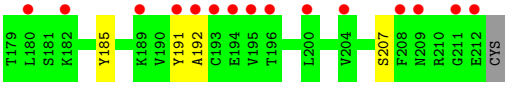


• Molecule 2: BA.2-13 light chain

Chain D:

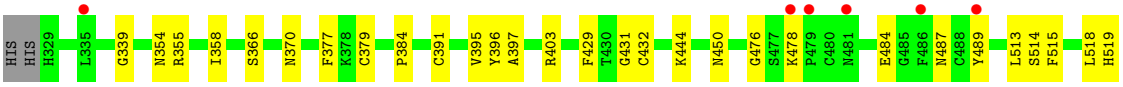






• Molecule 3: Spike protein S1

Chain R:

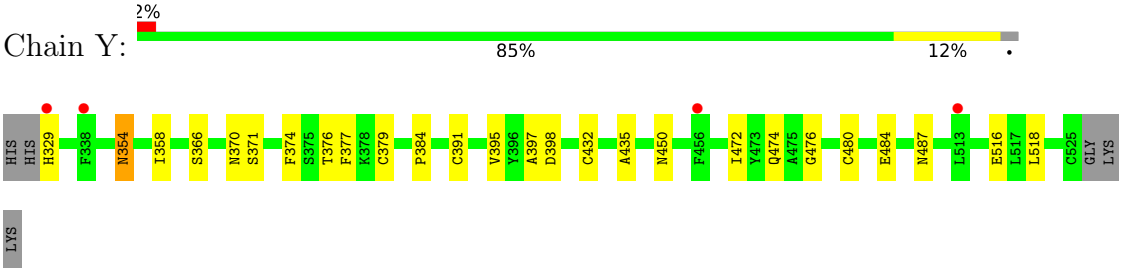


• Molecule 3: Spike protein S1

Chain X:

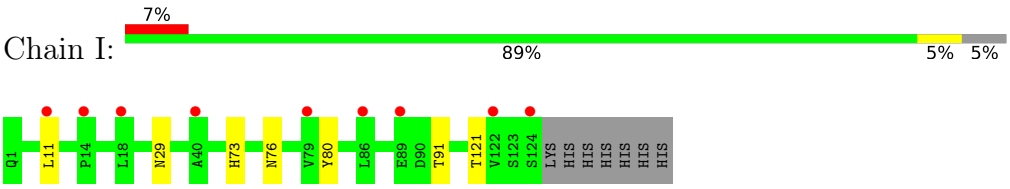
• Molecule 3: Spike protein S1

Chain Y:



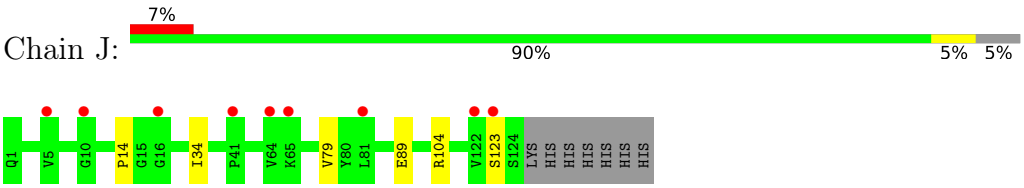
• Molecule 4: Nanobody C1

Chain I:



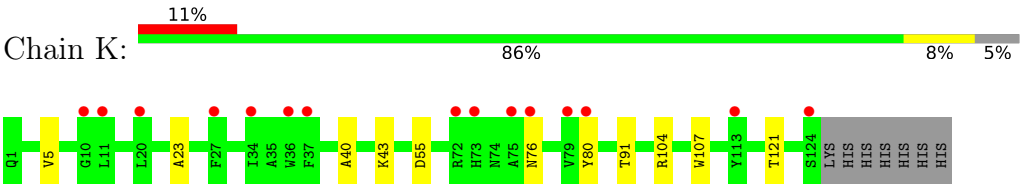
• Molecule 4: Nanobody C1

Chain J:



• Molecule 4: Nanobody C1

Chain K:

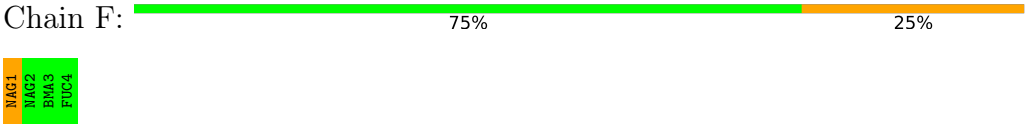


• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 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 F:



