wwPDB X-ray Structure Validation Summary Report (i)

May 28, 2025 – 04:45 PM EDT

PDB ID	:	9ML8 / pdb_00009ml8
Title	:	Crystal structure of the SARS-CoV-2 RBD in complex with the rabbit M8b-B1 Fab
Authors	:	Fan, C.; Bjorkman, P.J.
Deposited on	:	2024-12-18
Resolution	:	2.40 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 (i)) were used in the production of this report:

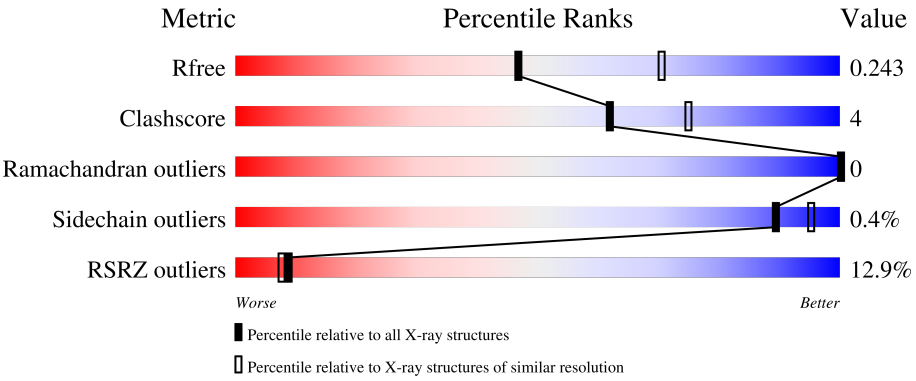
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 <=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	212	3% 82% 11% 8%
1	B	212	5% 85% 7% 8%
1	C	212	8% 83% 10% 8%
1	D	212	11% 77% 15% 8%
2	E	235	19% 87% 9% 5%

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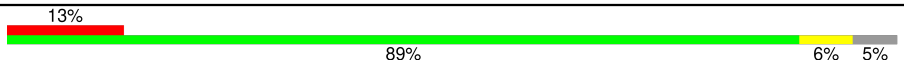
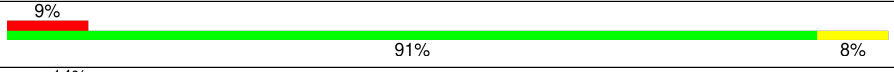
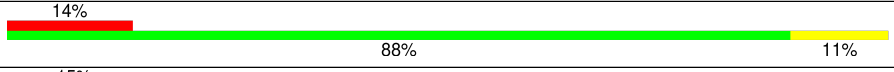
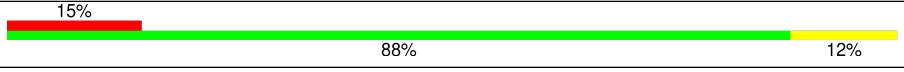
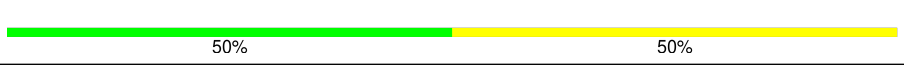
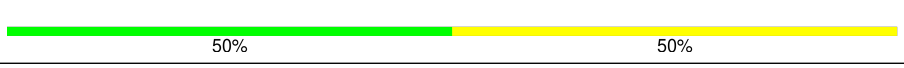
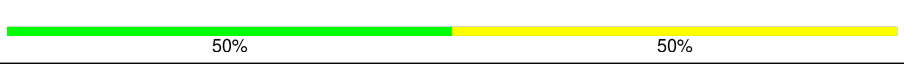
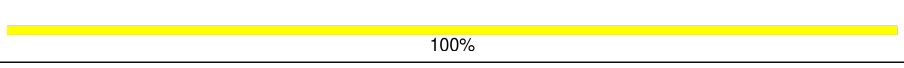
Mol	Chain	Length	Quality of chain
2	H	235	
2	M	235	
2	P	235	
3	F	217	
3	L	217	
3	N	217	
3	Q	217	
4	G	2	
4	I	2	
4	J	2	
4	K	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20452 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 protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	1	0
			1560	1000	262	290	8			
1	B	196	Total	C	N	O	S	0	1	0
			1560	1000	262	290	8			
1	C	196	Total	C	N	O	S	0	2	0
			1568	1004	264	292	8			
1	D	196	Total	C	N	O	S	0	1	0
			1558	999	260	291	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2
B	537	HIS	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2
C	538	HIS	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	537	HIS	-	expression tag	UNP P0DTC2
D	538	HIS	-	expression tag	UNP P0DTC2
D	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called M8b-B1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	H	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	M	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			
2	P	224	Total	C	N	O	S	0	0	0
			1683	1078	271	325	9			

- Molecule 3 is a protein called M8b-B1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	L	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	N	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			
3	Q	216	Total	C	N	O	S	0	1	0
			1643	1030	269	339	5			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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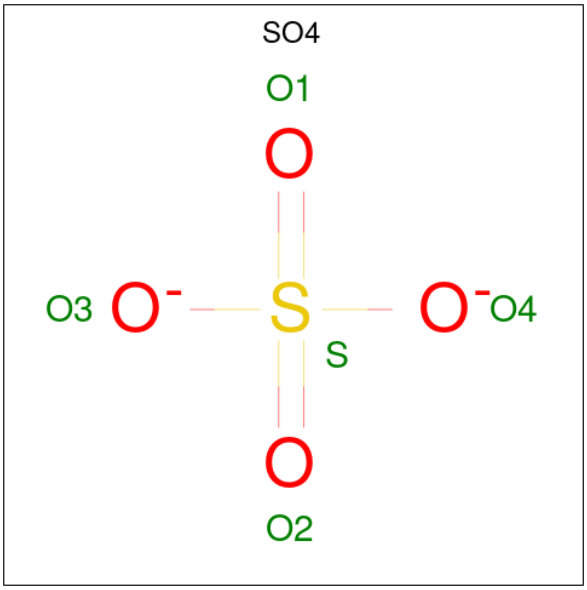
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0

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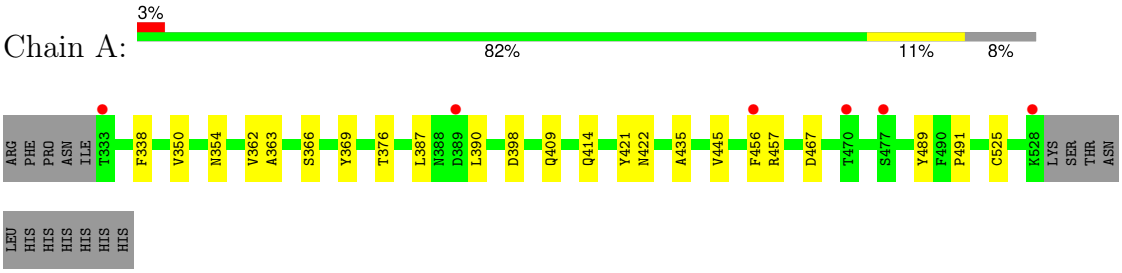
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	63	Total O 63 63	0	0
6	C	31	Total O 31 31	0	0
6	D	24	Total O 24 24	0	0
6	E	102	Total O 102 102	0	0
6	F	47	Total O 47 47	0	0
6	H	105	Total O 105 105	0	0
6	L	51	Total O 51 51	0	0
6	M	94	Total O 94 94	0	0
6	N	52	Total O 52 52	0	0
6	P	81	Total O 81 81	0	0
6	Q	47	Total O 47 47	0	0

3 Residue-property plots

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.

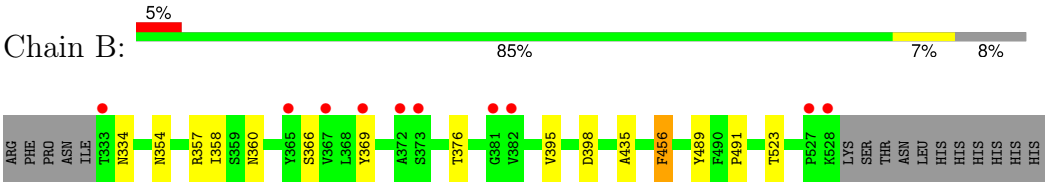
• Molecule 1: Spike protein S1

Chain A:



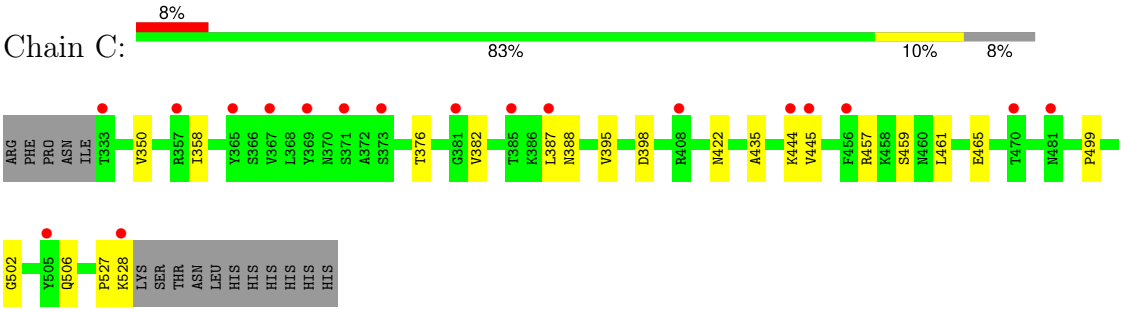
• Molecule 1: Spike protein S1

Chain B:



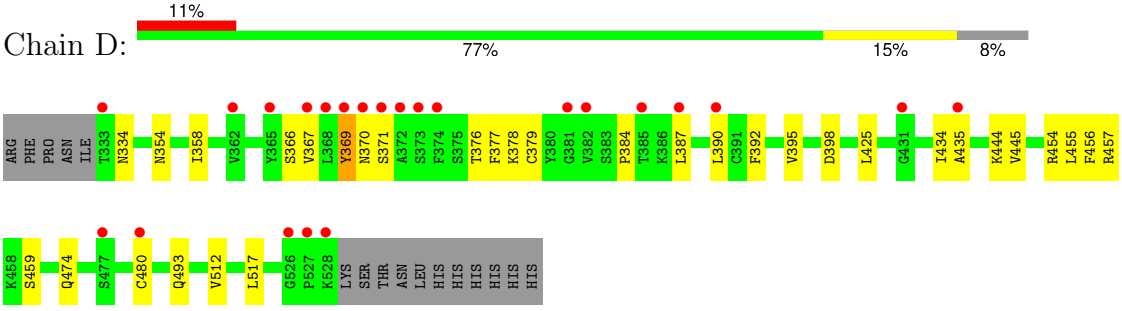
• Molecule 1: Spike protein S1

Chain C:



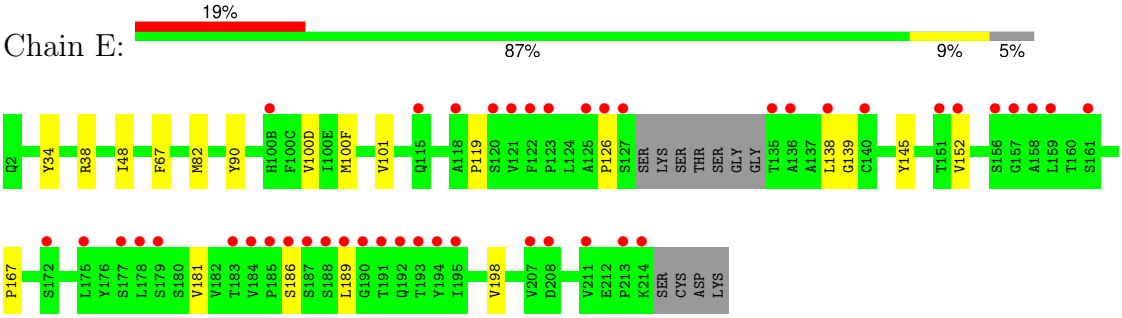
• Molecule 1: Spike protein S1

Chain D:



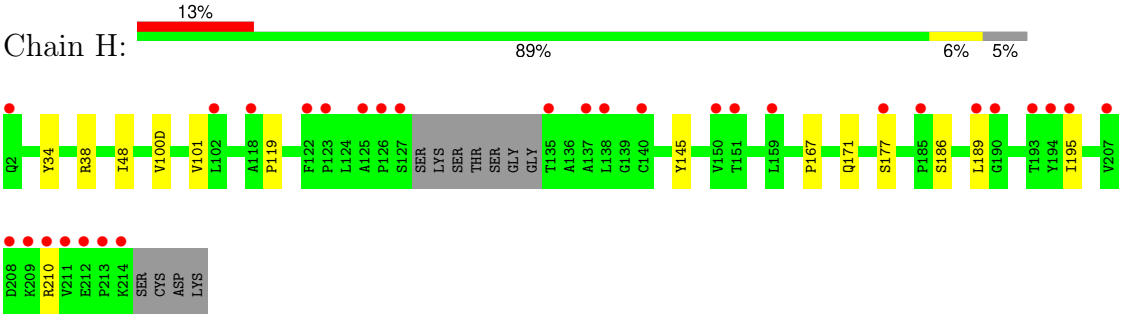
• Molecule 2: M8b-B1 heavy chain

Chain E:



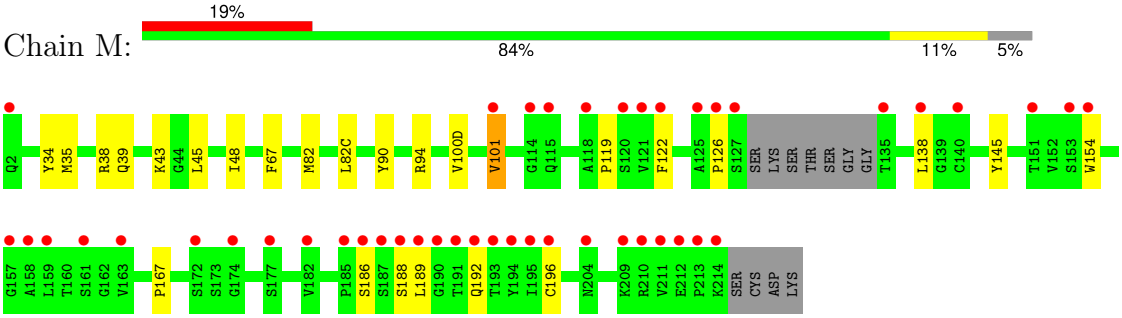
• Molecule 2: M8b-B1 heavy chain

Chain H:



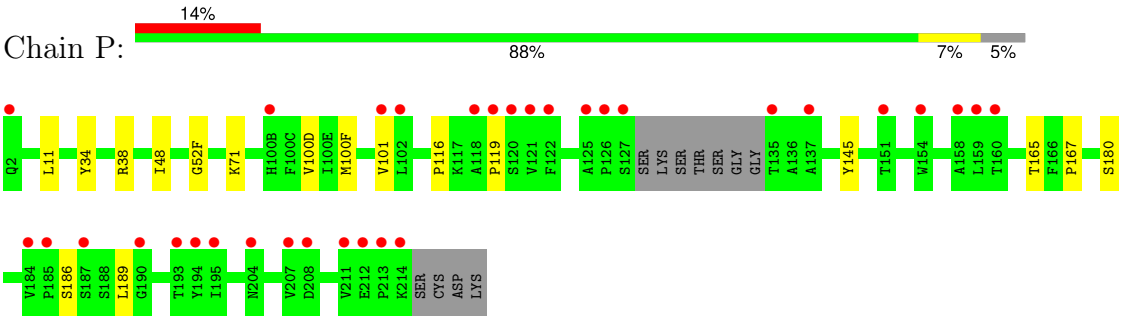
• Molecule 2: M8b-B1 heavy chain

Chain M:



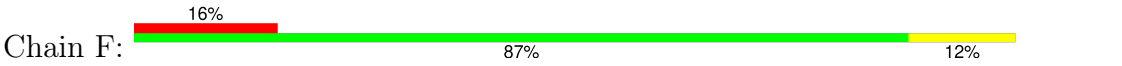
• Molecule 2: M8b-B1 heavy chain

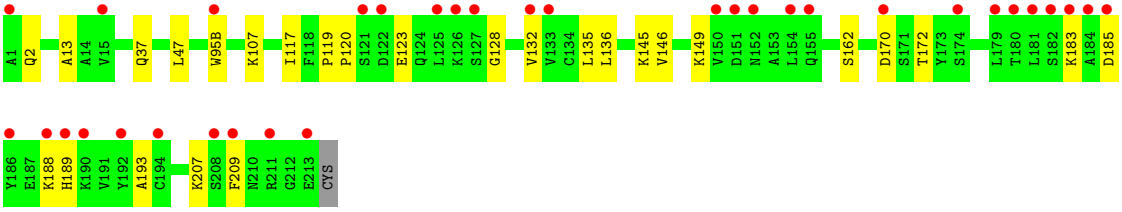
Chain P:



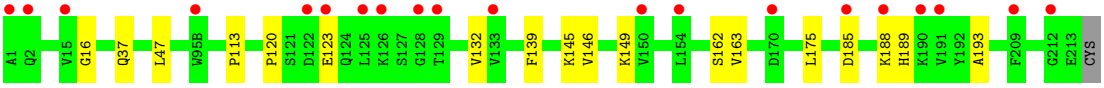
• Molecule 3: M8b-B1 light chain

Chain F:

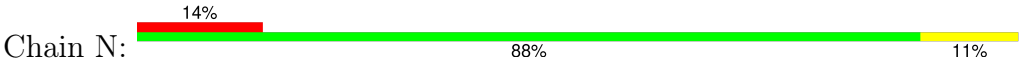


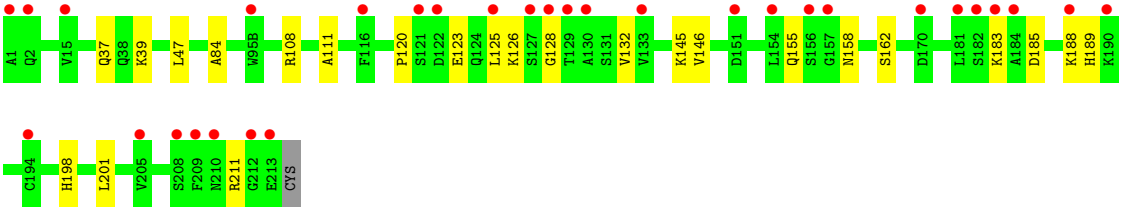


• Molecule 3: M8b-B1 light chain

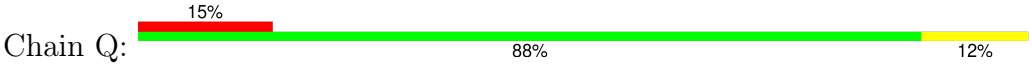


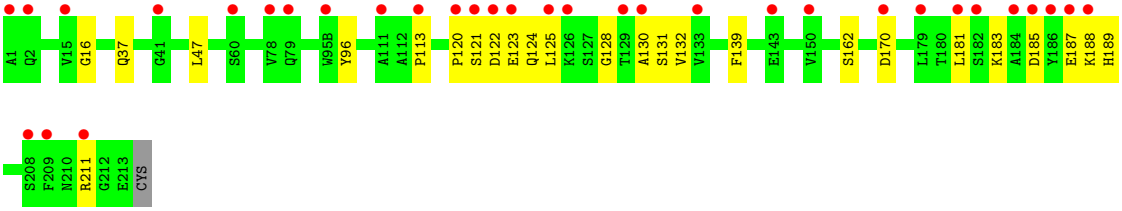
• Molecule 3: M8b-B1 light chain





• Molecule 3: M8b-B1 light chain





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

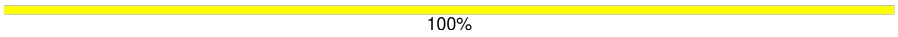
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain J:

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

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.07Å 173.44Å 129.93Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	39.15 – 2.40 39.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.15-2.40) 98.4 (39.15-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.223 , 0.247 0.221 , 0.243	Depositor DCC
R_{free} test set	131265 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20452	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.29% 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: NAG, SO4

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	0.10	0/1607	0.31	0/2186
1	B	0.10	0/1607	0.29	0/2186
1	C	0.10	0/1615	0.31	0/2197
1	D	0.12	0/1605	0.33	0/2184
2	E	0.10	0/1730	0.29	0/2362
2	H	0.09	0/1730	0.28	0/2362
2	M	0.10	0/1730	0.28	0/2362
2	P	0.09	0/1730	0.28	0/2362
3	F	0.15	0/1684	0.33	0/2293
3	L	0.09	0/1684	0.30	0/2293
3	N	0.10	0/1684	0.31	0/2293
3	Q	0.10	0/1684	0.30	0/2293
All	All	0.10	0/20090	0.30	0/27373

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	1560	0	1485	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1560	0	1485	9	0
1	C	1568	0	1490	12	0
1	D	1558	0	1480	21	0
2	E	1683	0	1630	12	0
2	H	1683	0	1630	7	0
2	M	1683	0	1630	19	0
2	P	1683	0	1630	9	0
3	F	1643	0	1576	16	0
3	L	1643	0	1576	11	0
3	N	1643	0	1576	16	0
3	Q	1643	0	1576	19	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	L	5	0	0	0	0
5	N	5	0	0	0	0
5	Q	5	0	0	0	0
6	A	58	0	0	0	0
6	B	63	0	0	1	0
6	C	31	0	0	0	0
6	D	24	0	0	0	0
6	E	102	0	0	0	0
6	F	47	0	0	0	0
6	H	105	0	0	0	0
6	L	51	0	0	0	0
6	M	94	0	0	1	0
6	N	52	0	0	0	0
6	P	81	0	0	0	0
6	Q	47	0	0	0	0
All	All	20452	0	18864	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 155 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:D:366:SER:HA	1:D:369:TYR:CE1	2.21	0.76
3:L:16:GLY:HA3	3:Q:16:GLY:HA3	1.70	0.74
1:D:367:VAL:O	1:D:371:SER:HB3	1.88	0.74
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.70	0.73
3:Q:123:GLU:OE2	3:Q:123:GLU:N	2.17	0.73