• Molecule 7: 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 G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.92Å 160.82Å 172.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.87 – 2.74 80.41 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.87-2.74) 99.9 (80.41-2.74)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.258 0.224 , 0.267	Depositor DCC
R_{free} test set	3941 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17807	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GOL, NAG, MAN, FUC, PG0, PG4

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	0.26	0/1725	0.53	0/2352
1	C	0.26	0/1708	0.53	0/2329
1	H	0.26	0/1719	0.52	0/2344
2	B	0.27	0/1650	0.52	0/2234
2	D	0.27	0/1650	0.52	0/2234
2	L	0.27	0/1650	0.53	0/2234
3	R	0.28	0/1624	0.51	0/2208
3	X	0.29	0/1624	0.50	0/2208
3	Y	0.29	0/1624	0.51	0/2208
4	I	0.28	0/990	0.54	0/1347
4	J	0.27	0/990	0.52	0/1347
4	K	0.28	0/990	0.52	0/1347
All	All	0.27	0/17944	0.52	0/24392

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

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	1685	0	1637	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1668	0	1625	26	0
1	H	1679	0	1632	19	0
2	B	1618	0	1575	14	0
2	D	1618	0	1575	10	0
2	L	1618	0	1575	11	0
3	R	1577	0	1485	18	0
3	X	1577	0	1485	15	0
3	Y	1577	0	1485	19	0
4	I	965	0	906	6	0
4	J	965	0	906	5	0
4	K	965	0	906	7	0
5	E	60	0	52	2	0
6	F	49	0	43	4	0
7	G	60	0	52	5	0
8	A	6	0	8	2	0
8	I	18	0	24	0	0
8	J	12	0	16	3	0
8	K	12	0	16	1	0
8	R	12	0	16	1	0
8	X	12	0	16	0	0
8	Y	12	0	16	1	0
9	J	8	0	12	0	0
9	R	8	0	12	1	0
10	X	13	0	18	4	0
10	Y	13	0	18	5	0
All	All	17807	0	17111	170	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 5.

The worst 5 of 170 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:9:GLY:HA2	1:A:18:LEU:HD21	1.55	0.86
1:C:9:GLY:HA2	1:C:18:LEU:HD21	1.58	0.83
3:X:476:GLY:H	3:X:487:ASN:HB3	1.50	0.76
1:C:11:LEU:HD11	1:C:160:PRO:HG3	1.72	0.72
1:H:9:GLY:HA2	1:H:18:LEU:HD21	1.71	0.72

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	220/231 (95%)	214 (97%)	6 (3%)	0	100	100
1	C	217/231 (94%)	212 (98%)	5 (2%)	0	100	100
1	H	219/231 (95%)	214 (98%)	5 (2%)	0	100	100
2	B	210/213 (99%)	201 (96%)	9 (4%)	0	100	100
2	D	210/213 (99%)	202 (96%)	8 (4%)	0	100	100
2	L	210/213 (99%)	201 (96%)	9 (4%)	0	100	100
3	R	195/202 (96%)	183 (94%)	12 (6%)	0	100	100
3	X	195/202 (96%)	183 (94%)	12 (6%)	0	100	100
3	Y	195/202 (96%)	187 (96%)	8 (4%)	0	100	100
4	I	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
4	J	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
4	K	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
All	All	2237/2331 (96%)	2160 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	186/194 (96%)	186 (100%)	0	100	100
1	C	184/194 (95%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	185/194 (95%)	185 (100%)	0	100 100
2	B	185/186 (100%)	185 (100%)	0	100 100
2	D	185/186 (100%)	185 (100%)	0	100 100
2	L	185/186 (100%)	184 (100%)	1 (0%)	88 92
3	R	171/175 (98%)	166 (97%)	5 (3%)	42 62
3	X	171/175 (98%)	169 (99%)	2 (1%)	71 83
3	Y	171/175 (98%)	169 (99%)	2 (1%)	71 83
4	I	103/110 (94%)	103 (100%)	0	100 100
4	J	103/110 (94%)	103 (100%)	0	100 100
4	K	103/110 (94%)	103 (100%)	0	100 100
All	All	1932/1995 (97%)	1922 (100%)	10 (0%)	88 92

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	403	ARG
3	Y	354	ASN
3	Y	377	PHE
3	R	403	ARG
3	R	484	GLU

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

Mol	Chain	Res	Type
4	I	29	ASN

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)