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	195/212 (92%)	190 (97%)	5 (3%)	0	100	100
1	B	195/212 (92%)	191 (98%)	4 (2%)	0	100	100
1	C	196/212 (92%)	190 (97%)	6 (3%)	0	100	100
1	D	195/212 (92%)	192 (98%)	3 (2%)	0	100	100
2	E	220/235 (94%)	217 (99%)	3 (1%)	0	100	100
2	H	220/235 (94%)	218 (99%)	2 (1%)	0	100	100
2	M	220/235 (94%)	217 (99%)	3 (1%)	0	100	100
2	P	220/235 (94%)	218 (99%)	2 (1%)	0	100	100
3	F	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	L	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	N	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
3	Q	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
All	All	2521/2656 (95%)	2465 (98%)	56 (2%)	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	170/185 (92%)	169 (99%)	1 (1%)	84 92
1	B	170/185 (92%)	169 (99%)	1 (1%)	84 92
1	C	171/185 (92%)	171 (100%)	0	100 100
1	D	170/185 (92%)	168 (99%)	2 (1%)	67 82
2	E	186/195 (95%)	185 (100%)	1 (0%)	86 94
2	H	186/195 (95%)	185 (100%)	1 (0%)	86 94
2	M	186/195 (95%)	185 (100%)	1 (0%)	86 94
2	P	186/195 (95%)	185 (100%)	1 (0%)	86 94
3	F	187/187 (100%)	187 (100%)	0	100 100
3	L	187/187 (100%)	187 (100%)	0	100 100
3	N	187/187 (100%)	187 (100%)	0	100 100
3	Q	187/187 (100%)	186 (100%)	1 (0%)	86 94
All	All	2173/2268 (96%)	2164 (100%)	9 (0%)	89 95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	101	VAL
3	Q	170	ASP
1	D	456	PHE
2	E	101	VAL
2	H	101	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	199	ASN
3	Q	38	GLN
3	F	158	ASN
3	Q	124	GLN

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Mol	Chain	Res	Type
2	P	39	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	G	1	1,4	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.99	0
4	NAG	I	1	1,4	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
4	NAG	I	2	4	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	J	1	1,4	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	0.80	0
4	NAG	K	1	1,4	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	0.95	1 (5%)

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	G	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C1-O5-C5	3.03	116.24	112.19
4	K	1	NAG	C1-O5-C5	2.45	115.47	112.19
4	G	1	NAG	C2-N2-C7	2.20	125.85	122.90
4	I	1	NAG	C1-O5-C5	2.18	115.11	112.19
4	J	1	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

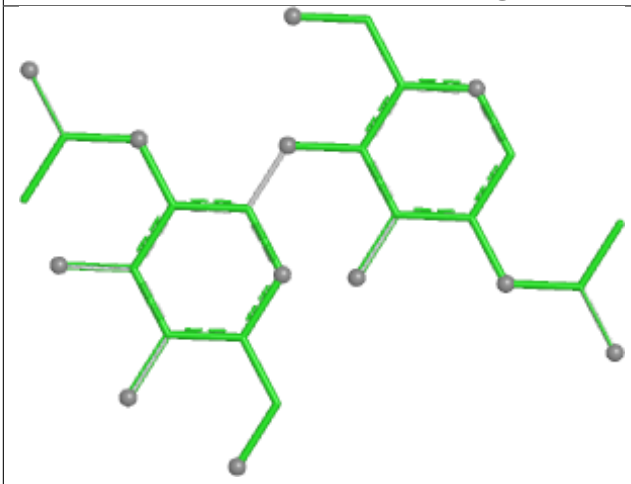
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2

There are no ring outliers.

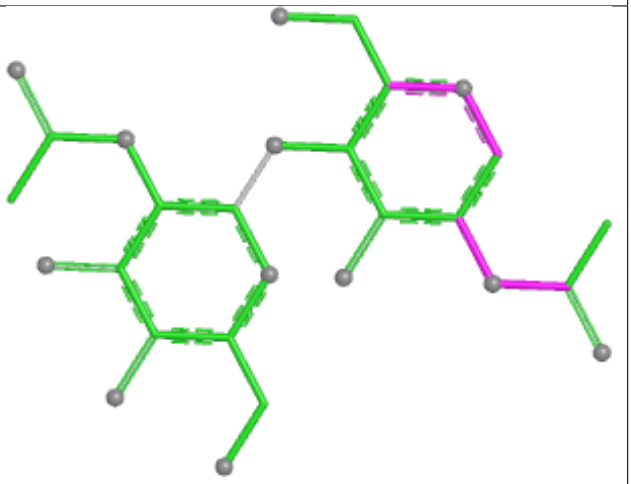
No monomer is involved in short contacts.

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

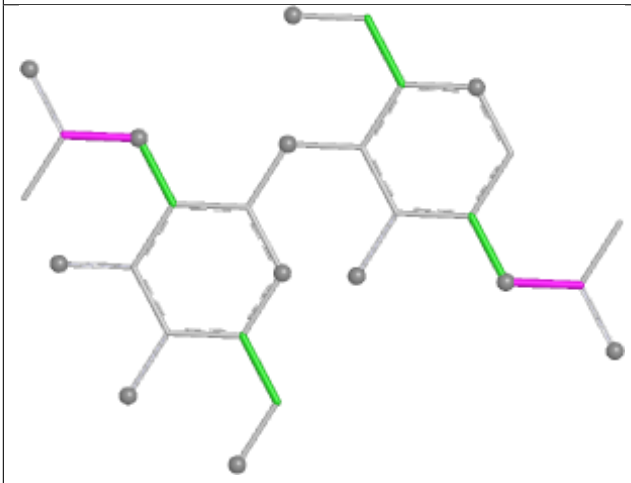
Oligosaccharide Chain G



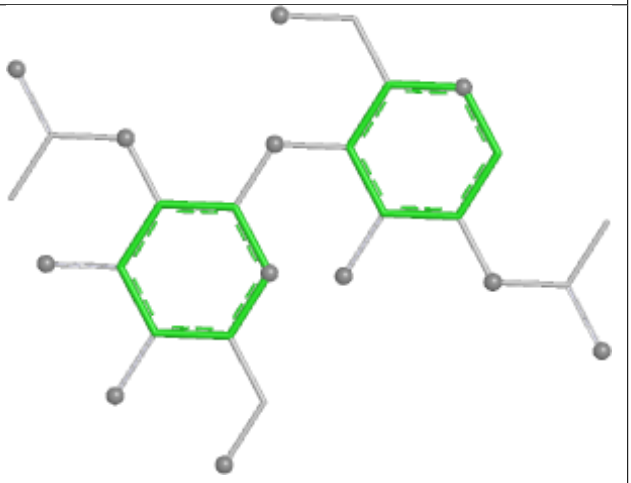
Bond lengths



Bond angles

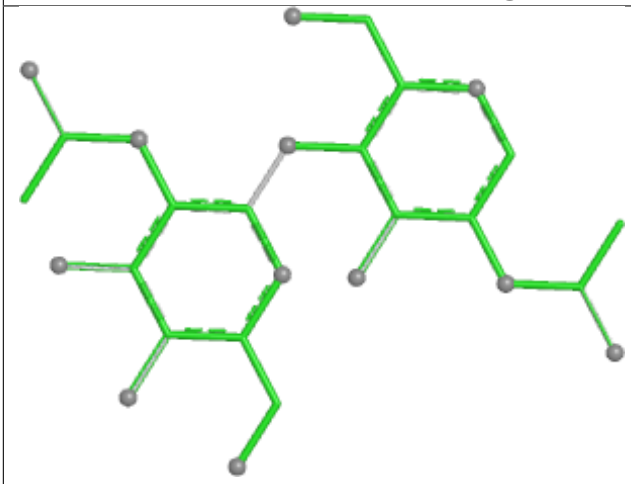


Torsions

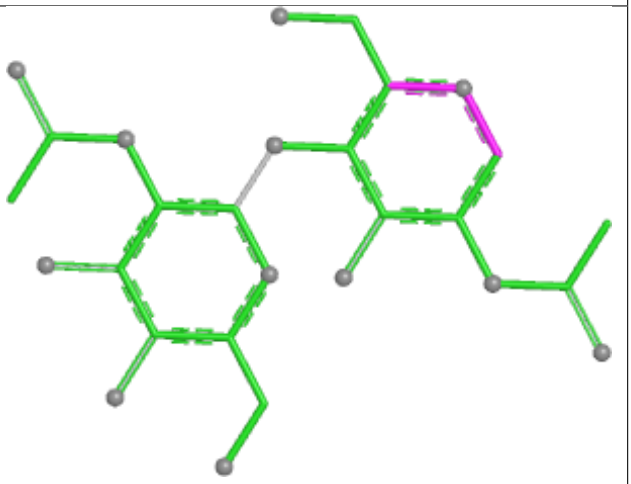


Rings

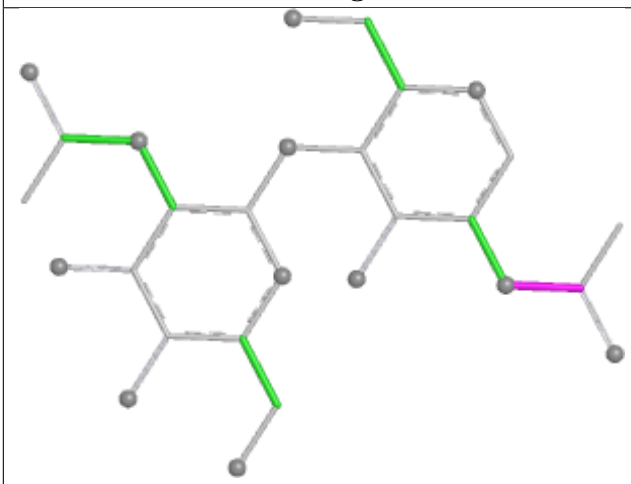
Oligosaccharide Chain I



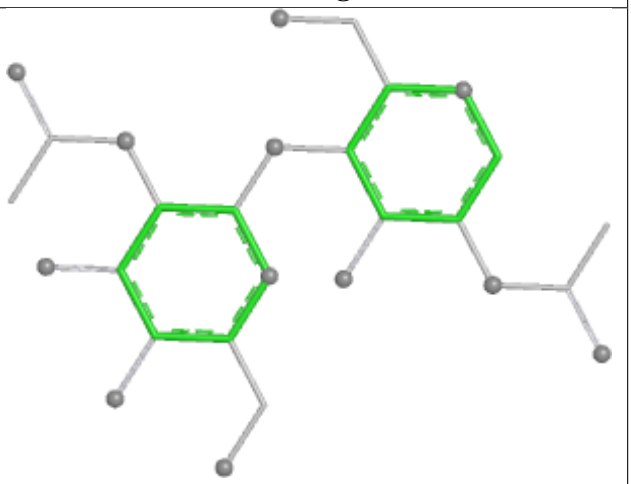
Bond lengths



Bond angles

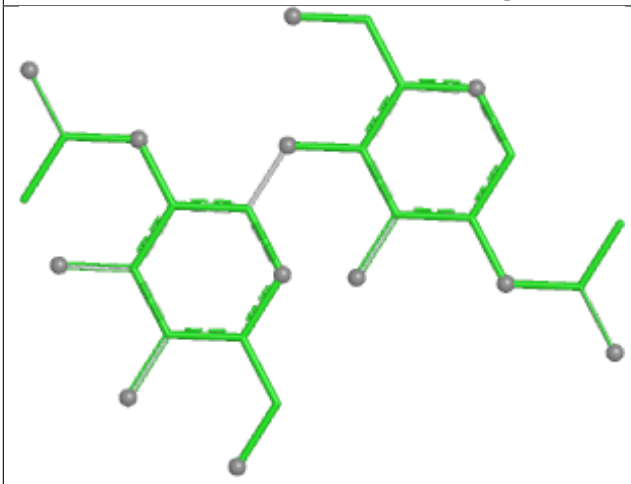


Torsions

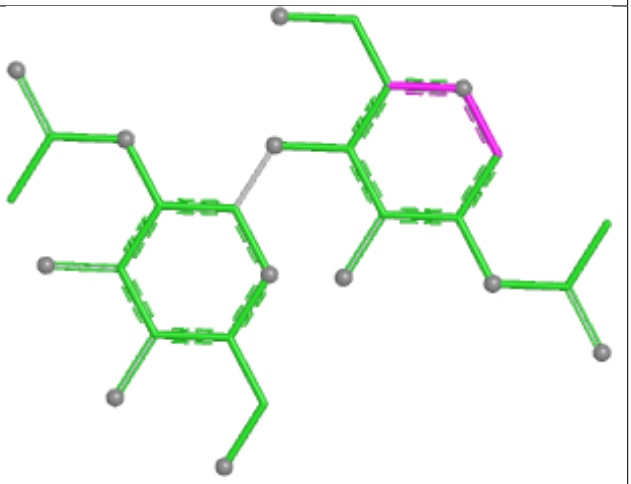


Rings

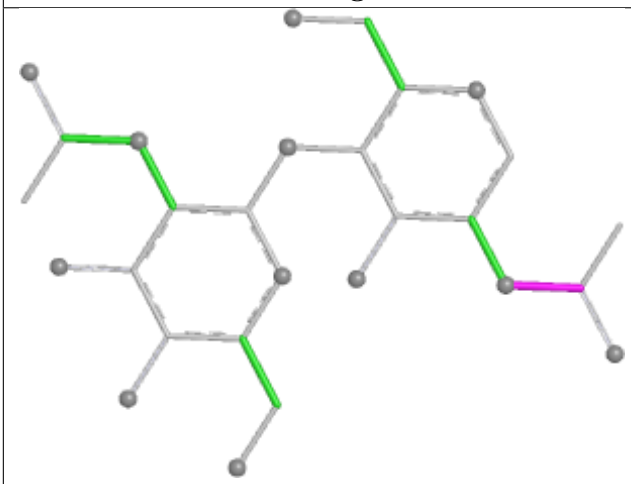
Oligosaccharide Chain J



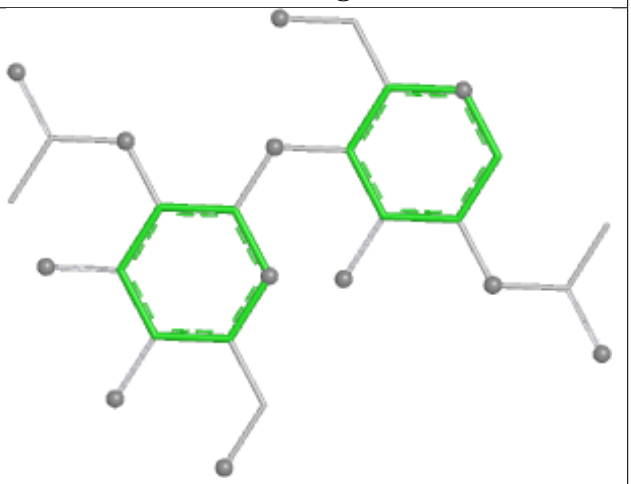
Bond lengths



Bond angles

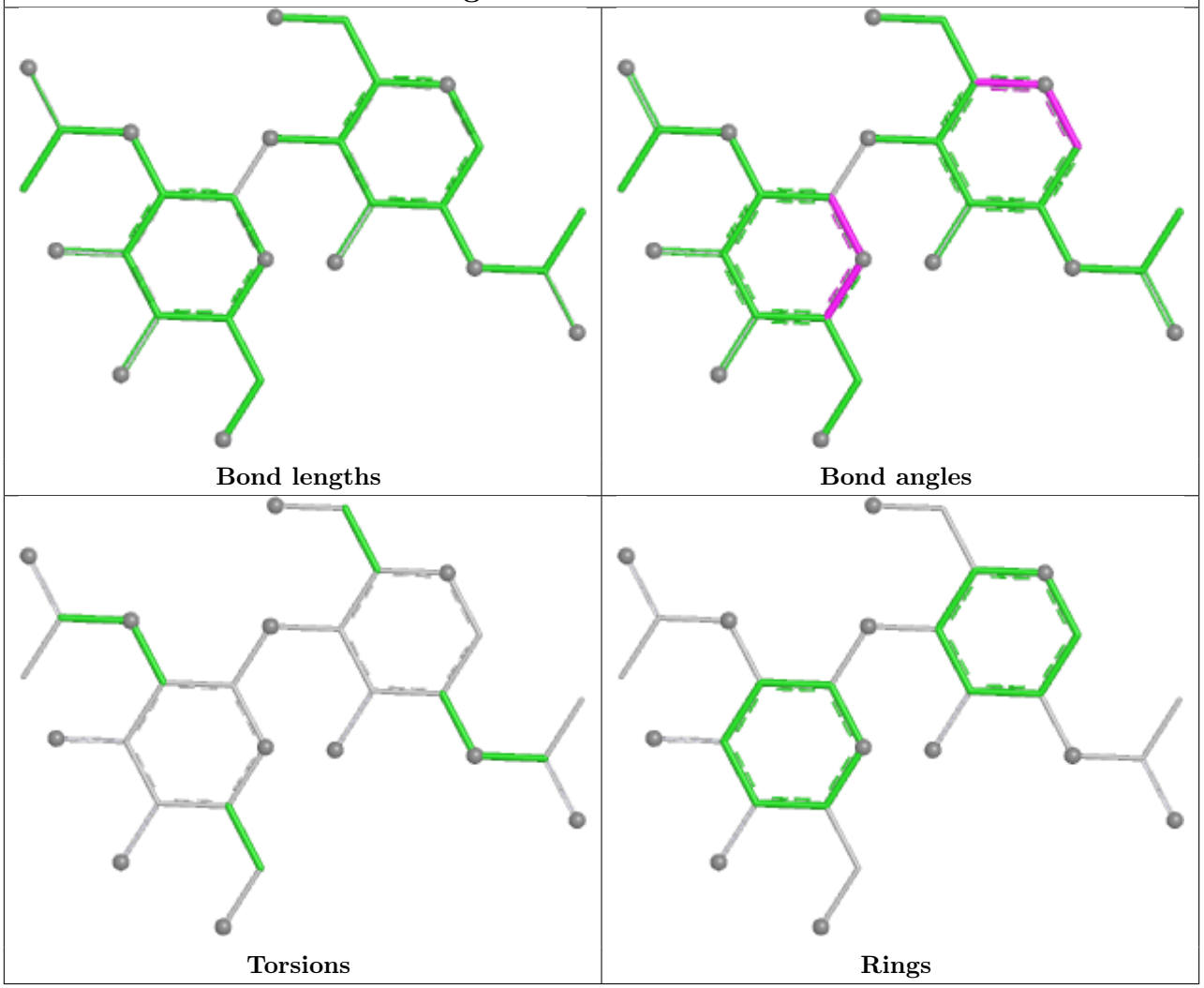


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