14 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	$\#\|Z\| > 2$
5	NAG	E	1	3,5	14,14,15	0.52	0	17,19,21	0.62	0
5	NAG	E	2	5	14,14,15	1.02	1 (7%)	17,19,21	0.99	2 (11%)
5	BMA	E	3	5	11,11,12	1.54	2 (18%)	15,15,17	1.53	3 (20%)
5	MAN	E	4	5	11,11,12	1.07	1 (9%)	15,15,17	1.21	2 (13%)
5	FUC	E	5	5	10,10,11	0.87	0	14,14,16	0.63	0
6	NAG	F	1	3,6	14,14,15	0.76	1 (7%)	17,19,21	0.49	0
6	NAG	F	2	6	14,14,15	0.49	0	17,19,21	0.46	0
6	BMA	F	3	6	11,11,12	1.05	0	15,15,17	0.90	0
6	FUC	F	4	6	10,10,11	0.90	0	14,14,16	0.69	0
7	NAG	G	1	3,7	14,14,15	0.75	1 (7%)	17,19,21	0.57	0
7	NAG	G	2	7	14,14,15	0.45	0	17,19,21	0.53	0
7	BMA	G	3	7	11,11,12	0.97	1 (9%)	15,15,17	1.41	3 (20%)
7	MAN	G	4	7	11,11,12	1.02	1 (9%)	15,15,17	1.15	2 (13%)
7	FUC	G	5	7	10,10,11	0.97	1 (10%)	14,14,16	0.63	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
5	NAG	E	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	FUC	E	5	5	-	-	0/1/1/1
6	NAG	F	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUC	F	4	6	-	-	0/1/1/1
7	NAG	G	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	FUC	G	5	7	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2	NAG	O5-C1	-3.57	1.38	1.43
5	E	3	BMA	C4-C3	3.18	1.60	1.52
5	E	3	BMA	C4-C5	2.81	1.58	1.53
5	E	4	MAN	C1-C2	2.68	1.58	1.52
6	F	1	NAG	C1-C2	2.56	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3	BMA	C1-C2-C3	-3.61	105.23	109.67
5	E	4	MAN	C1-C2-C3	2.40	112.62	109.67
7	G	3	BMA	O6-C6-C5	-2.39	103.08	111.29
5	E	2	NAG	C3-C4-C5	2.36	114.44	110.24
7	G	3	BMA	C1-C2-C3	-2.36	106.77	109.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	NAG	2	0
7	G	1	NAG	4	0

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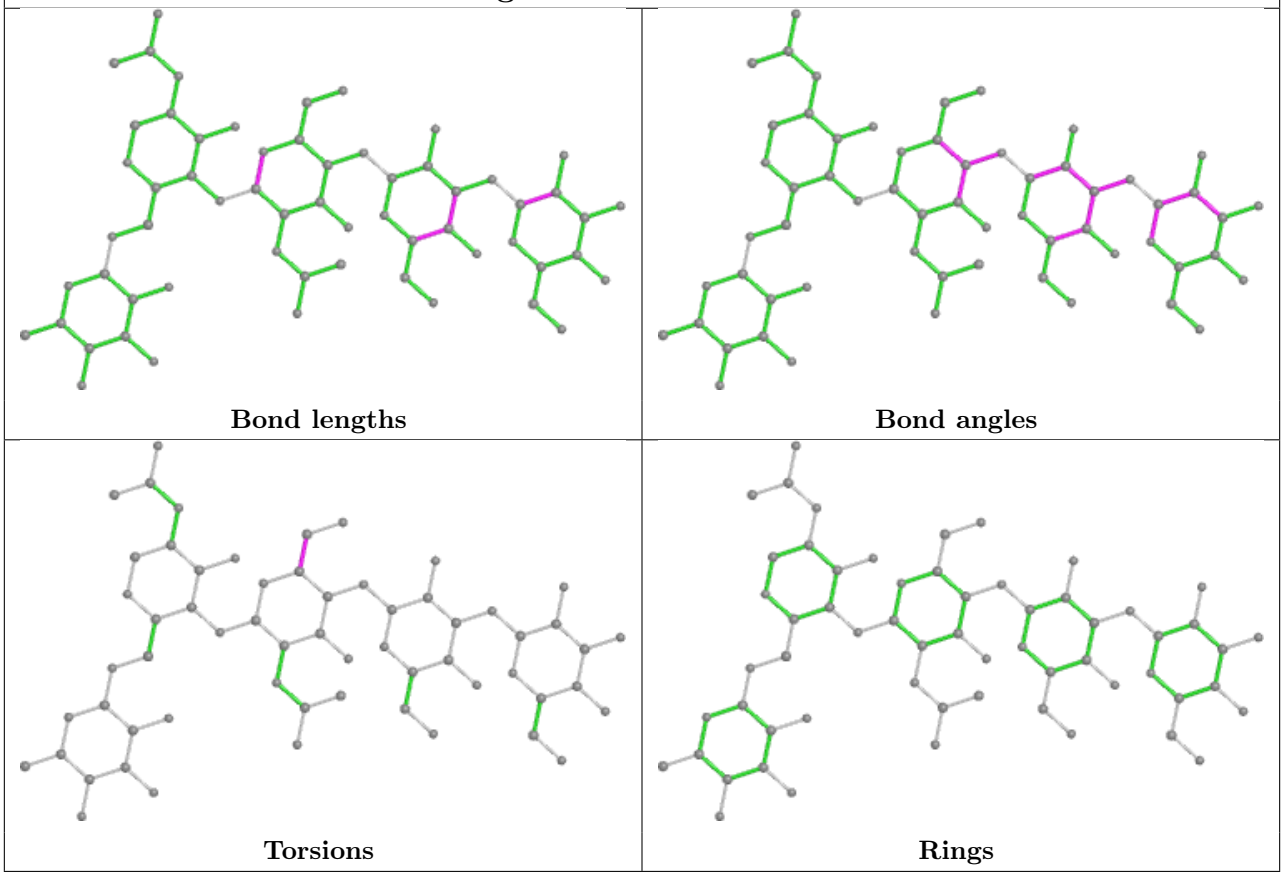
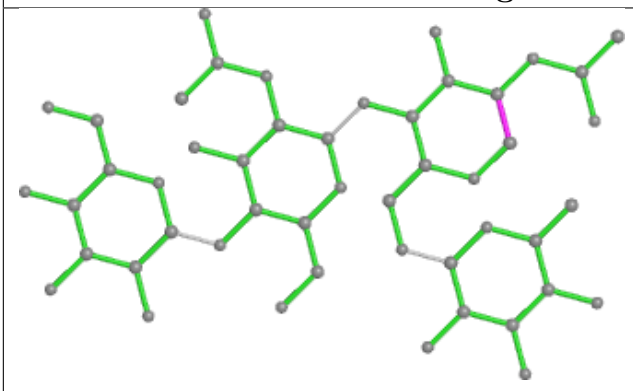
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	4	MAN	1	0
5	E	1	NAG	2	0
6	F	1	NAG	4	0