5	SO4	D	601	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	A	601	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	C	601	-	4,4,4	0.68	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	N	301	-	4,4,4	0.67	0	6,6,6	0.10	0
5	SO4	L	301	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.10	0
5	SO4	Q	301	-	4,4,4	0.68	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	196/212 (92%)	0.27	6 (3%) 51 48	24, 45, 65, 92	1 (0%)
1	B	196/212 (92%)	0.39	10 (5%) 34 32	26, 46, 81, 95	1 (0%)
1	C	196/212 (92%)	0.64	18 (9%) 16 14	23, 53, 84, 100	2 (1%)
1	D	196/212 (92%)	0.79	23 (11%) 10 9	37, 57, 101, 124	1 (0%)
2	E	224/235 (95%)	0.67	44 (19%) 4 3	24, 41, 102, 124	0
2	H	224/235 (95%)	0.59	30 (13%) 8 7	23, 40, 97, 124	0
2	M	224/235 (95%)	0.74	45 (20%) 3 3	26, 43, 108, 129	0
2	P	224/235 (95%)	0.67	33 (14%) 7 6	27, 44, 101, 132	0
3	F	216/217 (99%)	0.96	34 (15%) 6 5	30, 56, 108, 129	1 (0%)
3	L	216/217 (99%)	0.78	20 (9%) 16 14	29, 54, 105, 122	1 (0%)
3	N	216/217 (99%)	0.96	31 (14%) 7 6	29, 56, 109, 136	1 (0%)
3	Q	216/217 (99%)	1.03	33 (15%) 6 6	33, 59, 107, 127	1 (0%)
All	All	2544/2656 (95%)	0.71	327 (12%) 9 7	23, 51, 101, 136	9 (0%)

The worst 5 of 327 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1	ALA	6.6
3	N	125	LEU	6.3
3	F	1	ALA	6.2
3	Q	1	ALA	5.6
3	N	1	ALA	5.4

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)

SUGAR-RSR INFOmissingINFO

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, 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
5	SO4	Q	301	5/5	0.61	0.15	91,91,97,102	0
5	SO4	F	301	5/5	0.62	0.13	81,86,92,100	0
5	SO4	N	301	5/5	0.64	0.16	80,84,96,98	0
5	SO4	L	301	5/5	0.72	0.12	77,79,90,93	0
5	SO4	C	601	5/5	0.80	0.21	62,62,80,80	0
5	SO4	D	601	5/5	0.86	0.16	66,69,82,82	0
5	SO4	A	601	5/5	0.89	0.13	48,53,69,73	0

6.5 Other polymers (i)

There are no such residues in this entry.