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

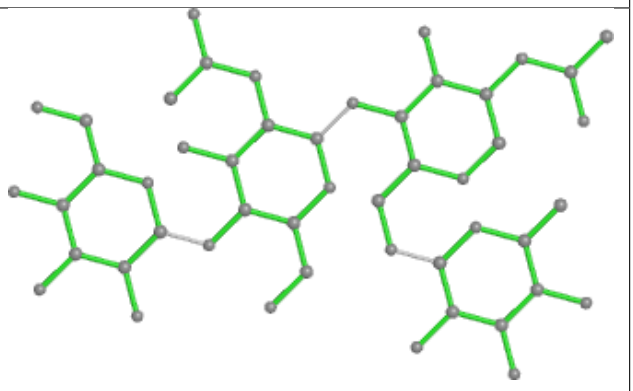
Oligosaccharide Chain E



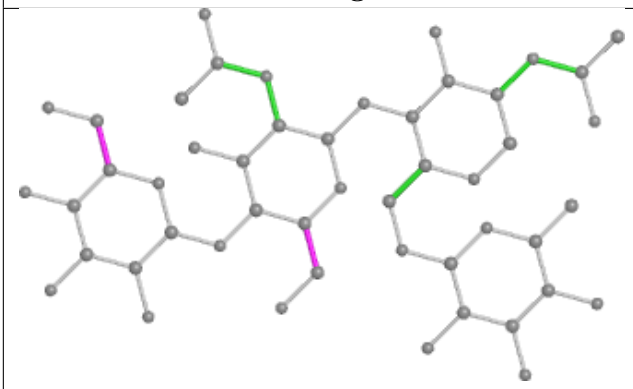
Oligosaccharide Chain F



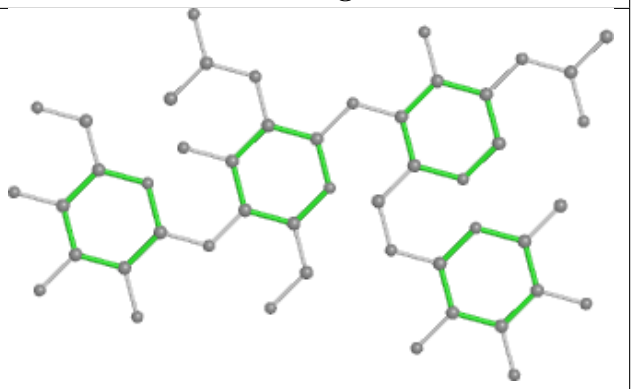
Bond lengths



Bond angles

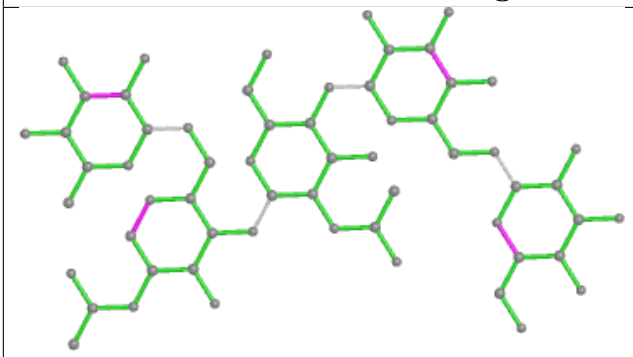


Torsions

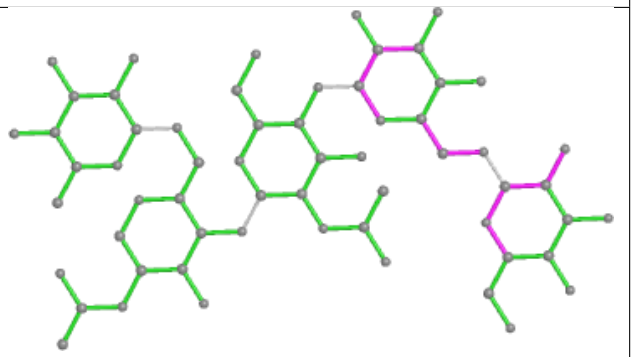


Rings

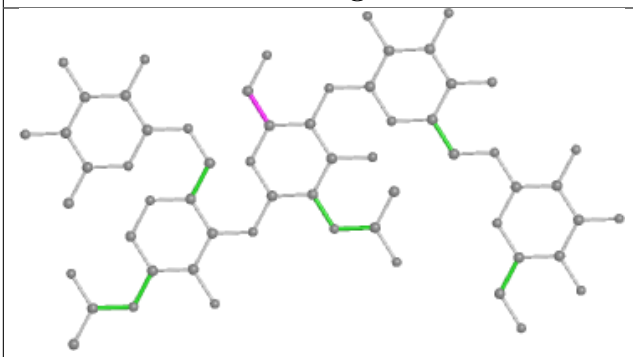
Oligosaccharide Chain G



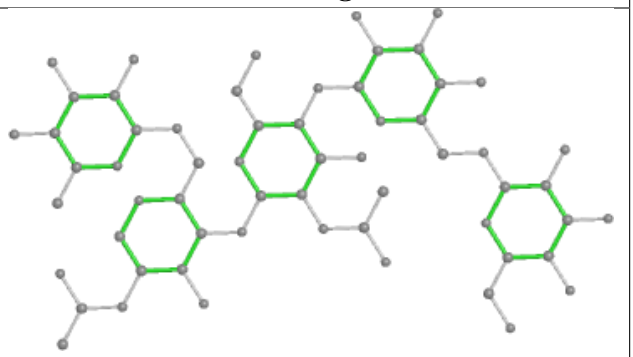
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	GOL	I	201	-	5,5,5	0.65	0	5,5,5	1.06	0
8	GOL	J	201	-	5,5,5	0.62	0	5,5,5	1.07	0
10	PG4	X	603	-	12,12,12	0.20	0	11,11,11	0.70	0
8	GOL	R	601	-	5,5,5	0.76	0	5,5,5	1.12	0
8	GOL	K	202	-	5,5,5	0.64	0	5,5,5	1.08	0
8	GOL	A	301	-	5,5,5	0.92	0	5,5,5	1.14	0
9	PG0	R	603	-	7,7,7	0.27	0	6,6,6	0.23	0
9	PG0	J	203	-	7,7,7	0.27	0	6,6,6	0.20	0
10	PG4	Y	603	-	12,12,12	0.21	0	11,11,11	0.69	0
8	GOL	Y	602	-	5,5,5	0.72	0	5,5,5	1.10	0
8	GOL	I	202	-	5,5,5	0.67	0	5,5,5	1.05	0
8	GOL	X	602	-	5,5,5	0.61	0	5,5,5	1.08	0
8	GOL	K	201	-	5,5,5	0.58	0	5,5,5	1.13	0
8	GOL	J	202	-	5,5,5	0.72	0	5,5,5	1.05	0
8	GOL	I	203	-	5,5,5	0.63	0	5,5,5	1.16	1 (20%)
8	GOL	Y	601	-	5,5,5	0.57	0	5,5,5	1.07	0
8	GOL	X	601	-	5,5,5	0.77	0	5,5,5	1.11	1 (20%)
8	GOL	R	602	-	5,5,5	0.85	0	5,5,5	1.11	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
8	GOL	I	201	-	-	0/4/4/4	-
8	GOL	J	201	-	-	0/4/4/4	-
10	PG4	X	603	-	-	5/10/10/10	-
8	GOL	R	601	-	-	4/4/4/4	-
8	GOL	K	202	-	-	1/4/4/4	-
8	GOL	A	301	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PG0	R	603	-	-	4/5/5/5	-
9	PG0	J	203	-	-	2/5/5/5	-
10	PG4	Y	603	-	-	8/10/10/10	-
8	GOL	Y	602	-	-	2/4/4/4	-
8	GOL	I	202	-	-	0/4/4/4	-
8	GOL	X	602	-	-	2/4/4/4	-
8	GOL	K	201	-	-	0/4/4/4	-
8	GOL	J	202	-	-	2/4/4/4	-
8	GOL	I	203	-	-	2/4/4/4	-
8	GOL	Y	601	-	-	2/4/4/4	-
8	GOL	X	601	-	-	4/4/4/4	-
8	GOL	R	602	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	203	GOL	C3-C2-C1	-2.11	103.48	111.70
8	X	601	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	601	GOL	O1-C1-C2-C3
8	I	203	GOL	C1-C2-C3-O3
8	X	601	GOL	C1-C2-C3-O3
8	X	602	GOL	O1-C1-C2-C3
8	J	202	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	603	PG4	4	0
8	R	601	GOL	1	0
8	K	202	GOL	1	0
8	A	301	GOL	2	0
9	R	603	PG0	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Y	603	PG4	5	0
8	Y	602	GOL	1	0
8	J	202	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	224/231 (96%)	0.88	35 (15%) 2 2	59, 105, 166, 180	0
1	C	221/231 (95%)	1.13	42 (19%) 1 1	62, 89, 162, 182	0
1	H	223/231 (96%)	0.33	3 (1%) 77 82	65, 86, 129, 180	0
2	B	212/213 (99%)	0.73	18 (8%) 10 12	65, 95, 143, 166	0
2	D	212/213 (99%)	1.03	41 (19%) 1 1	66, 116, 165, 198	0
2	L	212/213 (99%)	0.44	4 (1%) 66 73	66, 89, 114, 170	0
3	R	197/202 (97%)	0.47	6 (3%) 50 57	56, 70, 128, 190	0
3	X	197/202 (97%)	0.34	0 100 100	53, 65, 94, 114	0
3	Y	197/202 (97%)	0.43	4 (2%) 65 72	55, 68, 92, 124	0
4	I	124/131 (94%)	0.55	9 (7%) 15 17	66, 95, 132, 142	0
4	J	124/131 (94%)	0.61	9 (7%) 15 17	61, 99, 141, 175	0
4	K	124/131 (94%)	0.81	15 (12%) 4 4	71, 113, 147, 188	0
All	All	2267/2331 (97%)	0.65	186 (8%) 11 13	53, 86, 152, 198	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	TYR	10.4
1	C	208	ILE	8.4
1	C	224	VAL	8.0
1	A	167	TRP	7.8
1	A	224	VAL	7.6

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)

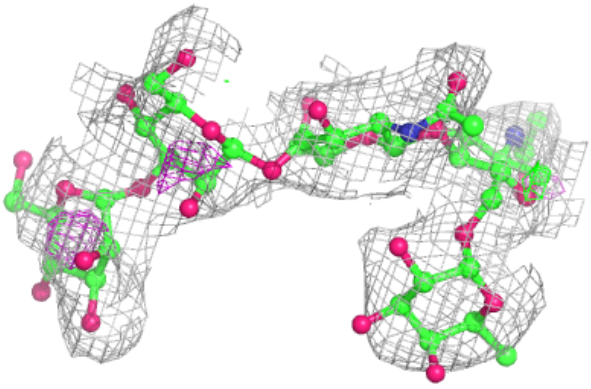
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

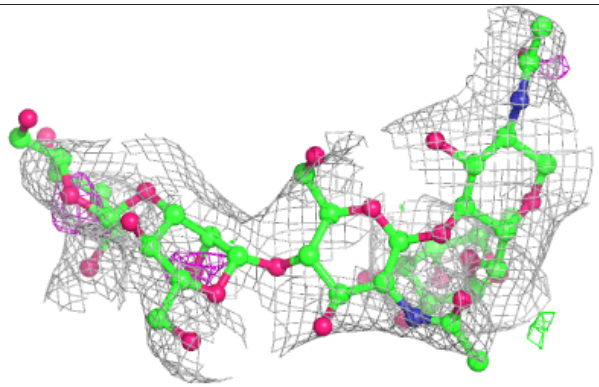
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BMA	G	3	11/12	0.57	0.26	127,130,132,135	0
5	BMA	E	3	11/12	0.60	0.19	129,134,139,139	0
5	MAN	E	4	11/12	0.62	0.34	134,143,146,146	0
6	BMA	F	3	11/12	0.76	0.14	124,127,131,133	0
6	FUC	F	4	10/11	0.82	0.35	115,121,125,127	0
7	MAN	G	4	11/12	0.83	0.21	125,132,137,138	0
5	NAG	E	2	14/15	0.84	0.17	117,121,130,135	0
7	NAG	G	2	14/15	0.85	0.18	106,112,118,124	0
5	FUC	E	5	10/11	0.87	0.19	112,123,126,130	0
6	NAG	F	2	14/15	0.88	0.21	112,117,125,128	0
5	NAG	E	1	14/15	0.89	0.20	75,97,117,120	0
7	FUC	G	5	10/11	0.91	0.16	107,115,118,118	0
7	NAG	G	1	14/15	0.92	0.18	80,90,105,107	0
6	NAG	F	1	14/15	0.94	0.17	78,92,112,120	0

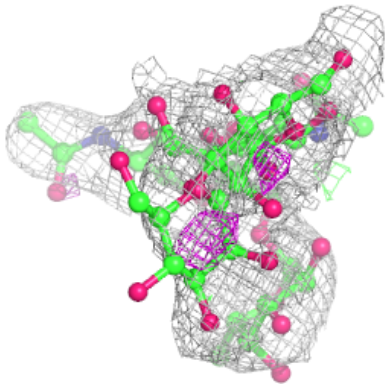
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

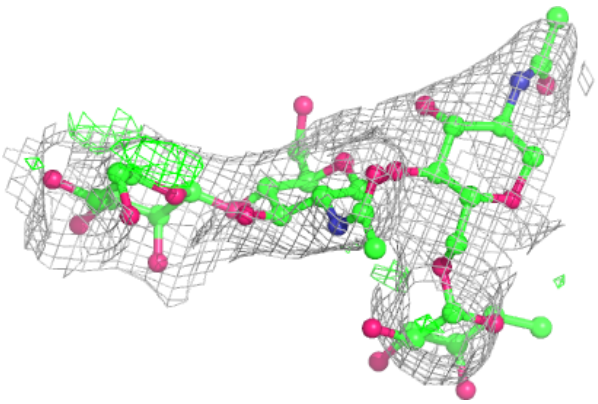


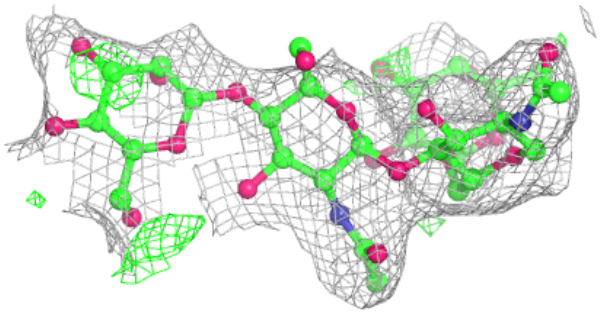


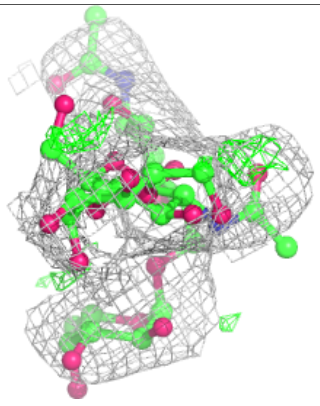


Electron density around Chain F:

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

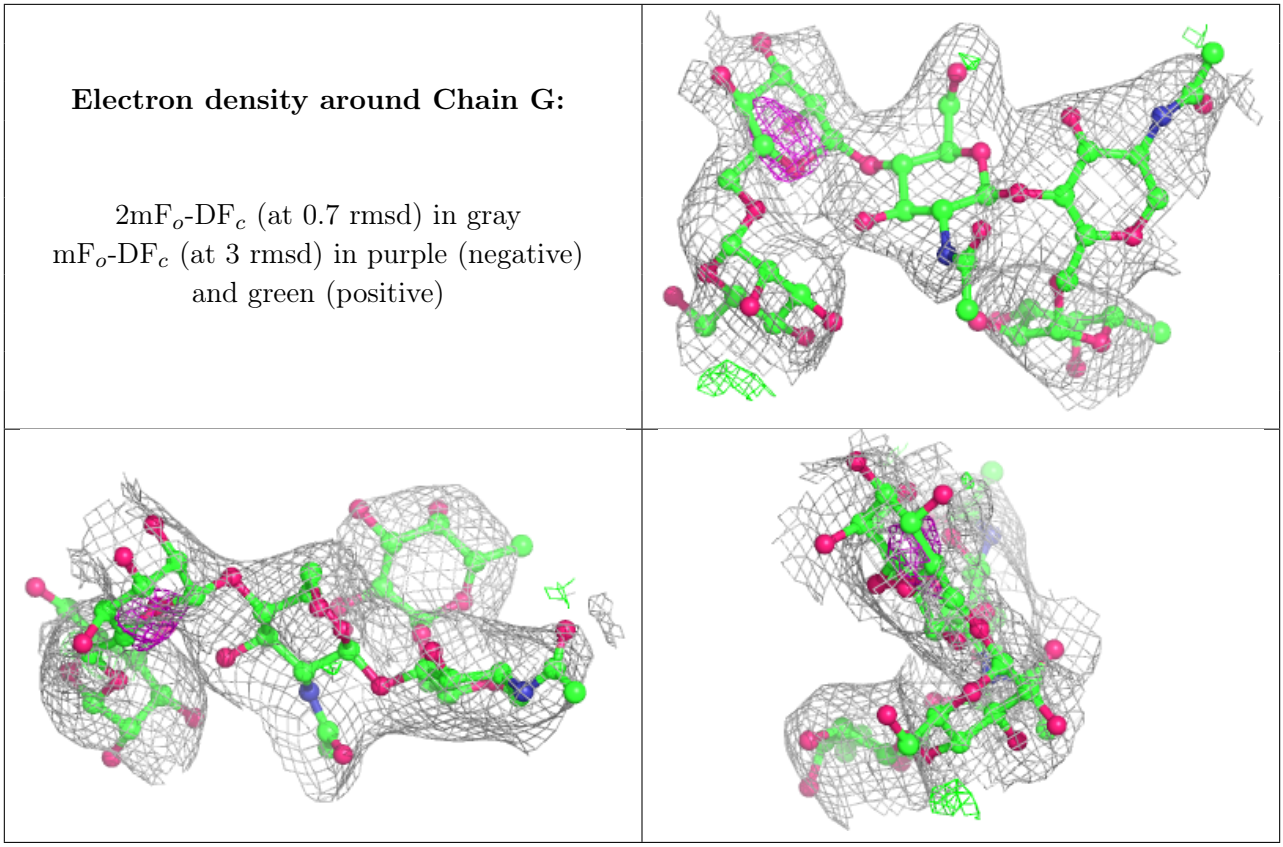






Electron density around Chain G:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	J	202	6/6	0.74	0.38	73,78,82,84	0
9	PG0	R	603	8/8	0.77	0.20	63,72,76,77	0
8	GOL	K	202	6/6	0.79	0.26	77,77,78,83	0
9	PG0	J	203	8/8	0.81	0.36	60,73,76,81	0
8	GOL	X	602	6/6	0.82	0.28	70,74,77,86	0
8	GOL	J	201	6/6	0.82	0.30	82,85,87,93	0
8	GOL	I	201	6/6	0.83	0.42	78,79,84,87	0
10	PG4	X	603	13/13	0.84	0.38	61,88,99,103	0
8	GOL	Y	601	6/6	0.88	0.23	61,69,70,71	0
8	GOL	R	602	6/6	0.88	0.24	64,69,70,71	0
8	GOL	A	301	6/6	0.88	0.45	65,69,76,90	0
10	PG4	Y	603	13/13	0.89	0.29	56,85,100,122	0
8	GOL	K	201	6/6	0.90	0.26	85,86,94,108	0
8	GOL	I	203	6/6	0.92	0.22	82,83,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	R	601	6/6	0.92	0.20	66,68,71,71	0
8	GOL	I	202	6/6	0.92	0.18	72,79,81,85	0
8	GOL	Y	602	6/6	0.94	0.23	63,64,67,74	0
8	GOL	X	601	6/6	0.94	0.26	61,63,66,70	0

6.5 Other polymers (i)

There are no such residues in this entry.